# Special Report No. 16

# GREAT-ER User Manual

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European Centre for Ecotoxicology
and Toxicology of Chemicals

Avenue E Nieuwenhuyse 4 (Bte 6)
B - 1160 Brussels, Belgium

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# INTRODUCTION

Risk represents the likelihood that the hazard will be realised - i.e. that due to the exposure an adverse effect may occur. Risk assessment is defined as the process that evaluates the likelihood that adverse ecological or human health effects may occur, are occurring, or have occurred as a result of exposure to one or more physical, chemical, or biological agents.

Fundamental to the risk assessment definition is the recognition that risk requires two elements: (1) a chemical or material's inherent ability to cause adverse effects and (2) the exposure or interaction of the chemical or material with an ecological component or with a human population at sufficient intensity and duration to elicit the adverse effect(s). The risk assessment process is a step-wise process in which assessment of potential adverse effects and exposure is integrated and compared with increasing realism. The ratio of the Predicted Environmental Concentration (PEC) to the Predicted No Effect Concentration (PNEC) is used as a measure of this risk.

The assessment of risk can require an in-depth assessment of the intrinsic physico-chemical properties, biodegradability, bioaccumulation potential and hazard or potential effects of the chemical. In addition, a thorough assessment of the release pathway, environmental fate and distribution of the chemical is required based on exposure measurements and/or mathematical models. In environmental exposure assessment the concentration of a substance in the different environmental compartments is estimated based on physico-chemical properties, the production and emission processes, the use and disposal patterns and the properties of the environmental compartments.

Since the introduction of risk assessment legislation in the EU, separate guidance documents have been prepared for the evaluation of risk for both New and Existing Chemicals (1993 and 1994, respectively). Because the Risk Assessment Directive of New Substances and Risk Assessment Regulation of Existing Substances were supported by a number of different technical guidance packages which resulted in different risk assessment conclusions, and possibly could lead to different risk management strategies, the Commission agreed to develop a uniform guidance package. This package (EEC, 1996) was released together with the supporting risk assessment computer model EUSES (European Uniform System for Evaluating Substances, 1996). The EUSES modelling approach estimates PECs for fictive environments via a generic multimedia ‘unit world’ approach and does not account for spatial and temporal variability in landscape characteristics, river flows and/or chemical emissions. Hence, the results are merely applicable on a generic screening level since these models do not offer a realistic prediction of actual steady-state background concentrations. In addition, the default EU generic regional environment (EEC, 1996) assumes treatment of only 70% of the waste water mass loading, leaving 30% of mass loading to this generic region untreated.

The objective of the GREAT-ER project is to develop and validate a powerful and accurate chemical exposure prediction tool for use within the EU environmental risk assessment schemes. This new database, model and software system is developed 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.

The GREAT-ER software system uses a Geographic Information System (GIS) for data storage and visualization, combined with simple mathematical models for the prediction of chemical fate. Hydrological databases and models have been used to determine river flows in the pilot study areas. GREAT-ER provides an accurate prediction of aquatic chemical exposure and allows the calculation of a realistic distribution of environmental concentrations of down-the-drain chemicals for use within the EU environmental risk assessment schemes. The aim of GREAT-ER is to enable the prediction of the concentrations of chemicals at any specific 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 the prototype runs in the first instance for the Aire, Calder, Went, Don (UK) and Lambro (I) regions, and for parts of Belgium and Germany.

The refined exposure assessment tool should greatly enhance the accuracy of current local and regional exposure estimation methods, and ultimately allow assessments on a pan-European scale.

This special report will allow you to install GREAT-ER and help you with key questions on how to run GREAT-ER.

# 1. INSTALLATION

## 1.1 REQUIREMENTS

GREAT-ER is a collection of models and scripts set on top of the geographic information system (GIS) ArcView, a product developed and marketed by the Environmental Systems Research Institute (ESRI). The development was based on the software package ArcView **3.0 with the patch for version 3.0a**. GREAT-ER is also compatible with the new version ArcView **3.1**.

The operating system GREAT-ER is designed for **WINDOWS NT 4.0**. Please note that GREAT-ER will not work properly under WINDOWS 95 although ArcView 3.0 and 3.1 do. Compatibility with WINDOWS 98 was not tested.

The GREAT-ER system contains a set of scripts for ArcView, models and other programs for data analysis. It also comes with a set of data and additional information for selected pilot regions.

The installation requires a minimum **free hard disk space of approximately 50 MB**.

## 1.2 SET-UP

GREAT-ER comes with its own set-up program, specifically designed for the installation of the complete modelling system. It can be found in the root directory of the GREAT-ER CD-ROM. It is recommended to exit all other running applications while installing GREAT-ER on your computer.

Installation steps (some terms are language dependent and may be different on your WINDOWS NT 4.0 version):

1. Insert the GREAT-ER CD-ROM into your CD-ROM drive. Run the setup program by selecting "Execute" from the WINDOWS NT 4.0 "Start Menu". Type e.g. `\setup.exe` and click the "OK" button. Please note that `D` may have to be replaced by the letter of your CD-ROM drive.

2. The first dialog appears, showing you the licence text of GREAT-ER. Please ensure you have carefully read and understood all the terms of the licence agreement. If you agree to the licence agreement, proceed with the installation by clicking the "Accept" button. If not, select "Cancel". The installation will then be aborted and GREAT-ER will not be installed on your system. At any time during the installation you can return to a previous dialog to modify settings by clicking the "Back" button.

3. Select the type of installation: either *full installation* or *CD-based installation*. It is recommended to proceed with the full installation. The CD-based installation should only be chosen for evaluation purposes. The required disk space is reduced to the amount of data resulting from simulation runs; all scripts, programs and additional data are loaded for a GREAT-ER application from the CD-ROM. This means the CD-ROM needs to be inserted in your CD-ROM drive while working with GREAT-ER. On the other hand, it is not possible to add new substances to the systems data base or to include further catchments or additional geo-referenced data.

4. If you have selected the full installation, the following dialog will enable you to specify the directory in which to install GREAT-ER. A directory can be specified by typing in the path directly or by browsing through the directory tree. If you type in a non-existing directory, the setup program will create it for you. Please note that only the last directory in a path can be created, new multi-stage directories are not possible. (E.g. if `C:\programs` is an existing path, `greater` and therefore `C:\programs\greater` would be a possible directory for the GREAT-ER installation. `C:\programs\models\greater` would not be allowed if `models` is not an existing directory. It has to be created manually using the Windows NT options before proceeding with the installation.)

5. For both types of installation a directory to store the scenarios has to be specified (see below). Restrictions are the same as for the GREAT-ER installation directory.

6. A final dialog enables you to review your settings. Click back to modify your settings, or complete the installation.

7. The set-up program evaluates the source files and starts to install GREAT-ER. Please note that on some systems the progress bar reporting the process of installation will not function properly.

8. It is recommended to restart the computer after installation to ensure correct recognition of new system settings.

9. Finally, you can create a link to the GREAT-ER program in any of the “Start Menu” program groups or on the desktop. The link target should be as follows:

   ```
   <ArcView path>\arcview.exe %GHOME%\great-er.apr
   ```

   where `<ArcView path>` has to be replaced by the path to your ArcView installation (e.g. `C:\ESRI\AV_GIS30\ARCVIEW\BIN32`).

   Alternatively, the link or shortcut can point directly to great-er.apr and ArcView will normally be started automatically.

## 1.3 GREAT-ER AND ArcView

As GREAT-ER is a software system built on top of the GIS ArcView, some familiarisation with the basic ArcView terminology and functions is recommended. It is outside the scope of this tutorial to explain all ArcView-specific terms used below. This is especially the case for all the ArcView features used to create a user-specific presentation of data.

The ArcView handbook gives some tutorials about how to use the basic functions of ArcView. In addition, the on-line help provides some useful information and the following sections are especially useful:

- *Introduction to ArcView* - This provides a useful introduction to the basics of ArcView, the different types of data and so-called ‘Documents’.
- *Creating and using maps* - This gives a useful description of ‘views’ which display maps and are therefore the central item of the GREAT-ER user interface.
- The sections on *Displaying a view* and *Choosing colours and symbols* are also useful. Both contain information on how to work with views and how to modify the presentation of maps and data.

These basics are sufficient to understand the terminology used in this user manual and to run simulations with GREAT-ER. If you intend to print or export maps to include simulation results in other documents or papers, you should read the chapter on *Laying out and printing maps*. The chapter in the ArcView handbook with the same name is also helpful. A basic understanding of the user interface facilities of ArcView (Menu Bar, Button Bar, Tool Bar) and Windows in general will be useful.

# 2. TUTORIAL

The essential steps to run a **first** simulation of GREAT-ER are printed within a grey shaded box (like this one). They represent the minimum contents of the tutorial. A 'typical' GREAT-ER session will generally involve a series of steps as outlined in Figure 2.1. The complete tutorial chapter is seen as a guided tour through all the main features of GREAT-ER and of the various options available. Finally, Chapter 3 of this User Manual provides a more detailed description of the different features and options available within GREAT-ER.

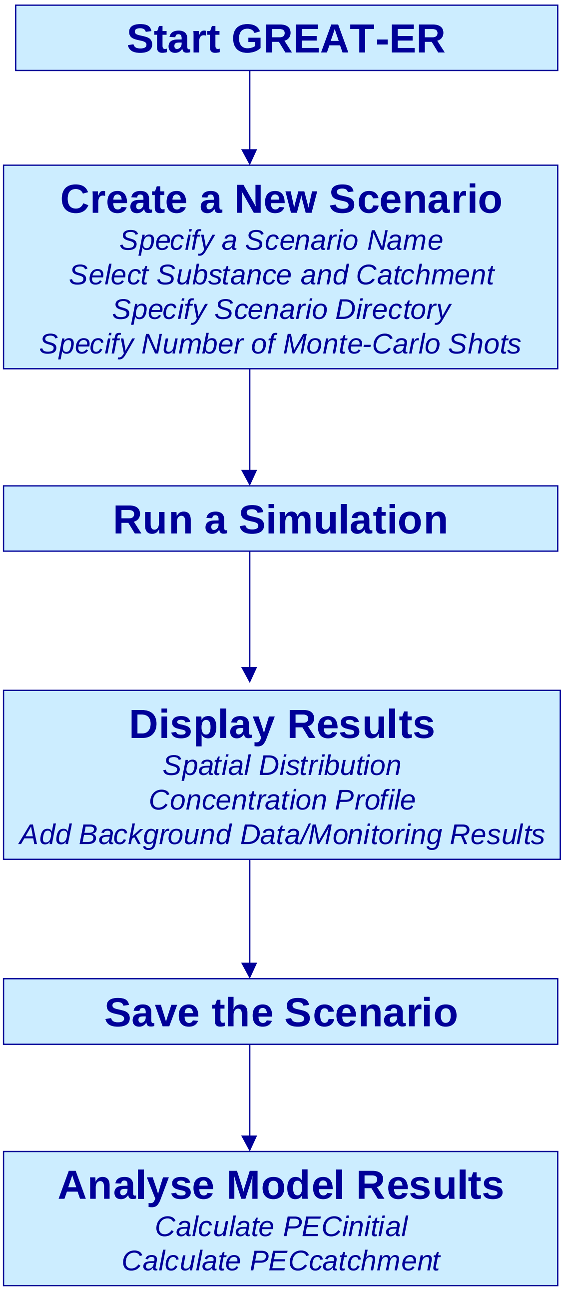


Figure 2.1: *Flow Chart of 'Typical' GREAT-ER Session*

## 2.1 BASIC CONCEPTS

### 2.1.1 Scenario Concept

The collection of data needed to perform a simulation is called a 'scenario'. Scenarios can be stored and loaded and thus offer the quick retrieval of certain situations. A unique title for each scenario assists the search of a specific one in a long list. Additionally, scenarios form the basis of the exchange of complete simulation data sets (see *Export / Import*).

A scenario consists of the following data:

1. **Title**: A unique name for the scenario.
2. **Catchment ID**: The (identity) ID is the name of the catchment (e.g. *Aire*). The catchment data themselves are not part of a scenario. Such data (e.g. river network) are fixed and cannot be edited.
3. **Substance**: The whole substance data set is stored within a scenario. The user can safely make changes to the substance properties for specific simulations without affecting the data stored in the substance database.
4. **Release Data**: Although the positions and number of discharge sites within a catchment are not editable, the attributes of the discharge sites can be modified. For this the set of attributes is stored with the scenario. In contrast to the substance database, modified data sets can not be written back to the GREAT-ER catchment database.
5. **Modified Flag**: The flag is set to *true* if any element of the scenario has been changed since the last save and hence the scenario is different to the scenario in the database with the same title. The flag is displayed in the scenario's view window title bar (see below).
6. **Model Parameter**: The complete model parameter data set needed by the GREAT-ER model is stored within a scenario.

The most important data of a scenario are given in the title bar of the corresponding view window. This makes the title, catchment ID, substance ID, modified state of scenario/substance and the simulation state permanently visible and avoids confusion when managing several open scenarios.

#### 2.1.1.1 *Scenario Database:*

A GREAT-ER installation always has only one scenario database. As mentioned in the section 1.2 on installation, the basis for the GREAT-ER scenario database is a directory. All scenarios are stored in separate sub-directories under this specific GREAT-ER scenario directory. Each sub-directory contains several tables (with data, such as discharge data, editable by the user) and all additional settings mentioned above.

Simulation results are also stored in this directory. It is suggested to store further analysis results under this sub-directory, too. This will increase the transparency of simulation results if all coherent data are stored in one directory structure. But please note, that in this case deleting a scenario will also delete any results derived from this scenario!

Given the described scenario database structure it should be noted that the exchange of scenarios with other GREAT-ER users will not work via scenario database files, but with the export/import feature described later (see Sections 2.7 and 3.1.8).

#### 2.1.1.2 *Active and Open Scenarios*

In GREAT-ER you can have many *open scenarios*, only one of which can be *active* at one time. The name of the active scenario is shown in the ArcView title bar. Scenario-related operations always are performed on the active scenario (e.g. Close Scenario, Edit Data Start Simulation, etc). The view window that corresponds to the active scenario is usually visible at the front. If a catchment has not yet been specified, the overview of Europe is visible.

The active scenario can be set by creating a new scenario, selecting a scenario from the scenario database or by activating the corresponding View window.

### 2.1.2 Substance Database

The substance database contains all the substance-specific information for any substances that have been included. The data may include physico-chemical properties, partitioning, degradation, sewage treatment removal, in-stream removal and market data, depending on what information are available. It also includes various identification parameters such as the substance name, CAS No. (Chemical Abstract Service Number) etc. The substance unique ID (key) which is displayed on the screen is actually made up from the substance name and its CAS No.
It is easy to add new substances or edit substance data as required. However, note that the default data delivered with GREAT-ER for Boron and LAS have been quality assured and it is not recommended that these data are modified unless new quality assured data become available.

### 2.1.3 Expert Mode vs. Easy-To-Use Mode

GREAT-ER offers two modes for the user interface: The *expert mode* and the *easy-to-use mode*.

'Expert' in this context requires familiarisation with ArcView. The expert mode gives access to ArcView operations and commands. This includes the possibilities of undocumented changes or deletion of basic GREAT-ER data sets. Obviously, this feature provides additional capabilities but also contains a hidden danger. The user should therefore decide carefully whether to perform operations in the expert mode or not.

'Easy-to-use' basically makes it is impossible to harm the system and/or the underlying GREAT-ER data sets. For undertaking model simulations and viewing the basic results, this mode is sufficient.

### 2.1.4 Model System

The current version of GREAT-ER comes with a model system covering three sub-models: sewer, treatment plant and river. There are three *complexity modes* for each of these sub-models. In the simplest mode only first-order elimination rates or percentage removal are considered, whereas higher modes consider elimination processes in more detail.

All of the sub-models are deterministic in principle. However, using the Monte-Carlo method set on top of these models, results are returned as distributions of concentrations. GREAT-ER delivers results for all considered geographic objects: sewers (i.e. the influent of a treatment plant), all treatment plants (effluent) and all river stretches within the catchment under investigation. See the model description for more details.

Model results are displayed by colouring river stretches on a map, or as concentration profiles along a river. GREAT-ER provides users with several options to analyse the results and to derive further values from them. For further details see below in the tutorial and menu description.

### 2.1.5 Parameter Handling

Depending on the selected models, different parameters will be used to run a simulation. These parameters are sorted according to their relation to a substance, catchment or model. GREAT-ER provides several dialogs to enter or modify the parameters.
To display the required parameters according to the selected model's complexity modes, GREAT-ER aids users with a colour coding within the dialogs. Parameters colour-coded green are definitely not used by the current model selection, nevertheless, it is possible to edit these parameters. Black parameters *might* be used within the current model selection and if so these need to be specified.

Additionally, GREAT-ER contains a ‘knowledge’ database of parameters to avoid wrong data entries. Values are compared against two ranges: a warning range and an error range. The warning range specifies the usual range of a parameter. If an entry exceeds the parameter warning range, a dialog will point out this possible mistake. Nevertheless, it is possible to run a simulation with such settings. In contrast, the error range defines the logical range of a parameter. Values outside this range are impossible and will lead to errors. If an entry exceeds the error range it is not possible to leave the dialog until a value within the warning range has been entered. A dialog will give an error message and hints on the logical range of the parameter. Finally, for better documentation and transparency of simulation results a separate comment can be entered for each parameter. This comment may provide additional information for example, about the source of the data, such as quality aspects.

## 2.2 STARTING GREAT-ER

If you have created a shortcut as mentioned under item 9 of the installation procedure, start GREAT-ER using its icon. Alternatively, start ArcView and select from the menu *File* the item *Open Project...* Browse through the directory tree to the directory of your GREAT-ER installation. Open the project file `great-er.apr`.

After the start-up GREAT-ER presents the initial screen. It shows a map of Europe and all currently available catchments.

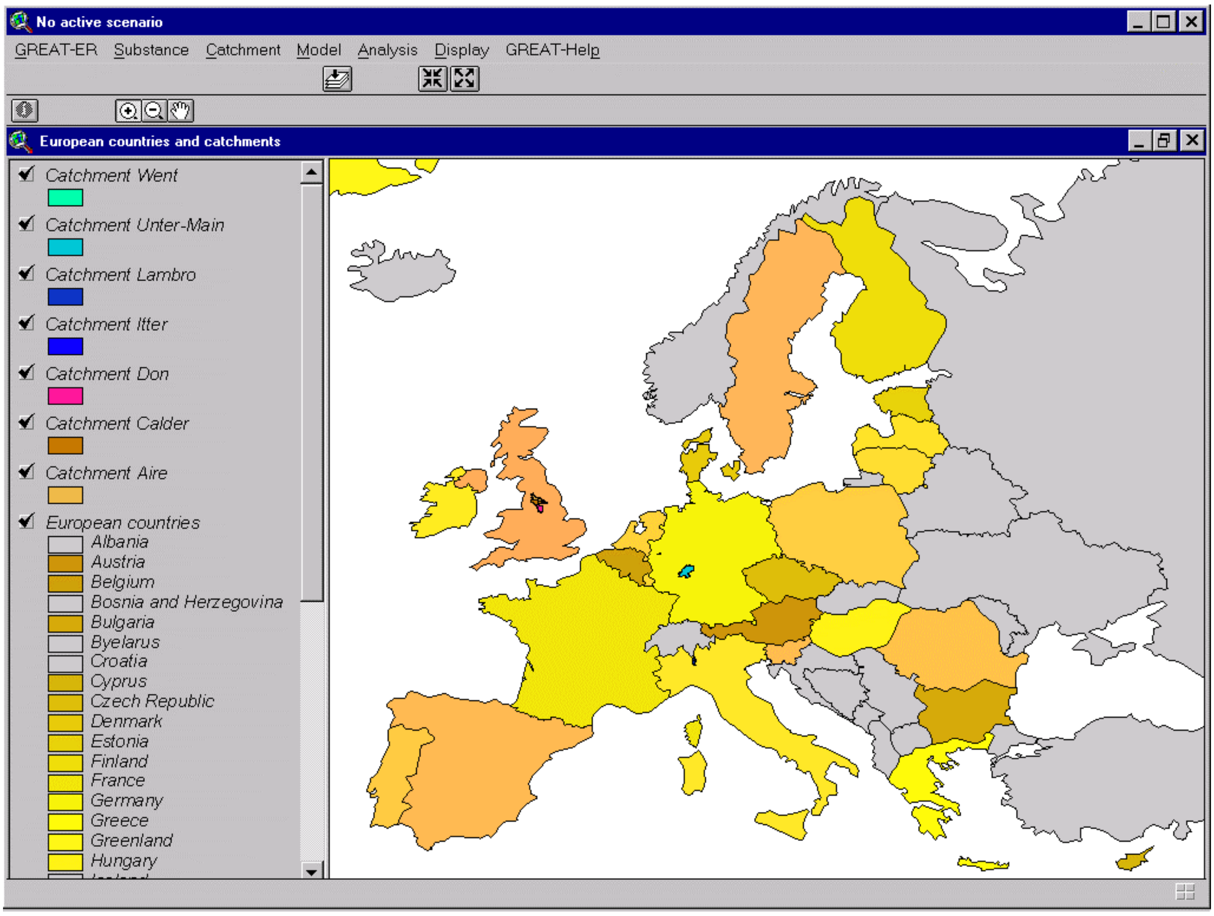


Figure 2.2: *GREAT-ER - initial screen*

GREAT-ER starts by default in the *Easy-to-use mode*: the ArcView menu bar is replaced by a specific GREAT-ER menu bar, the number of buttons and tools is reduced to the set needed for GREAT-ER. Please note that each menu item (when highlighted) is explained briefly in the bottom left corner of the ArcView window.

The menu items are ordered according to the usual work flow of a simulation session. Initially you have to create or select a scenario. The next step is to modify the data. Usually users will simulate a specific substance with several catchments and may want to use more detailed models if the simple ones identify issues. Hence the menu bar reflects this order of steps: *Substance*, *Catchment* and *Model*. The following items enable you to analyse the simulation results and offer various options to display accessory data or to modify the presentation of data based on additional information.

## 2.3 SETTING UP A SCENARIO

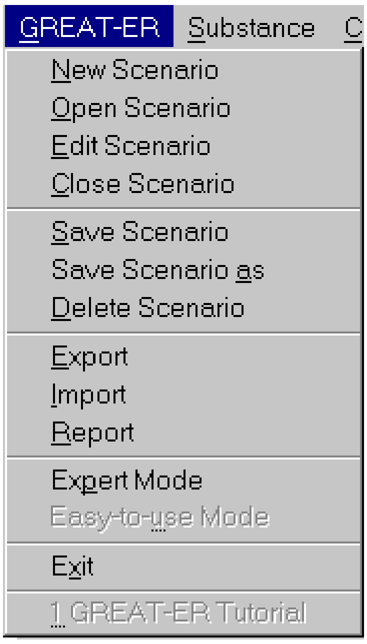


Figure 2.3: *GREAT-ER Menu*

The first menu of the GREAT-ER user interface, called *GREAT-ER*, covers all options to manage scenarios: creating new or loading existing ones, saving, deleting or exchanging with other users. As usual for Windows applications, this menu also includes the exit item and a list of currently open documents (here GREAT-ER scenarios).

### 2.3.1 Creating a New Scenario

To create a new scenario, select the ‘New Scenario’ item from the GREAT-ER menu. A new dialog appears:

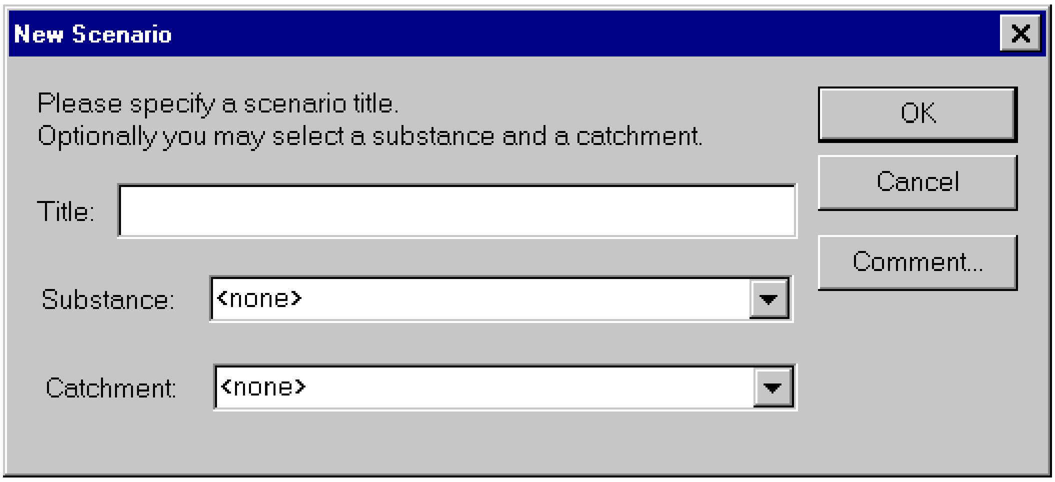


Figure 2.4: *New Scenario Dialog*

To create a new scenario you have to specify a *scenario name* at this stage. The name is used to identify the scenario in all further steps of GREAT-ER application. You may also select a substance and a catchment at this stage, although this can be left until later. Finally, you can enter a comment on the scenario to give additional remarks.

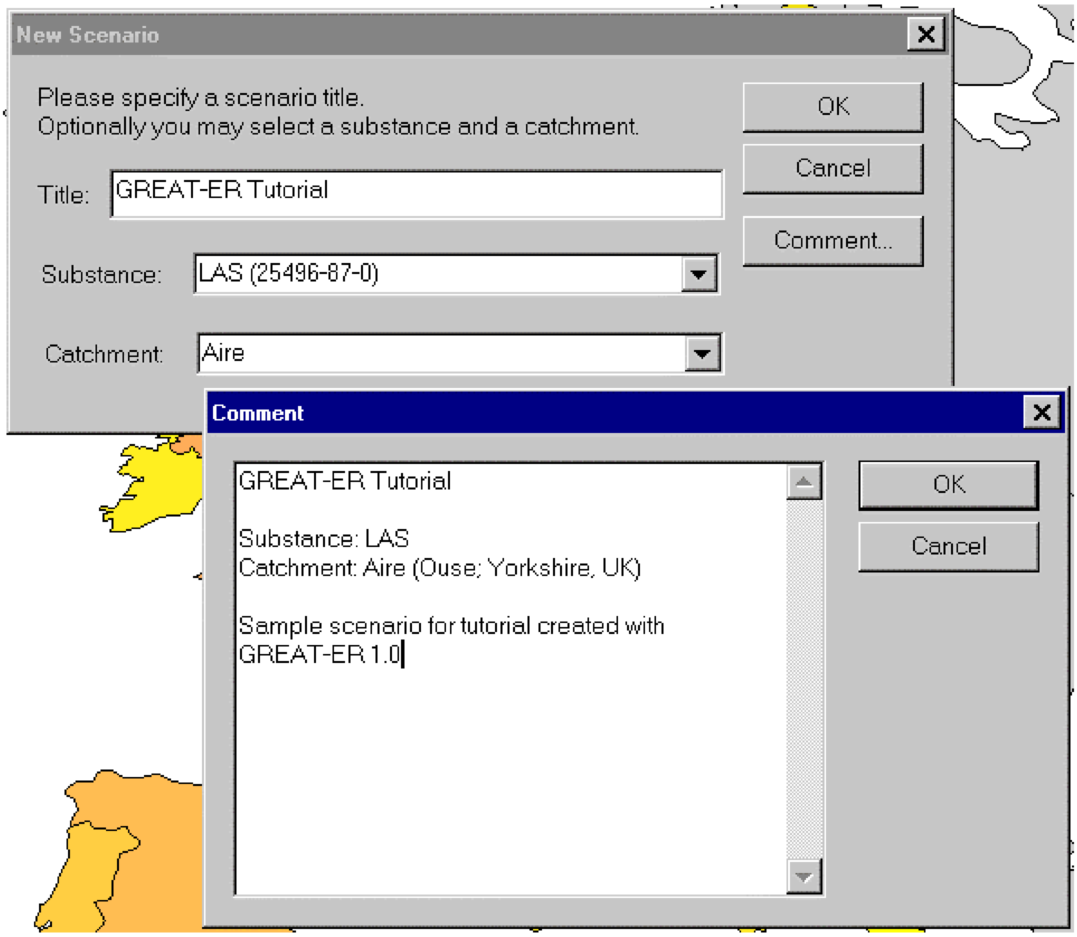


Figure 2.5: *Scenario Comment Dialog*

As an example, enter the name `GREAT-ER Tutorial` and select the substance *LAS* with the catchment *Aire,* then click on OK to leave the New Scenario dialog. You are then asked to specify a scenario directory name. Enter a non-existent subdirectory name (e.g. `tutorial`). The directory will then be created automatically. Each scenario is stored in a separate directory.

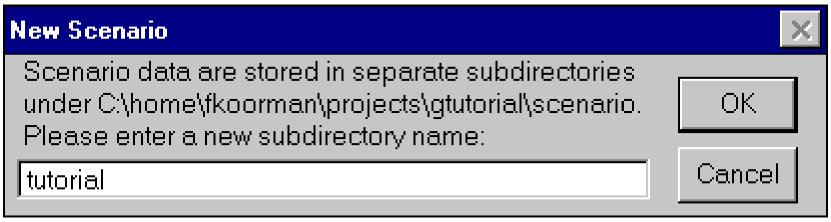


Figure 2.6: *Scenario Directory Dialog*

Finally, to accomplish the generation of scenario data structures, two dialogs will be presented to you (*Model Selection* and *Catchment Data*). Once you are more familiar with the software you may use these dialogs to speed up the input process for a simulation. Currently you only have to leave them with "OK". The dialogs will be explained later in this tutorial. Upon leaving these dialogs GREAT-ER loads the data and displays the selected catchment on the screen (Figure 2.7).

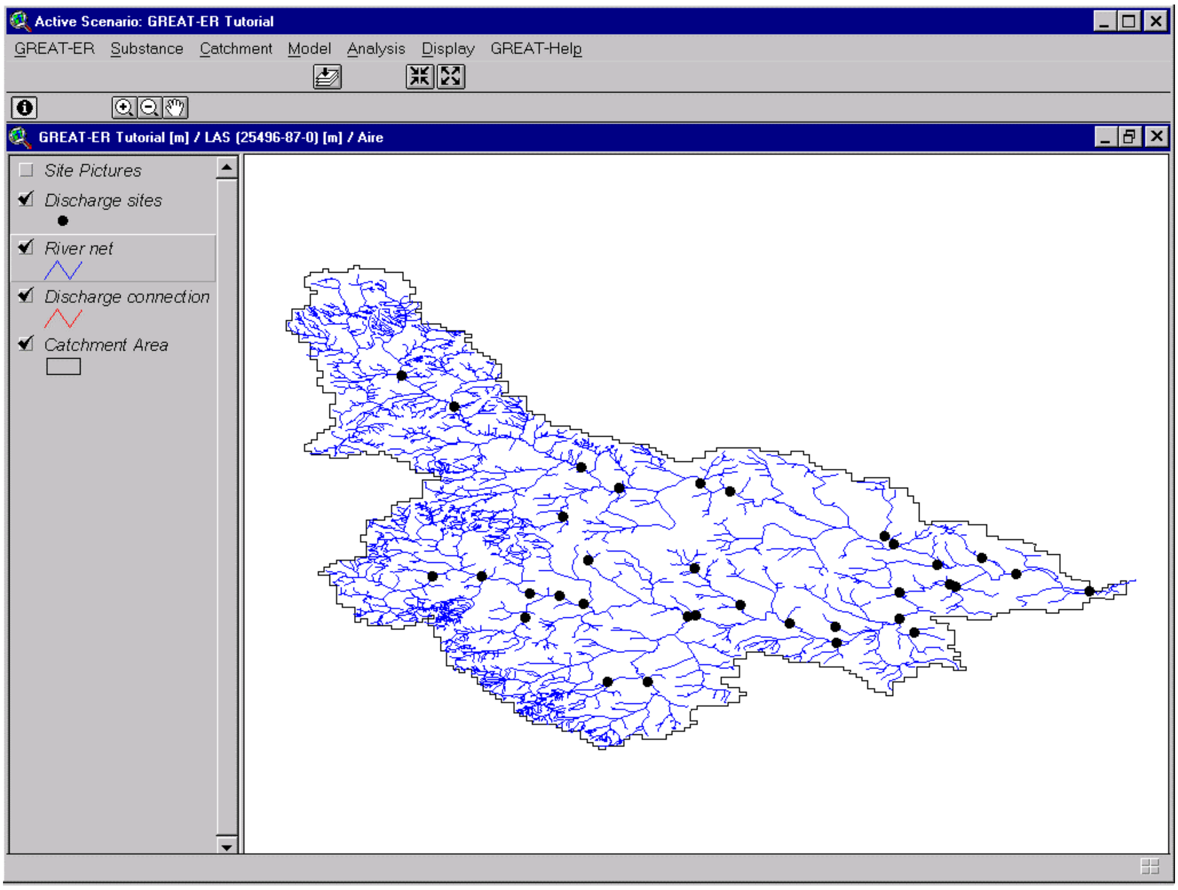


Figure 2.7: *Scenario Tutorial with Catchment Aire*

The view now displays the Aire catchment with *river network*, *discharge sites* and *catchment boundary*, as mentioned in the view's table of contents (to the left of the map). The user can 'check' (tick) the different map 'themes' in this table to select those required on the display.

The *discharge connections* are needed because sewage treatment plants may be situated at some distance from the actual discharge point into the river. Usually the distance is too small to be seen on the full catchment scale. The *site pictures* theme is a special theme which is only visible if photos are available to give users a better impression of the catchment.

The view title bar now gives some summary information about the data displayed: the name of the scenario, the substance and the catchment. The *m* in brackets warns users that there are unsaved changes. It can either appear for the scenario or the substance.

To also see the comments of a scenario, click with the *right* mouse button on the main display (map). A dialog with the scenario settings will appear.

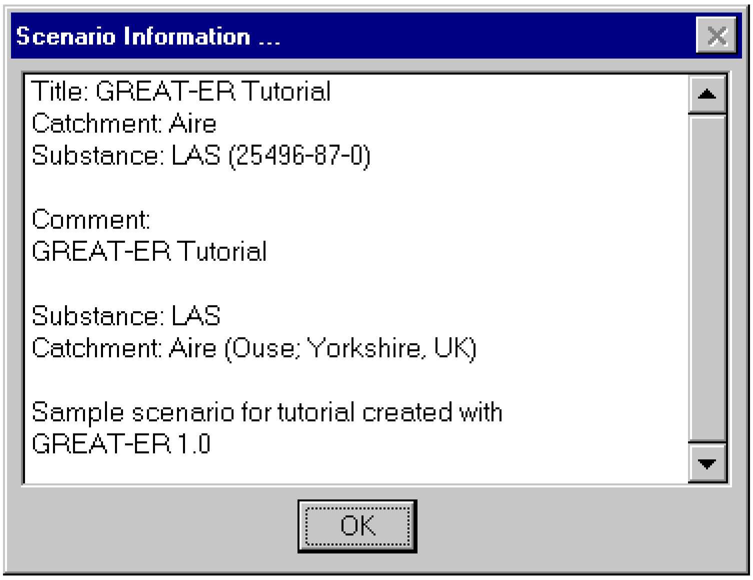


Figure 2.8: *Scenario Information Dialog*

The title bar of the ArcView application now displays the name of the active scenario (see above). This is helpful if more than one scenario is open and visible on the screen.

At this stage the user can experiment with the some of the tools (e.g. identify, zoom, pan). The *identify* tool presents the attributes of selected geographic objects. The user can select a theme from the table of contents (e.g. discharge sites), click on the 'i' icon and then click on a relevant map object (e.g. a discharge site) to view the various attributes associated with that object. Sometimes, due to the scale of detail, more than one object might be selected by a click. If this happens, the attributes of each object selected are presented sequentially in separate dialogs. To see them all, click "OK", to abort "Cancel".

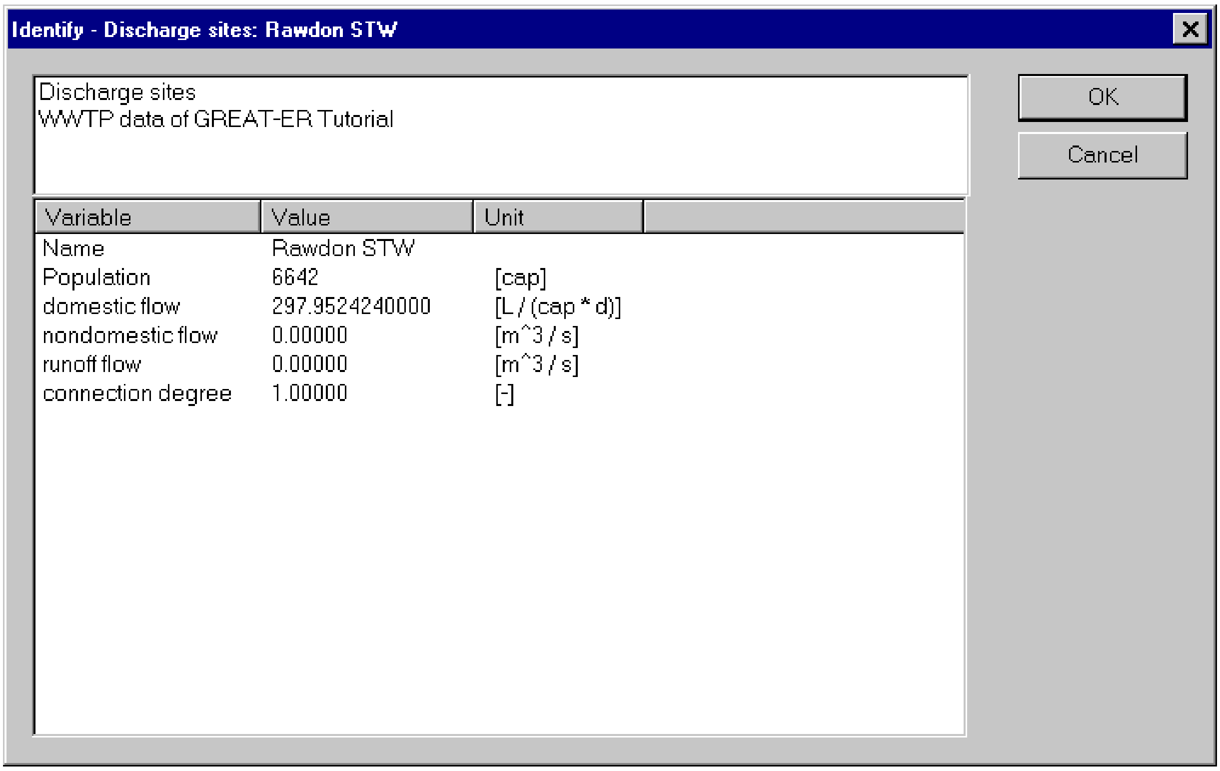


Figure 2.9: *Identify Tool Dialog*

### 2.3.2 Needed Inputs

Having now created a new scenario you may use the settings and data loaded from the databases (by selecting substance and catchment) or modify them.

As mentioned above, GREAT-ER provides three complexity modes for each of the various models. Obviously, the amount of required data increases with the complexity mode of a model. The GREAT-ER user interface accentuates this by colouring parameter values within the dialogs: Parameters coloured *green* are definitely not used in the current model mode selection, whilst those coloured *black* might be used.

Please refer to the technical documentation for a detailed description of the model complexity modes and the required parameters. By default, all sub-models (sewer, waste water treatment and river) are set to complexity mode one. The parameters needed at this complexity level are mentioned in the sections below.

### 2.3.3 Editing Substance Data

Having selected a substance within the scenario creation, the substance data set is loaded from the database. To view the data, select *Edit Substance* from the substance menu.

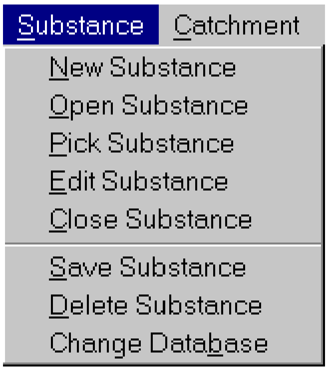


Figure 2.10: *Substance Menu*

The substance menu is split into seven categories presented on seven different ‘cards’:

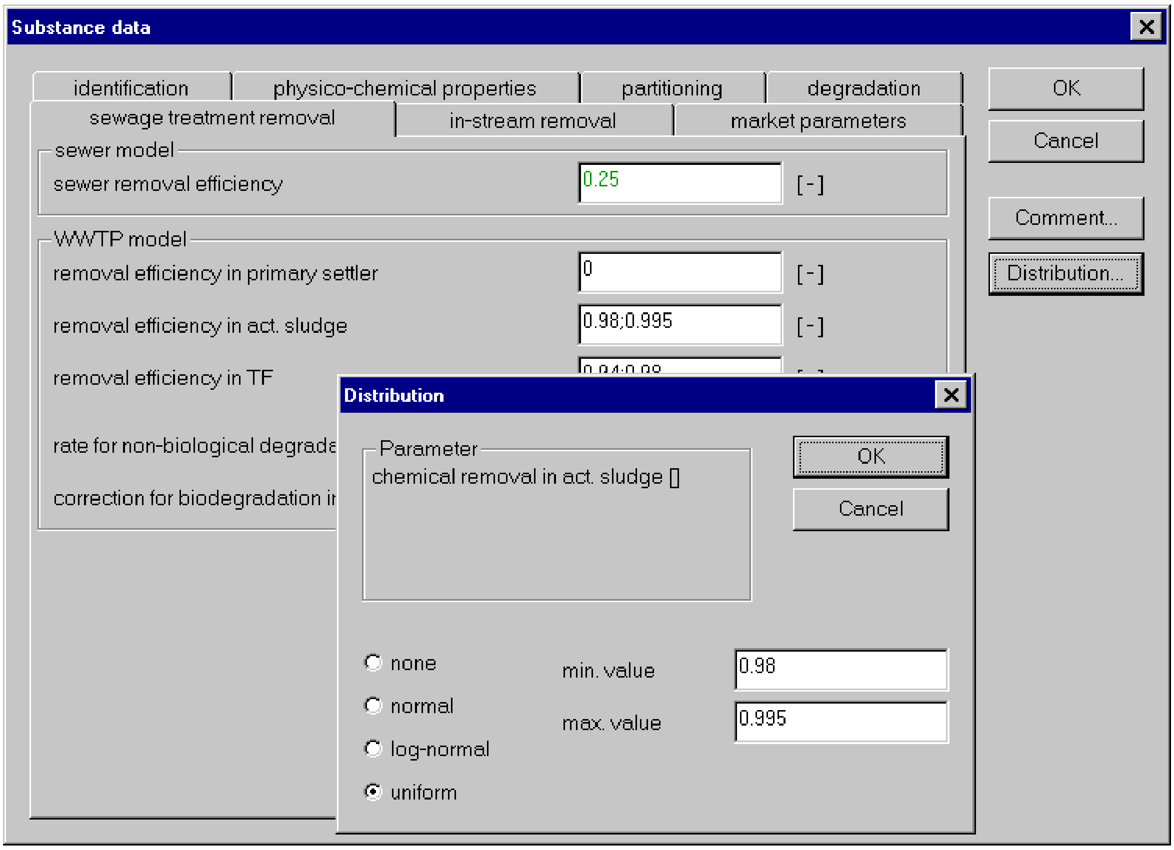


Figure 2.11: *Substance Data*

The various substance data are described briefly below.

***identification***

The identification card is the first one presented to the user upon entering the substance data. It is compulsory to give the substance a name; all other parameters which may ease identification are optional.

***physico-chemical properties***

In the simplest model modes these data are not required. They are only relevant for the higher modes as follows :

***partitioning***

The partition coefficients, if entered here, will override any estimated values calculated from physico-chemical properties. In the simplest model modes these data are not required. They are only relevant for the higher modes.

***degradation***

In the simplest model modes these data are not required. The parameters are only relevant for the higher modes.

***sewage treatment removal***

These data determine how much removal can occur during sewage treatment. In the simplest mode, GREAT-ER requires a fixed removal efficiency (expressed as the fraction removed) during primary, activated sludge or trickling filter treatment. All other parameters are related to higher model modes.

Please note that the plant types currently related to the treatment plant in the various catchments delivered with GREAT-ER always consider a primary settler as the first step in sewage treatment. If you only have an overall removal fraction (e.g. a combined removal fraction for primary and secondary treatment) you can set one of them to zero and enter the combined rate in the other.

The sewage treatment card also gives information on another fundamental GREAT-ER concept (if you have selected the sample LAS substance data set). As described briefly under the basic concepts, the GREAT-ER models perform a stochastic simulation on top of a deterministic model by the Monte-Carlo method. This covers the variations within the catchment's hydrologic regime but also considers other parameters. For most parameters it is possible to specify a distribution. These can be either normal, logarithmic normal or uniform. Depending on the selected distribution a set of values has to be entered to describe the distribution. Leaving the distribution dialog you may notice that distributions are coded by the descriptive values separated by a semicolon. Do not try to specify a distribution by entering the values directly. Obviously further information is needed to describe a distribution. Always use the distribution dialog (invoked by the related button) if you want a parameter to be considered as distributed.

***in-stream removal***

The *in-stream removal* card enables you to control the elimination processes within the river. Only an aggregated first-order elimination rate is needed for the simplest river fate model (mode 1). The other parameters are only used in higher model modes.

Another GREAT-ER feature is the option to enter a special comment for each value. This is useful to document the data sources for the various parameters. Try the comment button to obtain further information on the elimination rate.

***market data***

The *market data* card enables you to specify a general consumption value for the substance. This is slightly different from the *Edit Market Data* dialog discussed later in this tutorial which enables you to specify consumption values for selected discharge sites. The current version of GREAT-ER (1.0) does not allow a distribution to be given for product consumption.

Upon leaving the substance dialog, all substance settings for a first simulation run are made.

#### 2.3.4 Pick Substance and Change Database

The Pick Substance and the Change Database function somewhat differently: The *Pick Substance* enables you to copy the substance data from another open scenario. This makes it easier to transfer specific parameter settings to several scenarios. The *Change Database* item enables you to change the database from which substance data are loaded. If you intend to work with a large amount of substances this feature gives users the opportunity to group substances by classes into different databases. This increases the transparency of data storage and speeds up data retrieval.

### 2.3.5 Editing Catchment Data

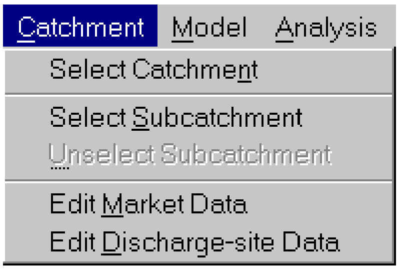


Figure 2.12: *Catchment Menu*

The catchment data mainly consist of spatial data sets which are not editable within the easy-to-use mode. The user can only select a new catchment for the currently active scenario. However, it is possible to select a subset of the current catchment (e.g. the Aire upstream the confluence with the Calder in the tutorial sample scenario) to focus on the area of interest and to speed up the simulation.

As with the sub-catchment selection, the main items of the catchment menu, *Edit Market Data* and *Edit Discharge-Site Data*, are also managed by 'tools'. After selection, the mouse pointer style changes to identify the new mode. Click on the catchment map to choose the object to be edited.

*Edit Market Data*

The *Edit Market Data* dialog enables you to specify site-specific consumption data. To cover industrial sites, users can enter an additional input into the treatment plant This input reflects discharges resulting from the production processes and can be calculated from the production volume. Please note that 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 input considered here is the mass flow independently of substance into the treatment plant in [kg/a]. As with the loads from domestic inputs, the industrial input is subsequently processed by the treatment plant model, if present, for the selected location.

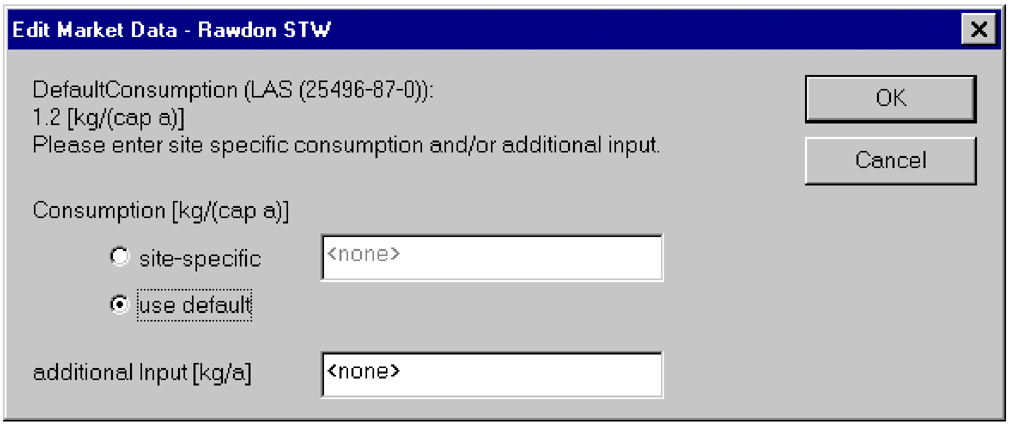


Figure 2.13: *Edit Market Data Dialog*

*Edit Discharge-Site Data*

Similar to the *Edit Market Data* dialog, the *Discharge-Site Data* dialog enables users to modify the parameters of a specific treatment plant.

Several site-specific parameters can be changed. These include population, the elimination rate (used for complexity mode I), the treated fraction of incoming sewage (e.g. bypass or overflow) and in general the type of treatment plant. Incoming waste waters from separate "sources" are also considered such as domestic input, non-domestic input (this covers mainly industrial inputs) and run-off. If only an overall value is available for treatment plants this should be entered as domestic flow.

Please note that domestic flow is given in [litre / (capita * day)], whilst non-domestic flow and run-off are considered as [$m^3$ / second].

Please note furthermore that it is possible to specify a distribution for a general removal efficiency, but not for a site-specific removal efficiency. Nevertheless, it is possible to have a distributed removal efficiency for, e.g. activated sludge plants, and a fixed rate for a selected site.

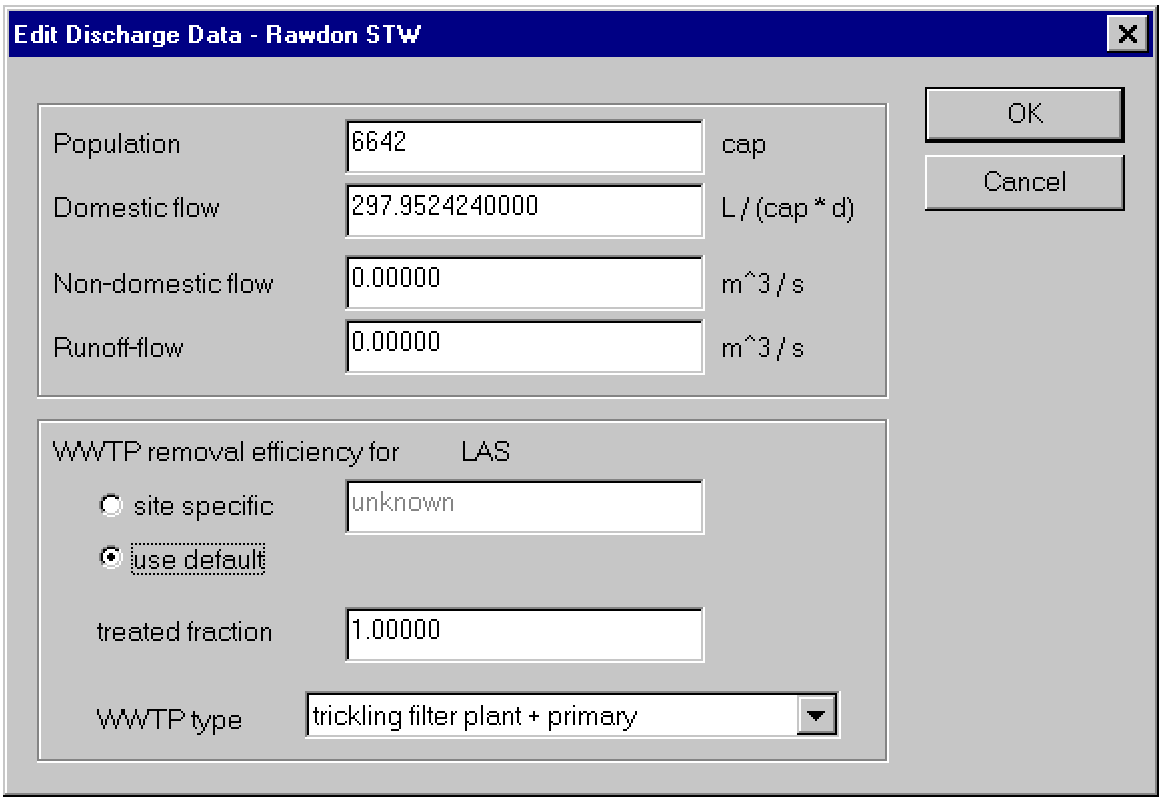


Figure 2.14: *Edit Discharge-Site Data Dialog*

## 2.4 RUNNING A SIMULATION

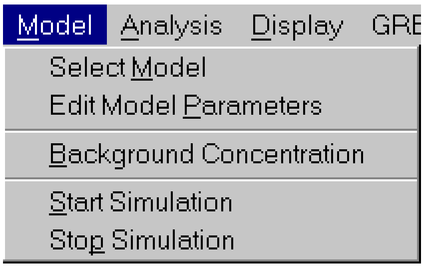


Figure 2.15: *Model Menu*

Having created a scenario and selected the substance and catchment data, the user can then select the required model parameters and start a simulation.

There are three additional dialog options which the user can select at this stage; *Select Model*, *Edit Model Parameters* and *Background Concentration*. These are described briefly below:

*Select Model*

The *Select Model* dialog also allows the user to select the complexity mode for the different models. Figure 2.16 shows the options for the river model and similar options exist for the sewer and wastewater treatment models.

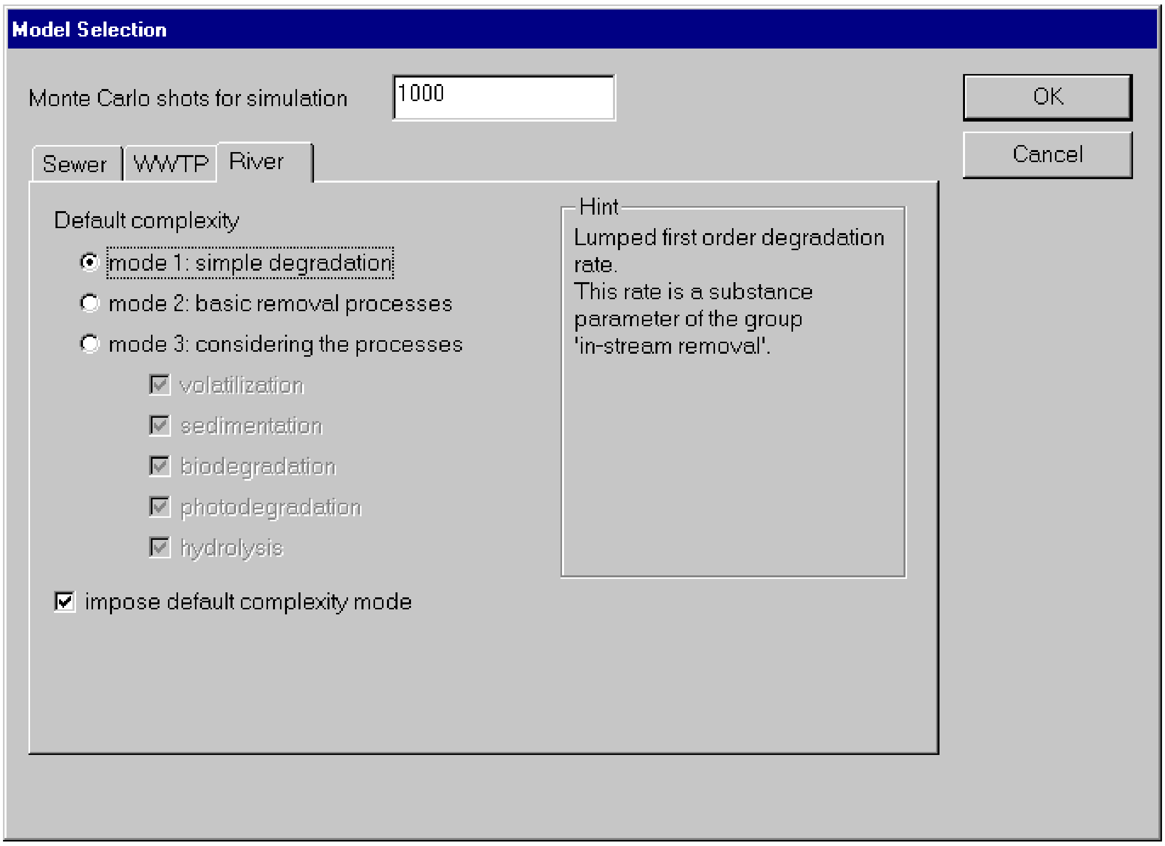


Figure 2.16: *Model Selection Dialog*

The text field on the right provides some summary information (hints) on the selected mode. If you increase complexity modes, it may be necessary to go back to earlier data dialogs to enter additional parameters. For example, if you need in-sewer removal to be considered, you have to go back to the substance data dialog to enter a removal rate for sewers. Please note that in-sewer removal is the only 'higher' model in which only one parameter has to be entered. All other 'higher' models require a somewhat larger data set.

Since GREAT-ER uses the Monte-Carlo method to provide a stochastic approach, the number of Monte-Carlo shots performed during a simulation also has to be entered within the *Model Selection* dialog. As a rule of thumb, the minimum number of shots recommended to obtain a stable simulation result are as shown in Table 1:

**Table 1. Monte-Carlo Simulation**

| | small catchments / simple | large catchments / complex |
|---|---|---|
| $C_{sim\ mean}$ | 500 | 2500 |
| $C_{sim\ 90\%}$ | 2500 | 5000 |

*Edit model Parameters*

The *Model Parameters* dialog allows the user to edit various environmental data and specific properties of the sewer, wastewater treatment plant and river models. For higher complexity modes, a useful feature is the "Default" button which can be used to assign pre-selected values to different parameters. However, please note, that each default value has to be set individually. If you want a set of all default values to be used for some scenarios this is currently only possible by creating a generic scenario without a substance or catchment. All further scenarios can then be created from this generic one and saved to new scenario (use *Save As*).

*Background concentration*

*Background Concentrations* are included to consider additional loads within the river network which may be found upstream from the first known discharge. Note that the given value is simply added to the model results after the simulation. The background concentration is not considered within the elimination processes.

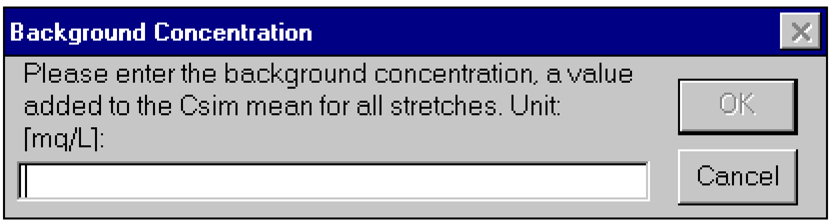


Figure 2.17: *Background Concentration Dialog*

You are now able to start a simulation. Click on *Start Simulation*. Initially, GREAT-ER 'exports' all the data needed for the simulation. Depending on your computer system, this could take a while. Then a new window appears, displaying the progress of the simulation:

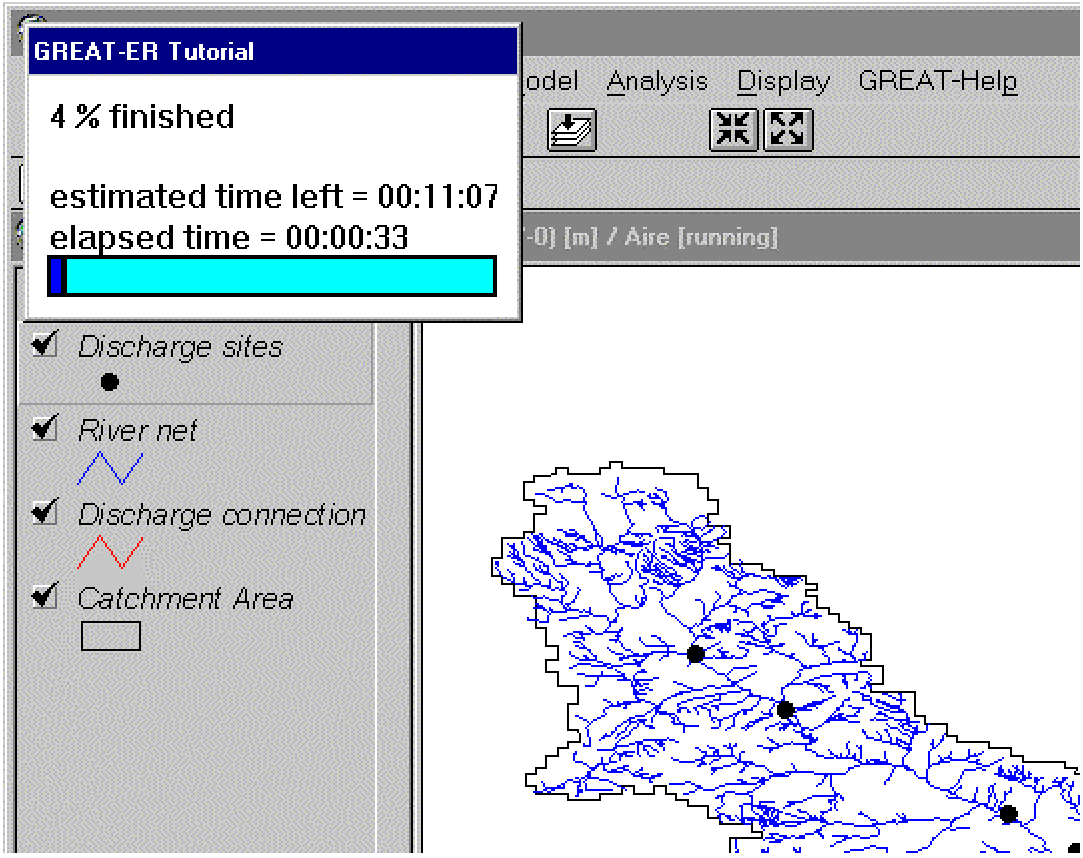


Figure 2.18: *Running simulation on Aire catchment*

Due to some system timings it is not possible to change to another window during this initial phase. After a short delay, window control becomes available again and you may change back to the ArcView window, running the simulation in the background. A remark `[running]` in the window title bar identifies that a simulation is running for the active scenario. The user may now proceed to work with another scenario or even on the scenario view currently under simulation. You should not modify scenario parameters while a simulation is running. You should also bear in mind that any user interaction while a simulation is running may significantly increase the simulation running time.

After the simulation has finished, the results will be displayed on the screen. The river stretches will be coloured according to the model results. A new theme will also be visible in the view's table of contents entitled *Csim mean*. Csim stands for *simulated concentration* (in contrast to *monitored concentration*); *mean* indicates that the different colours represent the mean concentrations resulting from the Monte-Carlo method. [More specifically, the mean value is given as $C_{sim,\ internal}$ which is described later in more detail].

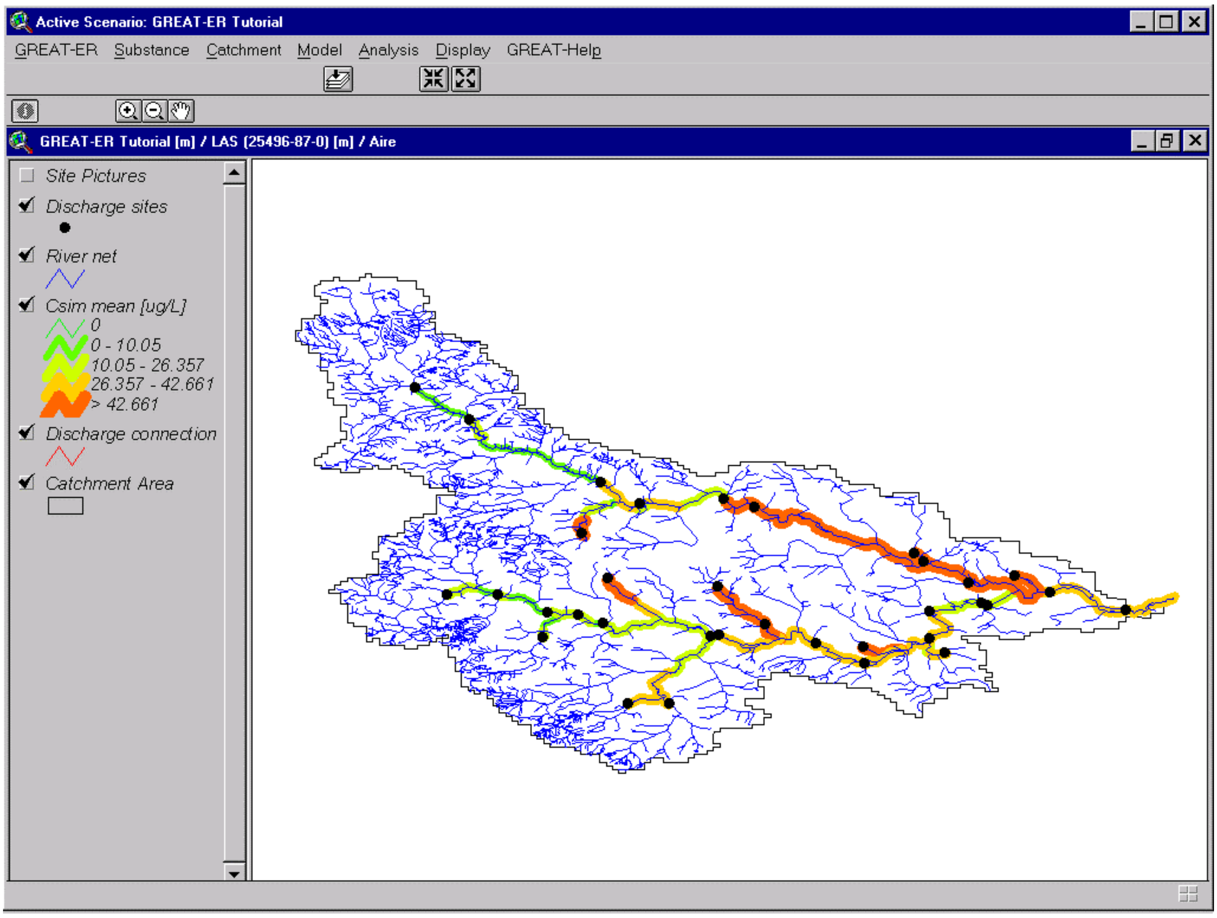


Figure 2.19: *Visualisation of simulation results for the Aire catchment*

If you need to abort a simulation for some reason, click on the simulation progress window. A dialog appears, asking you if the simulation should be continued.

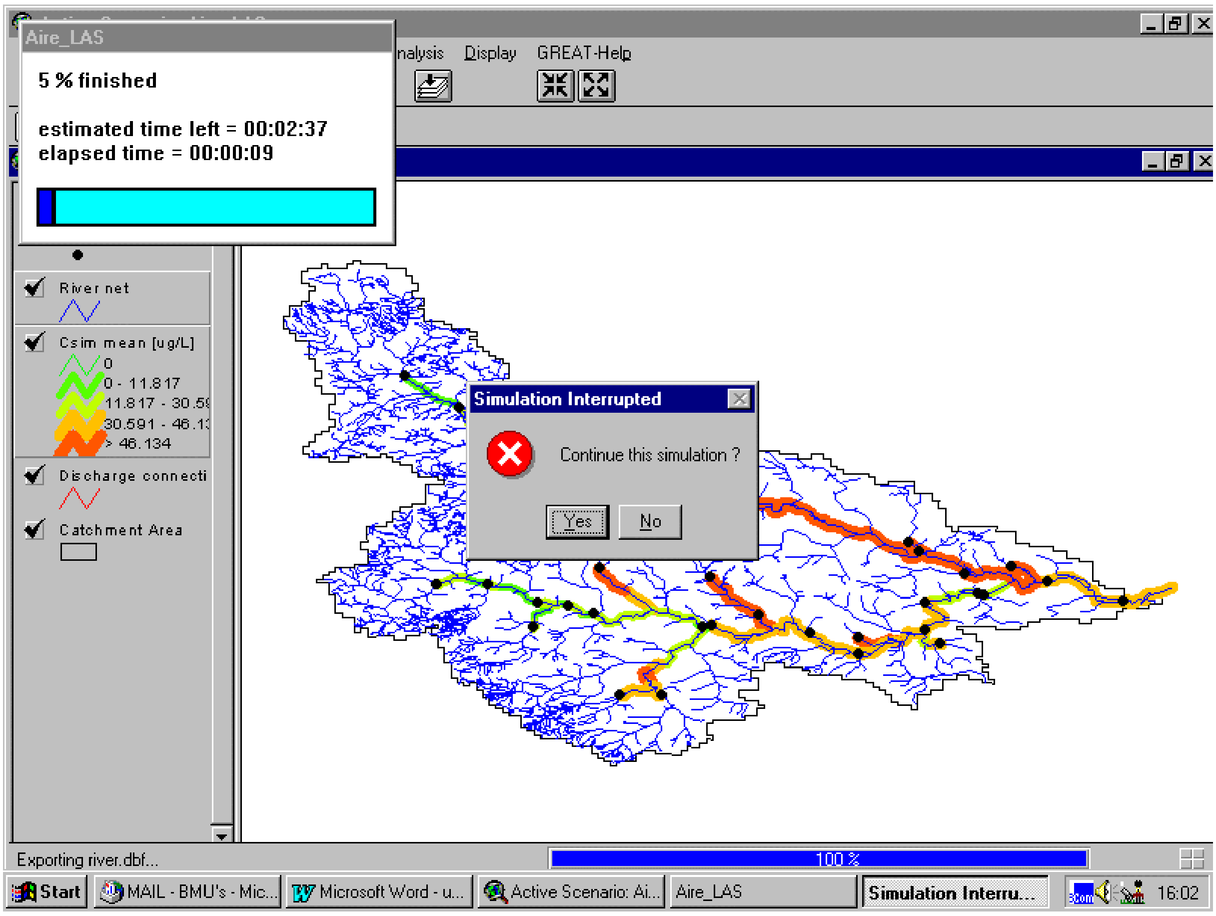


Figure 2.20: *Process of simulation abortion*

If you then select "No", the simulation will be aborted and a report will inform you about the message sent back from the simulation system to the GREAT-ER user interface:

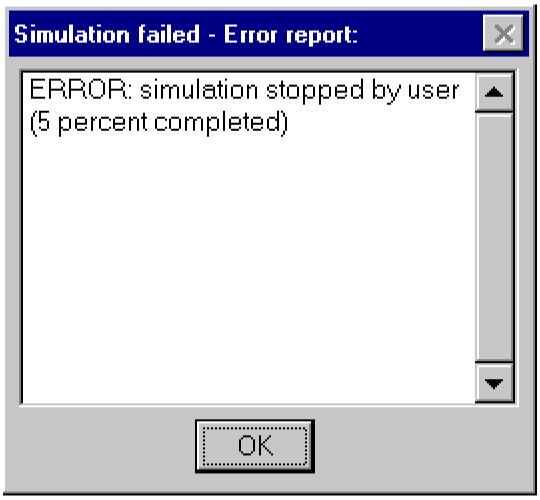


Figure 2.21: *Process of simulation abortion*

The meaning of the menu item *Stop Simulation* is not the same. This item is a kind of safety guard. If a simulation fails for some reason (identified for example, by an error message titled `rsxnt`) you should select the *Stop Simulation* menu item. This will change some settings behind the user interface and enable you to safely save any remaining open scenarios. After selecting this item you should close GREAT-ER and restart. Errors may occur if attempting a very large number of Monte-Carlo shots, for example, or if the numerical solution becomes unstable for some reason.

### 2.4.1 Save a Scenario

Before proceeding to analyse the model results it is advisable to return to the beginning, the *GREAT-ER* menu, to save the scenario: select *Save* from the menu: all scenario settings and the model results will be saved in the scenario's directory. A dialog informs you of its successful completion.

The GREAT-ER user interface provides users with two options to save scenario data: *save* and *save as*.

**Save Scenario**

This option writes all data from the active scenario to the file system under the directory specified for the scenario, reports successful completion and lets you proceed with the active scenario.

**Save Scenario As**

This option works slightly differently. First you have to specify a new name for the scenario (scenarios are identified by their names, so unique names are recommended) and enter any comments to help future identification of the new scenario. You then click on "OK" and specify a new scenario directory, which will then be created automatically.

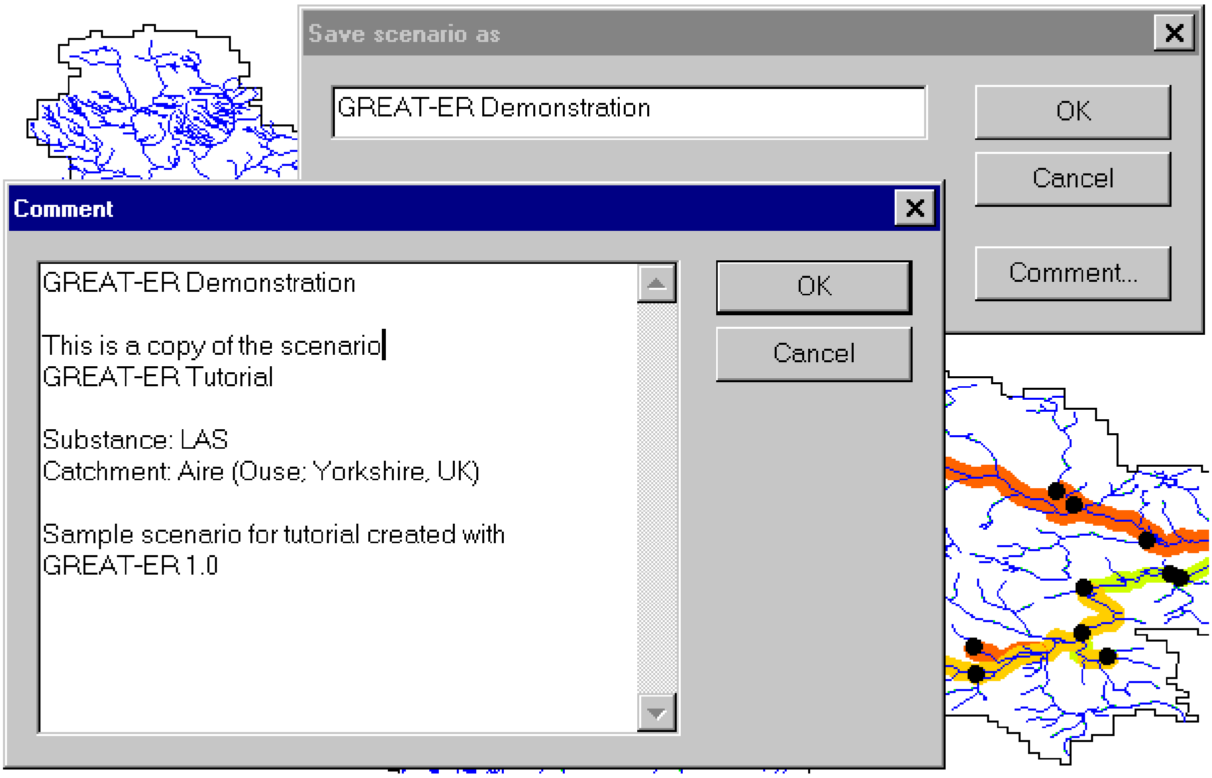


Figure 2.22: *Save As Dialog*

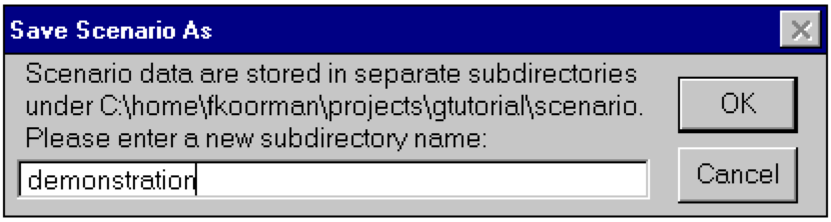


Figure 2.23: *Save As Directory Dialog*

After using *Save Scenario As* a message will appear reporting successful completion and reminding the user of something very important: *The active scenario stays the original one. This means that if you intend to continue working on the scenario just saved, you have to load it again separately. To avoid confusion it is recommended that the original scenario is also closed prior to loading in the new one. Warning: If you make changes to a scenario, then use 'Save As', then subsequently use 'Save' the ORIGINAL scenario is overwritten. This is different to the way other familiar programs work (e.g. WORD or EXCEL) which is why it is being highlighted here.*

## 2.5 ANALYSING MODEL RESULTS

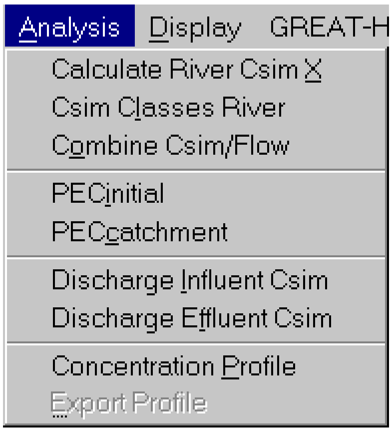


Figure 2.24: *Analysis Menu*

After a model run has been completed, the analysis menu provides various facilities for analysing the results. Since the results are stored as frequency distributions, it is possible to calculate percentiles of concentrations (using *Calculate River Csim X*) for the different river stretches. Alternatively the menu provides you with features to modify the presentation of results: either by *classification* or a colour coded *combination of concentrations with flows*. The analysis tools most relevant to risk assessment are the functions to calculate PEC (Predicted Environmental Concentration) values.

Please note that the GREAT-ER analysis tools are designed to analyse distributions of values. Although it is possible to run a simulation with only one Monte-Carlo shot the analysis functions may fail if this is attempted.

### 2.5.1 PEC Calculations

Figure 2.19 shows clearly that GREAT-ER is able to predict the spatial distribution of concentration, based on real catchment data and known properties of a substance. This is a much more advanced tool than the generic regional or multi-media approaches.

GREAT-ER also proposes some novel PEC concepts for characterising exposure in river catchments (Boeije *et al*, 1999). Several values are provided which are split into two categories: $PEC_{initial}$ and $PEC_{catchment}$. Detailed discussion of the underlying concepts is beyond the scope of this user manual, although a brief description is given below. For further information refer to the technical manual.

**$PEC_{initial}$**

This is the spatial aggregation of concentrations in the river directly after emission. This is similar to the $PEC_{local}$ as defined in the EU Technical Guidance Documents, although its calculation is different.

Based on the $C_{sim,\ start}$ mean values (see Appendix A), the mean is calculated for all stretches receiving treated or untreated discharges:

$$PEC_{initial} = \sum_{i=1}^{n} \frac{Csim, start, i}{n}$$

$C_{sim,\ start,\ i}$ is the concentration at the beginning of river stretch *i*, directly receiving treated or untreated waste water emissions.

By definition, the $PEC_{initial}$ is calculated from the $C_{sim,\ start}$ mean values. This calculation is started by selecting the item *PECinitial*.

Please note that PEC calculations are not available if a Sub-catchment is selected.
After the calculation a dialog displays the result alongside additional information.

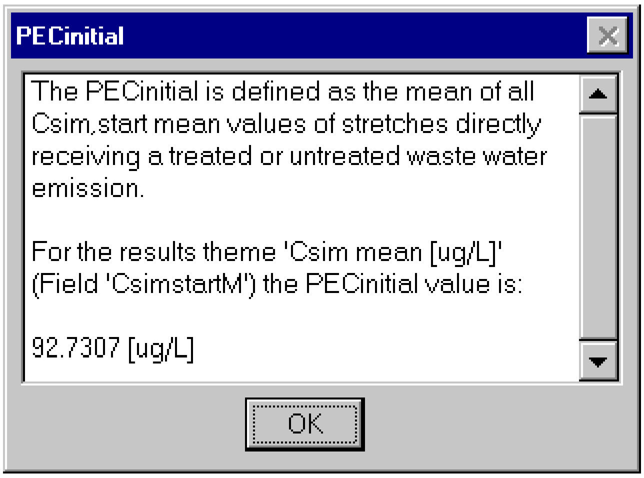


Figure 2.25: *$PEC_{initial}$ calculation results*

**$PEC_{catchment}$**

This is the average of representative concentrations over the entire catchment. This is a new concept for geo-referenced exposure assessment, although there is some analogy with the $PEC_{regional}$ in the EU Technical Guidance Documents.

The "most representative" value for the concentration in the stretch is taken as $C_{sim,\ internal}$ (the average concentration for the stretch). However, different values could be used and in order to demonstrate the effect of using different possible definitions, GREAT-ER computes four different $PEC_{catchment}$ values. These values differ in the set of stretches selected for the calculation and in the weighting of concentrations.

All $PEC_{catchment}$ values are defined as the mean of the weighted concentrations of the selected stretches. Possible selections are (A) all stretches within a catchment or (B) only polluted stretches. Option (A) is more comparable to the current regional exposure assessment approach (unit world models) in which all surface waters in a region are considered to be available for the dilution of the chemical mass loading. In contrast, option (B) considers only the loaded river stretches and allows the user to focus on the river stretches potentially at risk.

Both approaches have to deal with different issues concerning scale dependencies or data requirements. The different weighting methods are discussed below:

1. **Weighting by stretch volume** for both stretch selections. The volume is calculated (assuming a rectangular cross section) by flow, flow velocity and length. This method places more weight (and therefore 'importance') on large rivers and therefore on high dilution situations.

2. **Weighting by stretch length** for both stretch selections. The interpretation of this weighting method is that stretches with equal length are of equal importance. Small rivers are considered to be equally valuable as large rivers.

Methods 1 and 2 depend on the scale and detail of the underlying digital river network, and the more that (unpolluted) headwaters are included, the lower the aggregated $PEC_{catchment}$ will be. Conversely, in a low detailed river network, small (and possibly more valuable) stretches are neglected. Hence these two methods are most relevant for option B, where only the loaded stretches are considered.

3. **Weighting by flow increment** considers all stretches within a catchment. The weighting of a stretch is calculated by the difference of flow in relation to its upstream stretch (two stretches in the case of a confluence). Thus the values related to stretches are similar to those in weighting by length. A slight accentuation might be given to receiving stretches because, in addition to the natural flow increment, these are also artificially influenced by the waste water flow.

   The initial stretch of a river is considered with its complete flow (there is no longer an upstream stretch and thus the increment is the flow). If these stretches are unpolluted, the weighting method is largely independent of the scale of detail of the digital river network. Regardless of how detailed rivers are digitised, the flow of a given stretch can be considered as the sum of all its upstream stretches and therefore the stretch representing the headwaters is of the same value as all stretches considered separately.

The calculation of $PEC_{catchment}$ can be based on any of the previously derived percentiles of the model results. When selecting *PECcatchment* the existence of previously calculated values is first checked because, depending on the catchment extent and detail of the digitised river network, the calculation may take several minutes. A progress bar will index the progress of the calculation. After completion the values mentioned above are listed in a small report window:

Note that the *PECcatchment* calculation may be based on mean or 90th percentile *Csim* values:

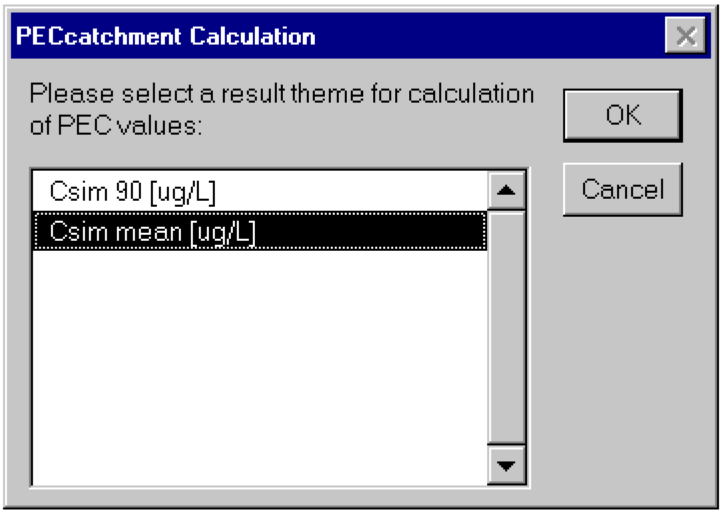


Figure 2.26: *PEC$_{catchment}$ calculation results*

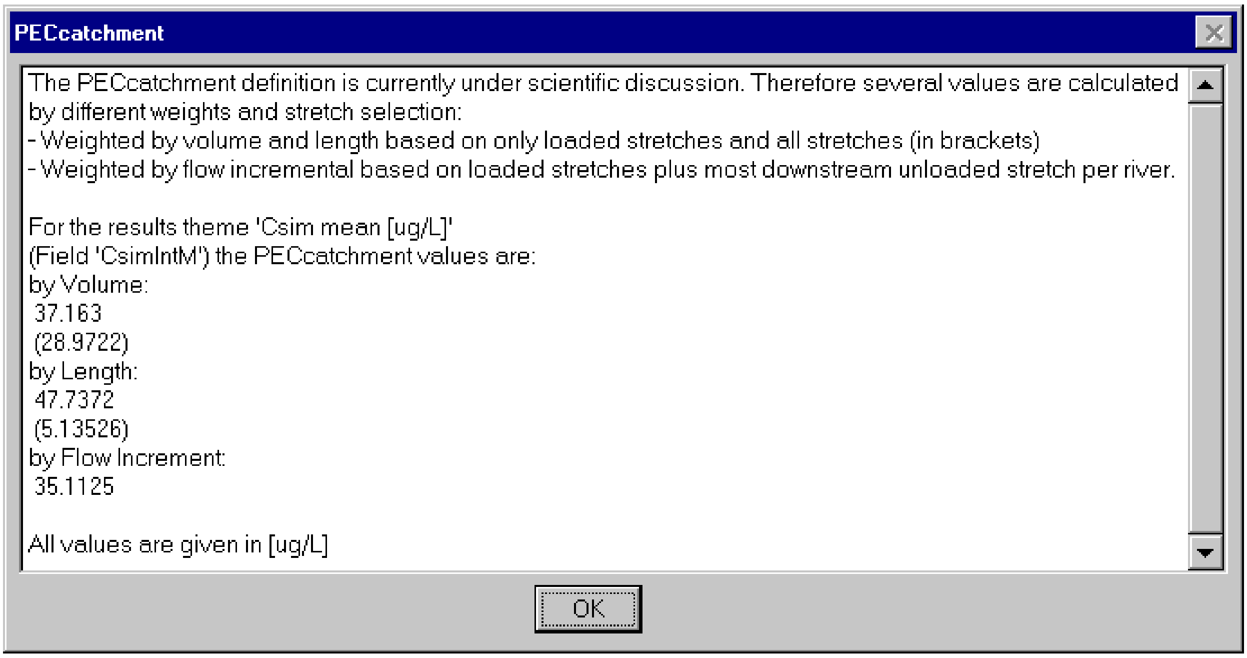


Figure 2.27: *PEC$_{catchment}$ calculation results*

## 2.6 ADDITIONAL DISPLAY OPTIONS

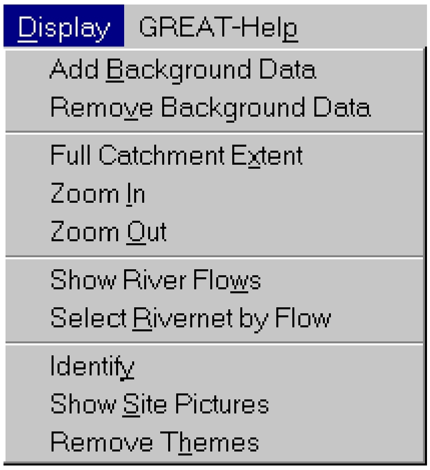


Figure 2.28: *Display Menu*

The monitoring programmes undertaken in the pilot areas of GREAT-ER form an integral part of the GREAT-ER project. The data obtained are stored as geo-referenced data (i.e. monitoring sites with monitoring data as attributes) within the GREAT-ER software. To display these data select *Add Background Data*. A dialog will then present a list of all background data available for the active scenario. Monitoring data will also be available among these.

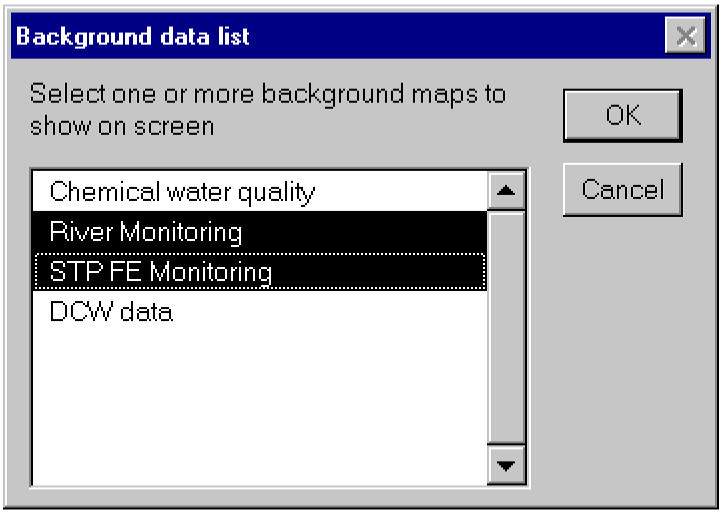


Figure 2.29: *Select Background Data Dialog*

The user may select one or more entries. For the purpose of this tutorial select `River Monitoring` and `STP FE Monitoring`, FE stands for Final Effluent and leave the dialog with "OK". Two new themes are displayed on the view.

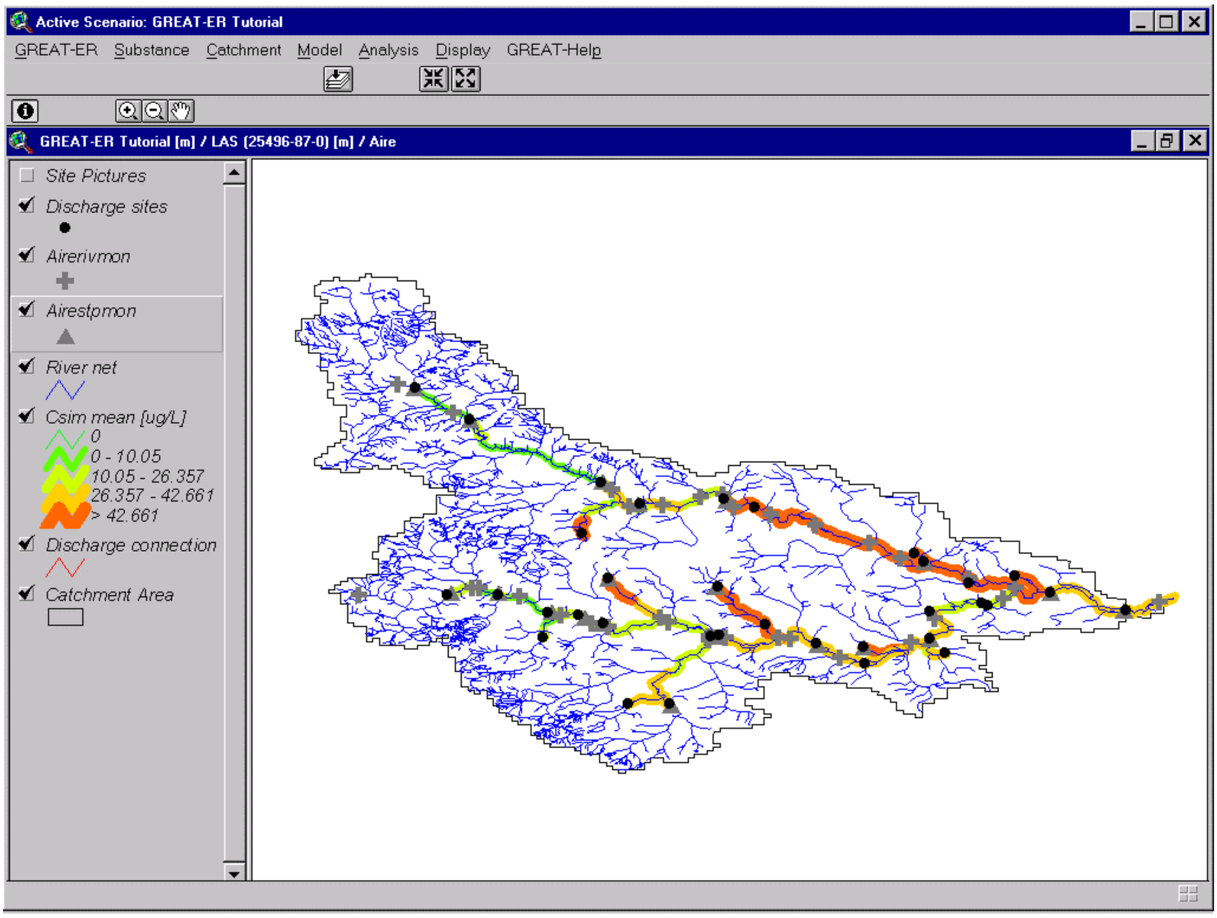


Figure 2.30: *Display of Monitoring Sites for Aire Catchment*

Once the data are visible on the display, the monitoring data can be investigated using the identify tool. In the same way, any other available background data can be displayed and interrogated.

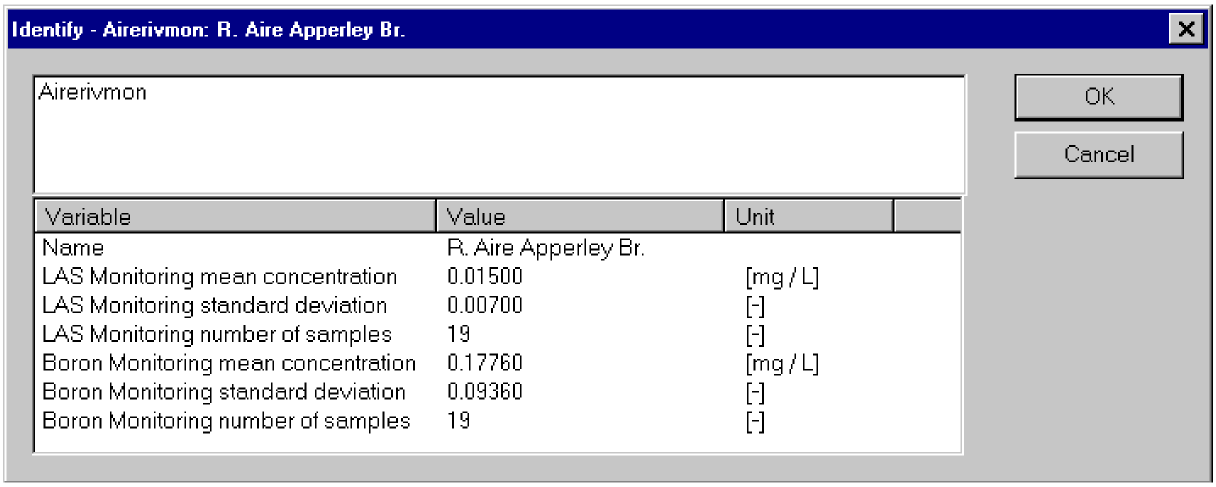


Figure 2.31: *Monitoring Data Identify Dialog*

## 2.7 DATA EXCHANGE

There are two options to exchange simulation results or complete scenarios using GREAT-ER:

- to share scenarios with other users for further discussion;
- to generate a report with results for further analysis or inclusion in other documents.

The first option is supported by providing an export / import functionality. Selecting *Export*, an export file will be created in the directory of the active scenario. The export file will cover all scenario settings and additional data derived from the results. Please note that the export / import feature does not include geographic data such as river network (due to possible licence restrictions). Therefore users have to ensure that they are working on equal geographic data sets if they want to exchange (and work with) scenario data. Conversely, an export file can be selected using the *Import* item and will then be added as a new scenario to the scenario database.

GREAT-ER provides some features for the second option within the expert mode. The menu item *Report* under the *GREAT-ER* menu can be used to write all scenario data and all results to a specified file. Specific parts can then be abstracted from this using a common text editor. Another option is to export a concentration profile for a selected river. By selecting *Analysis* / *Concentration Profile* a tool will be activated, then select a stretch by clicking on the view. Moving downstream the $C_{sim,\ internal}$ values are collected for each stretch. The collection will be displayed in a simple X/Y-profile. Alternatively there is the option to export the profile data to create a smarter presentation using a preferred data plotting or spreadsheet program.

It should be mentioned that the full set of simulation results for a scenario are stored under the scenario directory within the files *`Csim.dbf`* (river) and *`CsimSTP.dbf`* (treatment plants). C*opies* of these files may be used to further analyse the data.

Other options are available under ArcView in the expert mode. The most important function might be to export the resulting visualisation onto a map by colouring the river stretches. This can be done quite comfortably using the ArcView *layout* capabilities.

## 2.8 LIMITATIONS

### 2.8.1 ArcView

**Chart Display**

The chart options of ArcView are quite limited. Only 50 data points can be displayed within an X/Y plot used for the concentration profile along a river. For this reason the profile might not display all stretches downstream from the selected stretch. To deal with this limitation GREAT-ER provides users with the *Export Profile* feature to write the complete stretch set to a file (either plain ASCII or dBase) for further analysis or more comfortable plotting with the user's favourite data plotting or spreadsheet application.

**Error Calling Unlink**

GREAT-ER combines the data needed for simulations from various tables (which is usual for GIS and databases in general). ArcView, as the underlying database system, provides a complex sequential approach for this task. The ‘Error Calling Unlink’ message might occur (usually if a network is involved) as a result of timing problems while resolving these links (possibly while editing a scenario). If this error occurs it is recommended to close the scenario and GREAT-ER immediately.

**Error in Application**

Closing GREAT-ER and therefore ArcView might lead to a cryptic error message caused by ArcView. This is not an error of GREAT-ER but of ArcView itself. It may also occur if ArcView is opened and is left again without any further action.

### 2.8.2 User Interface

**Distributions**

Several substance-related parameters may not be entered as distributed values but the user interface does not warn about this directly. Classified according to the dialog's cards these are:

**Identification**:

Obviously none of the identifications can be entered as distributed.

**Physico-chemical properties**:

molar mass
acid versus basic dissociation parameter

**Degradation**:

anaerobic biodegradation correction factor
anoxic biodegradation correction factor
affinity constant for aerobic / anaerobic
sorbed biodegradation correction factor
temperature correction for biodegradation

**In-stream removal**:

correction factor for biodegradation in rivers

**Sewage treatment**:

correction for biodegradation in activated sludge

**Market Data**:

domestic product consumption.

Note furthermore, that it is possible to specify a distribution for a general elimination rate, but not for a site-specific elimination rate. Nevertheless, it is possible to have a distributed elimination rate for, e.g. activated sludge plants, and a fixed rate for a selected site.

**Default Values**

A set of all default values to be used for some scenarios is currently only possible via a workaround. Create a generic scenario without a substance or catchment. All further scenarios can be created from this generic one by saving them as new scenarios (use *Save As*).

**GREAT-ER Analysis Tools**

Note that the GREAT-ER analysis tools are designed to analyse distributions of values. Although it is possible to run a simulation with one Monte-Carlo shot, the analysis functions may fail if this is attempted.

Note that PEC calculations are not available if a sub-catchment is selected.

**GREAT-ER Help System**

Note that the start-up phase of the help system may take some time to initiate.

**Operating System WINDOWS NT 4.0**

The operating system GREAT-ER is designed for is **WINDOWS NT 4.0**. GREAT-ER **will not** work properly under WINDOWS 95, although ArcView 3.0 and 3.1 do. Compatibility with WINDOWS 98 was not tested.

**Creating Directories**

The feature of directory creation is limited within both the set-up and the GREAT-ER user interface (e.g. new scenario). The last directory in a path can be created, but new multi-stage directories are not possible.

### 2.8.3 Model System

The GREAT-ER simulation system includes detailed sub-models for rivers and activated sludge treatment plants but only a single percentage removal for sewer and trickling filter treatment plants.

## 2.9 ADDING A NEW CATCHMENT

The catchment data sets used in GREAT-ER are large and relatively complex structures. All catchments included in GREAT-ER have to be developed using the GIS system ARC/INFO. However, in addition to this, several software tools for creating a catchment have also been developed within the GREAT-ER project which might be useful for future development and inclusion of new catchments. These software tools are not included with the installation software but are available separately (please contact ECETOC for further information).

A general overview of the processing steps is given below:

The data required to build a GREAT-ER catchment may exist in several different formats and/or resolution. This problem is solved by the definition of an intermediate file format. For each data group a GREAT-ER pre-defined format is given. The required files have to be produced from the original raw data, either manually or from some customised software routines which could be developed if required.

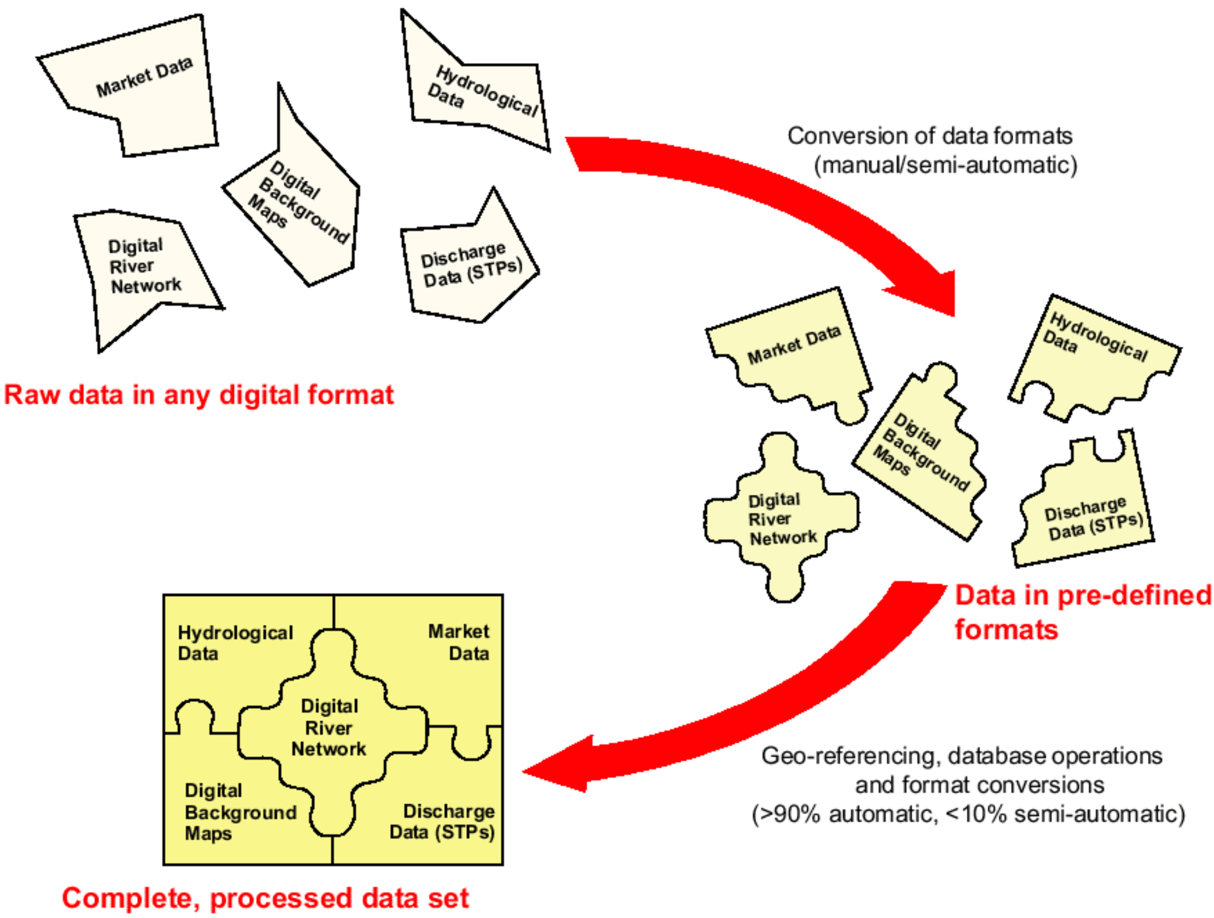


Figure 2.32: *Two step data processing*

Once all the required data have been converted, the second step is quite simple. Most of the work is done automatically via 'makefiles' and several 'scripts'. These will execute the necessary format conversions, data joining, etc. and finally the installation of the new catchment.

All routines used for the production of the currently included catchments are available as source codes (e.g. for MicroLowFlows datasets) and can be studied (contact ECETOC for further information).

# 3. MENU STRUCTURE

The following sections provide a brief description of all the menu items within GREAT-ER 1.0. Sections 3.1, 3.2, 3.3 etc correspond to the main menu groups (GREAT-ER, Substance, Catchment, Model, Analysis and Display). The various sub-sections then describe each of the options within these groups.

## 3.1 GREAT-ER

### 3.1.1 New Scenario

This item is always enabled. A dialog for the specification of a new scenario appears. The minimum set is to specify a *scenario name* for identification. The entered name is checked against the existing scenarios in the scenario database.

Optionally a *substance* and a *catchment* may be selected from the related databases. The editing of a comment is also optional. Leaving the dialog with "Cancel" will abort the creation of a new scenario, "OK" will bring you to a dialog in which to specify a non-existing directory for the new scenario. It will be created automatically.

The dialogs *Model Selection* and *Edit Catchment Parameters* then appear sequentially. Their invocation is necessary at this stage to complete the scenario data set. Finally, the new scenario is made active and the previously active scenario is deactivated.

It is not possible to create a new scenario without a title nor to specify a title already used for another open scenario. If a catchment has not been selected, the new scenario view will display a map of Europe.

### 3.1.2 Open Scenario

This item is only enabled if the scenario database contains at least one scenario. The scanning of the scenario database could take a while if you have already created a number of scenarios.

The dialog that appears is separated into two areas: on the left a list is presented containing all available scenarios. Select one by click or enter a name in the entry field at the top of the list.

Selecting a scenario by a single click, the fields in the right area display additional information on the scenario for better identification: substance, catchment, comment and the scenario directory.

To load the scenario, leave the dialog with "OK" or double-click the selected scenario.

If there is already an open scenario with the same title, the specified one will not be loaded. The one already open must be closed first.

### 3.1.3 Edit Scenario

This item is only enabled if there is at least one open scenario. The dialog is the same as under *New Scenario* to enable the user to modify the main settings of a scenario in a single dialog: name, substance, catchment and comment.

If the name has been modified a following dialog will ask you to change the scenario directory. If the dialog is cancelled or the directory name not changed, the scenario will be kept in the current scenario directory.

### 3.1.4 Close Scenario

This item is only enabled if there is at least one open scenario. If the active scenario is not identical to the scenario in the database with the same title, a dialog will appear giving the option to save the scenario. Confirmation of saving will also be requested if the active scenario is not in the scenario database.

However, if *Close Scenario* is selected, the active scenario will be closed and removed from the list of open scenarios.

### 3.1.5 Save Scenario

This item is only enabled if there is at least one open scenario. The active scenario will be saved to the scenario database. Confirmation is necessary to overwrite a scenario in the database with the same title.

### 3.1.6 Save Scenario As

This command is similar to *Save Scenario*, except that you first have to specify a new title and it is not checked whether the scenario has been modified. The dialog also provides the option to edit the scenario comments. Leaving the dialog with "OK" you have to specify a new, nonexisting directory for the new scenario.

After using *Save Scenario As* a message will appear reporting successful completion and reminding the user of something very important: *The active scenario stays the original one. This means that if you intend to continue working on the scenario just saved, you have to load it again separately. To avoid confusion it is recommended that the original scenario is also closed prior to loading in the new one. Warning: If you make changes to a scenario, then use ‘Save As’, then subsequently use ‘Save’ the ORIGINAL scenario is overwritten. This is different to the way other familiar programs work (e.g. WORD or EXCEL) which is why it is being highlighted here.*

### 3.1.7 Delete Scenario

This item is only active if at least one scenario is in the scenario database. It is only possible to delete a closed scenario. The deleting of open scenarios is prevented.

A selection dialog as under *Open Scenario* will appear giving you the option to specify the scenario you wish to delete. A simple confirmation dialog will follow if there is no open scenario with the same title.

### 3.1.8 Export / Import

The *Export* item is only active if there is at least one open scenario. The related function acts on the active scenario. The *Import* item is always active.

The *Export*/*Import* feature helps the exchange of simulation data and results between different users. The export function applies to the whole active scenario, including any additional documents derived from the model results and stored in the scenario subdirectory. Please note that the export / import feature does not include the geographic data such as river network (due to possible licence restrictions). Therefore users have to ensure that they are working on identical geographic data sets if they want to exchange (and work with) scenario data.

When "Export" is selected, a dialog appears in which you specify where a scenario is to be exported to: you have to enter a file name and can also select a directory. The complete scenario directory will be written to the export file.

When the inverse process of import is selected, a dialog appears asking you to select the export file. After "OK" the scenario data set will be included in the existing scenario database.

### 3.1.9 Report

This menu item is active if there is at least one open scenario. The complete scenario data settings and results will be written to a formatted ASCII-file which the user specifies in a file selection dialog.

This will also include any comments entered for the various parameters.

#### 3.1.10 Expert Mode / Easy-to-use Mode

The user can ‘toggle’ between these different modes.

Under the Easy-to-use Mode the item *Expert Mode* option will be visible and will launch the expert mode of GREAT-ER. The complete range of menus and tools will then be available.

In the Expert Mode the *Easy-to-use Mode* command sends users back from the expert mode to the easy-to-use mode. All additional menus and some tools, etc. are removed.

Many changes, such as new themes added to a view are not ‘reversible’ and these will still be active. If it is required to remove a theme the user must delete them manually, either using the expert mode or the menu item *Display* / *Remove Themes*.

#### 3.1.11 Exit

This command will quit ArcView after confirmation. For each still open modified scenario a save request will appear. If any major problem occurs during this procedure, the Exit routine will abort.

A possible error screen after closing GREAT-ER is related to the implementation of ArcView itself and is not a bug of GREAT-ER. Note that it is not possible to exit GREAT-ER by clicking on the ‘cross’ in the top right-hand corner as in other Windows applications. If this is attempted a message is given requesting the user to use the *Exit* command.

#### 3.1.12 *n* a scenario title

This item list shows all currently opened scenarios. Selecting a scenario title makes this scenario the active one. The menu item of the active scenario is not selectable (given in grey).

## 3.2 SUBSTANCE

The *Substance* menu contains all functions necessary to modify the substance related to a scenario. It also offers features to manage the substance database.

### 3.2.1 New Substance

This item is only enabled if there is an active scenario, because a substance must be connected to a scenario. The substance dialog is raised and the substance data should be specified.

As GREAT-ER uses the Monte-Carlo method, a distribution can be specified for most of the parameters. Depending on the selected distribution, various descriptive values have to be entered. Conversely, switching back from a distribution to a fixed value, GREAT-ER calculates the mean of the former distribution as its first guess.

The substance dialog is separated into seven cards:

**identification**

You can specify the substance name, CAS and EINECS number and additional synonyms to aid identification. The substance name is essential, the other parameters are optional. It is not possible to leave the substance dialog with "OK" (i.e. to use the entered data) without specifying a substance name. The only possibility would be to abort by "Cancel". For each parameter a comment can be entered.

**physico-chemical properties**

General physico-chemical properties can be edited on this card. More process-specific physico-chemical parameters are placed on the related cards.

**partitioning**

The necessity of declaring partitioning coefficients depends on the selected model.

**degradation**

The degradation card covers some very specific parameters for biodegradation and Mooned kinetics. See the model technical documentation description for a more detailed explanation of parameters.

**sewage treatment removal**

Depending on the selected models various parameters have to be entered to describe the substance fate in sewer and the different treatment plants.

**in-stream removal**

As with sewage treatment removal, more or less detailed elimination rates have to be entered, depending on the selected mode for the river sub-model

**market information**

You can specify a default consumption (kg per capita and year) of the substance assumed for any discharge site in the simulation area. See *Edit Market Data* to edit more site-specific data. Cancelling the dialog will cause you to return to the previous state. Otherwise confirm the new substance by selecting "OK". The substance is then added to the active scenario. If the previous substance of the scenario has been modified, a confirmation dialog will appear. If there is an open scenario with a substance that has the same ID, a hint will be prompted.

### 3.2.2 Open Substance

This item is enabled if the substance database contains at least one substance. You will be prompted by a list dialog to select one of the substances from the database. The chosen substance will be loaded for the active scenario. If the previous substance has been modified, a dialog will ask you to save the former substance data to the database. If there is an open scenario with a substance that has the same ID, a hint will be prompted.

### 3.2.3 Pick Substance

This item is enabled if you have more than one open scenario. It enables users to transfer substance data from a different scenario. By picking a substance it is easy to create a scenario with a substance that was perhaps once edited but not stored in the database (e.g. experimental parameter modifications, invalid parameter set).

If you select a substance, a confirmation dialog will ask if you wish to save the current substance data. The only way to avoid the replacing of the substance related to the active scenario is to say ‘No’ at this stage and prevent an existing data set being overwritten in the substance database.

### 3.2.4 Edit Substance

This item is enabled if the active scenario has a substance. The substance dialog will be shown to allow editing of any substance data in the active scenario. The dialog is described under *New Substance*.

### 3.2.5 Close Substance

This item is enabled if the active scenario has a substance. This command will remove the substance from the scenario. If the substance has been modified, a confirmation dialog appear.

### 3.2.6 Save Substance

This item is enabled if there is an active scenario containing a substance. If the substance is not modified (in relation to the substance data in the substance data base), a hint will be given and nothing will be done. Otherwise the substance will be saved to the substance database. If there is a substance in the database with the same ID, confirmation will be requested.

### 3.2.7 Delete Substance

This item is enabled if there is at least one substance in the database. A dialog with a list of all substances in the database will appear. After confirmation the selected substance will be removed from the database.

### 3.2.8 Change Database

Change database will offer a file dialog where another database file ( **.odb*) can be selected. It is possible to have many different substance databases. The default database delivered with GREAT-ER (*substance.odb*) should only be modified/extended if the new values are quality controlled (literature/laboratory reference). If you need to work with a large amount of substances, the substance database concept enables you to store substances in different databases by classes. This increases the transparency of data storage and speeds up data retrieval.

## 3.3 CATCHMENT

The *Catchment* menu provides the catchment-related functions available for a simulation session. The items in this menu are only available if there is an open scenario.

### 3.3.1 Select Catchment

A dialog is raised in which you can select a new catchment for the active scenario from the list of catchments in the database. If the scenario has been modified you will be requested to save it before selecting a new catchment.

### 3.3.2 Select Subcatchment

This item enables the selection of a sub-catchment for a simulation, by clicking on the appropriate river stretches. The new simulation will then only work on all upstream stretches.

If the active scenario already contains simulation results, these will be deleted (after confirmation from the user) before the new sub-catchment is selected.

For identification purposes the selected stretch is coloured red and the end of the simulated river network is marked with a red dot.

This feature reduces the simulation time if only a smaller sub-catchment is of interest. However, it should be noted that not all of the analysis functions will work on sub-catchment data.

### 3.3.3 Unselect Subcatchment

This item is only enabled if there is a sub-catchment selection within the active scenario. It will undo a former sub-catchment setting. If the scenario includes simulation results these will be deleted (after confirmation from the user) before the entire catchment is once again selected.

### 3.3.4 Edit Market Data

The *Edit Market Data* dialog enables you to specify site-specific consumption data. To cover industrial sites, users can enter an additional input into the treatment plant This input reflects discharges resulting from the production processes and can be calculated from the production volume. Please note that the calculation of the fraction of the production volume which will be released is not part of GREAT-ER but must be calculated manually beforehand. The input considered here is the mass flow of substance into the treatment plant in [kg/a]. As with the loads from domestic inputs, the industrial input is subsequently processed by the treatment plant model, if present, for the selected location.

After leaving the dialog, the market data tool is still active.

### 3.3.5 Edit Discharge-site Data

Similar to the *edit market data* dialog, the *discharge-site data* dialog enables users to modify the parameters of a specific treatment plant.

Several site-specific parameters can be changed. These include population, the elimination rate (used for complexity mode one), the treated fraction of incoming sewage water (e.g. bypass or overflow) and in general the type of treatment plant. Incoming water from separate "sources" is also considered such as domestic input, non-domestic use (this covers mainly industrial inputs) and run-off. If only an overall value is available for treatment plants this should be entered as domestic flow.

Please note that domestic flow is given in [litre / (capita * day)], where non-domestic flow and run-off are considered as [$m^3$ / second].

Please note furthermore that it is possible to specify a distribution for a general removal efficiency, but not for a site-specific removal efficiency. Nevertheless, it is possible to have a distributed removal efficiency for, e.g. activated sludge plants, and a fixed rate for a selected site.

Leaving the dialog the discharge data tool is still active.

## 3.4 MODEL

The *Model* menu provides items for model control. This includes the input of model-related parameters and settings and the control of a simulation run itself. The items in this menu are only enabled if there is an open scenario.

### 3.4.1 Select Model

The text field on the right provides some summary information (hints) on the selected mode. If you increase complexity modes, it may be necessary to go back to earlier data dialogs to enter additional parameters. For example, if you need in-sewer removal to be considered, you have to go back to the substance data dialog to enter a removal rate for sewers. Please note that in-sewer removal is the only ‘higher’ model in which only one parameter has to be entered. All other ‘higher’ models require a somewhat larger data set.

The "impose default complexity mode" check button should usually be checked. After reference to the technical description of the model input tables the (expert) user has the option to specify different complexity modes for selected geographic objects. However, these options are beyond the scope of this user manual and are only available within the ‘expert mode’.

Please refer to the model technical documentation for more information on the model's complexity levels.

### 3.4.2 Edit Model Parameters

The *Model Parameters* dialog allows the user to edit various environmental data and specific properties of the sewer, wastewater treatment plant and river models. For higher complexity modes, a useful feature is the "Default" button which can be used to assign pre-selected values to different parameters. However, please note, that each default value has to be set individually. If you want a set of all default values to be used for some scenarios this is currently only possible by creating a generic scenario without a substance or catchment. All further scenarios can then be created from this generic one and saved to new scenario (use *Save As*).
The set of WWTP-related parameters is so large that it does not fit on a single card. The most

important parameters are grouped on the card. To edit the complete data set launch the dialog using the "complete list ..." button. Please refer to the model documentation for more detailed information on the model's parameters.

### 3.4.3 Background Concentration

*Background Concentrations* are included to consider additional loads within the river network which might be monitored upstream from the first known discharge. Note that the given value is simply added to the model results after the simulation. The background concentration is not considered within the elimination processes.

The concentration has to be entered before running a simulation. The unit is always [mg/L]. After the simulation the specified background concentration will be added to the model results. If the model results are displayed in a different unit an automatic conversion will be activated for the background concentration. Depending on the extent of the catchment, the addition may take some time. Finally, a remark is added to the scenario's view title bar (`Background Concentration xxx [mg/L]`) to indicate that the background value has been added.

To remove a background concentration, enter a concentration of zero in the dialog.

### 3.4.4 Start Simulation

This command will start the simulation for the active scenario if all required data have been specified.

Only one simulation is possible at a time for the same catchment, but different catchments can be simulated simultaneously. In other words, if a simulation is launched for a scenario after some seconds (due to precise timing of the system) it is possible to proceed with other catchments. More details about starting a model are given in the tutorial section 2.4 of this user manual.

### 3.4.5 Stop Simulation

This item is a kind of safety guard. If a simulation fails for some reason (identified for example, by an error message titled `rsxnt`) you should select the *Stop Simulation* menu item. This will change some settings behind the user interface and enable you to safely save any remaining open scenarios. After selecting this item you should close GREAT-ER and restart. Errors may occur if attempting a very large number of Monte-Carlo shots, for example, or if the numerical solution becomes unstable for some reason.

## 3.5 ANALYSIS

The *Analysis* menu provides further functions for the analysis of model results. The menu items are only enabled if the active scenario contains model results.

Please note that the GREAT-ER analysis tools are designed to analyse distributions of values. Although it is possible to run a simulation with one Monte-Carlo shot the analysis functions will probably fail if this is attempted.

### 3.5.1 Calculate River Csim X

Since GREAT-ER calculates a distribution of concentrations for each stretch (based on the Monte-Carlo simulation) this menu item enables users to calculate any percentile from the distribution of $C_{sim, internal}$. The model results are considered as log-normal distributed. After specifying a percentile (the unit is per cent, hence the specified value must be greater than 0 and less than 100) the values will be derived per stretch and a new field will be added to the results table. After calculation a new theme is displayed in the scenarios view, entitled "`Csim xx [unit]`". The colouring is the same as that used for the mean values.

The analysis methods mentioned below are possible for either the default $C_{sim, internal}$ mean values or a derived percentile.

### 3.5.2 Csim Classes River

After a model run has been completed, the *analysis menu* provides various facilities for analysing the results. Since the results are stored as frequency distributions, it is possible to calculate percentiles of concentrations (using *Calculate River Csim X*) for the different river stretches. Alternatively the menu provides you with features to modify the presentation of results: either by *classification* or a colour coded *combination of concentrations with flows*. The analysis tools most relevant to risk assessment are the functions to calculate PEC values (Predicted Environmental Concentration).

### 3.5.3 Combine Csim / Flow

The *Combine Csim / Flow* feature generates a new theme considering both $C_{sim, internal}$ mean and mean flow. The resulting theme will display the $C_{sim, internal}$ mean classification by colour-coding the legend and the mean flow by stretch width. The user has the option to specify the number of classes per value. The classes will be formed on the definition: one class for zero values and equal distances for all other classes.

The automatically generated legend can be edited using the ArcView legend. You should save this manually created legend file to the scenario directory to reload on demand because the additionally generated analysis themes will not be saved with the scenario.

### 3.5.4 PEC*initial*

This is the spatial aggregation of concentrations in the river directly after emission. This is similar to the $PEC_{local}$ as defined in the EU Technical Guidance Documents, although its calculation is different. Based on the $C_{sim,\ start}$ mean values (see Appendix A), the mean is calculated for all stretches receiving treated or untreated discharges:

By definition, the $PEC_{initial}$ is calculated from the $C_{sim,\ start}$ mean values. This calculation is started by selecting the item *PECinitial*.

Please note that PEC calculations are not available if a sub-catchment is selected. After the calculation a dialog displays the result alongside additional information.

### 3.5.5 PEC*catchment*

This is the average of representative concentrations over the entire catchment. This is a new concept for geo-referenced exposure assessment, although there is some analogy with the $PEC_{regional}$ in the EU Technical Guidance Documents. $PEC_{catchment}$ is described in some detail in the tutorial (see Section 2.5.1) .

The calculation of $PEC_{catchment}$ can be based on any of the previously derived percentiles of the model results. When selecting *PECcatchment* the existence of previously calculated values is first checked because, depending on the catchment extent and detail of the digitised river network, the calculation may take several minutes. A progress bar will index the progress of the calculation. After completion the values mentioned above are listed in a small report window:

A progress bar will indicate the progress of the calculation. After completion the values are listed in a small report window. Three different results are given based on different weighting methods:

a) weighting by volume based on the subset of loaded stretches and on all stretches within the catchment;

b) weighting by stretch length based on the subset of loaded stretches and on all stretches within the catchment;

c) weighting by flow increment based on all stretches within the catchment.

### 3.5.6 Discharge Influent Csim / Discharge Effluent Csim

The GREAT-ER models calculate concentration distributions for both the catchment river network and the influent and effluent of the catchment's treatment plants.

These values are stored in the scenario directory in a separate file (`CsimSTP.dbf`). Using the corresponding menu item a new theme appears on the view, displaying the discharge sites classified by either influent or effluent concentration.

After executing one of these menu items once, the model results for treatment plants can be investigated using the identify tool.

### 3.5.7 Concentration Profile

Selecting the *Profile* menu item the cursor shape changes to identify the new mode. You then have to select a stretch by clicking on the view. Moving downstream the $C_{sim,\ internal}$ values are collected for each stretch. The collection will be displayed in a simple X/Y-profile. Alternatively you have the option to export the profile data to create a smarter presentation using your favourite data plotting or spreadsheet program.

The chart options of ArcView are quite limited. Only 50 data points can be displayed within an X/Y plot used for the concentration profile along a river. For this reason the profile might not display all stretches downstream from the selected stretch. To deal with this limitation GREAT-ER provides users with the *Export Profile* feature to write the complete stretch set to a file (either plain ASCII or dBase) for further analysis or more comfortable plotting with the user's favourite data plotting or spreadsheet application.

### 3.5.8 Export Profile

This item is only active if there is already a plotted river concentration profile. A file selection dialog appears enabling users to specify a file name for the profile. It is recommended to first select the target directory (by browsing through the directory tree). The file type can then be specified by the file name extension: use a `.txt` to export in plain ASCII or `.dbf` to export a dBase file. See Section 2.7 for more information.

## 3.6 DISPLAY

The *Display* menu provides several commands for extending or changing the visual appearance of the data under investigation. Some commands (*Full Catchment Extent*, *Zoom In*, *Zoom Out* and *Identify*) are standard ArcView features and also available in the tool bar.

None of the commands influence or change the simulation input or output.

#### 3.6.1 Add Background Data

This command will offer a selection of available background information. A set of transport and population data is provided for all GREAT-ER catchments (derived from the Digital Charts of the World, DCW). Selecting the DCW, Roads, Rail Roads, City Areas and City Names will be displayed for the whole country to which the catchments belong. The resolution of the DCW data is 1 : 1,000,000.

Furthermore, for most catchments monitoring and similar data (e.g. water quality classes) are available as background data.

You can select several background themes at the same time.

#### 3.6.2 Remove Background Data

All DCW themes can be removed by selecting this menu item. Other themes can be removed via the menu item *Remove Themes* (see below).

#### 3.6.3 Full Catchment Extent

The view of the active scenario will zoom to show the full size of the catchment boundary.

#### 3.6.4 Zoom In

This item activates the 'Zoom In' tool for all views. The change of the tool is also indicated by the change of the mouse pointer (when moved across a view). You may now draw a rectangle which will define the extent of the new area to be displayed. If the shape of the rectangle and the view is different, the zoom factor is automatically changed to cover the whole selected area. You can also click once anywhere in the view to zoom in with a fixed factor.

#### 3.6.5 Zoom Out

As the opposite command of 'Zoom In', the 'Zoom Out' tool works in the same way except that the selected rectangle indicates the area and factor for zooming out. The smaller the selected area the higher the zoom out factor.

### 3.6.6 Show River Flows

This function creates a copy of the current river network theme and associates the mean river flow ([$m^3/s$]) with the line thickness (considering the whole river network). The new theme shows a flow classification with 5 classes. The functionality of the command can also be reproduced by applying the legend editor (except for copying the theme).

### 3.6.7 Select Rivernet by Flow

This command allows users to reduce the number of displayed river segments using the criterion of minimum flow. A dialog will ask for the minimum flow value [$m^3/s$] to be displayed. Those river segments with a mean flow lower than this value will then be made invisible. This command is directly applied to the river network theme of the active scenario (no copy of the theme is created). Hence a value of '0' (or any negative number) means all stretches are displayed.

### 3.6.8 Identify

This command works in a similar fashion to the ArcView identify tool. By clicking anywhere in a view, attributes of features of all active themes are displayed in several (subsequent) dialogs. For some themes more than one data subset is available. The data set can be selected in the upper dialog list field.

Only those items which are known to GREAT-ER will be listed, together with an appropriate description and unit. Other items (possibly added in the expert mode) will not be displayed. After selecting 'OK', the information about the next theme is shown. 'Cancel' will stop the subsequent presentation.

In the expert mode this special Identify dialog is switched off and replaced by the standard ArcView Identify dialog.

### 3.6.9 Show Site Pictures

If the corresponding catchment offers site pictures, the mouse pointer will change its shape and the site pictures theme will become active. Locations at which pictures have been taken are marked with large dots. Clicking on a dot will launch a window showing the picture of the site in question (this dialog is a ArcView built-in dialog).

Note that the images are always scaled (see check box at the bottom). This means that the displayed ratio between width and height may not be the real one.

One problem is that scaling may be switched on by default on some small desktop size PCs. A picture exceeding the desktop size leads to the problem that the close window button is inaccessible to the mouse.

### 3.6.10 Remove Themes

For all selected themes, a message will appear requesting whether or not to remove the theme from the view. Exceptions are the standard themes 'River Net', 'Site Pictures', 'Discharge Sites', 'Discharge Connection' and 'Catchment Area'. It is not possible to delete these themes via this menu item.

## 3.7 GREAT-HELP

### 3.7.1 Contents

The GREAT-ER help system is implemented as a HTML structure similar to the menu structure description as published in the GREAT-ER manual. After selecting this menu item the default HTML-browser of the user's system will be launched with the table of contents of the on-line help as the opening window.

Please note that the start-up phase of the help system may take some time to initiate.

### 3.7.2 About GREAT-ER

This menu item provides basic information on the user interface and the GREAT-ER project itself.

### 3.7.3 About Model

This menu item provides basic information about the model system.

# 4. GREAT-ER MESSAGES

## 4.1 CONVENTIONS

We have set up certain typographic conventions to accentuate the meaning of words mentioned in this manual. The following table describes the main conventions:

| **Style** | **Meaning** |
|---|---|
| Serif | Usual text |
| *Italic* | Emphasis / menu items / input |
| CAPITALS | Products / Software |
| `Typewriter` | Software output, messages |
| *`Typewriter italics`* | File names, directories |
| **<PATH>** | System variables, e.g. *PATH* |

## 4.2 HINTS

Hints are provided to give information. They appear as messages informing the user that data cannot be found or some function is not allowed, for example. If these messages appear it does not normally indicate a serious problem, only that the user needs to make some selection or exit from the particular option. The following hint messages are given at various times and the additional remarks may help to clarify what action, if any, is required:

1. `No substance database found - creating new.`
   For some reason the default substance database could not be found. Therefore a new file entitled `substance.odb` was created to generate a new default database. You may try to install manually or to copying another substance database to the default name *`substance.odb`*.

2. `Sorry, it is not allowed to close this window.`
   You have tried to close the view of Europe (the GREAT-ER basic view) by the clicking on the close button ("*X*") on the window title bar. The resulting process would be similar to the menu item *Exit* but is not stable and may cause loss of data. For this reason the action is prevented. Please use the *Exit* item to close GREAT-ER.

3. `Sorry there is already an open scenario with this title.`
   It is not allowed to have two open scenarios with the same name. The scenario name is the key to identifying a scenario and must be unique. Please close the currently open scenario with the name in question if you want to open the new one.

4. `It is necessary to first save the scenario.`
   For reasons of stability and data safety it is only allowed to change catchment data for an unmodified scenario, i.e. a scenario directly saved before changing the catchment data.

5. `No substance specified for active scenario.`
   No substance found for active scenario. As market data and discharge-site data dialogs offer users the opportunity to overwrite general substance settings by site-specific values, these are only applicable if a substance has already been selected.

6. `A simulation for this scenario seems to be still in progress.`
   This is a typical hint: currently not available, the function can be executed some time later because it is not possible to run more than one simulation at a time for a scenario.

7. `This selection tool has to be applied to the active scenario view.`
   You have clicked on the view with the European overview while the Sub-catchment selection tool was active. The message appears, because it is not possible to select a stretch from the overview.

## 4.3 WARNINGS

Warnings are given if something has gone wrong. These are different to errors in the sense that they do not cause a loss of data and may be resolved with the use of the technical documentation.

1. `Environment variable <GHOME> not set.`
   This environment variable (specifying the GREAT-ER home directory) is established by the set-up program. However, if this error occurs it means it is now missing (maybe deleted manually). Following the warning a dialog will be given to enable you to specify the home directory for the current GREAT-ER session. However, it is recommended to set the variable permanently with the system settings.

2. `Environment variable <GSCENARIOS> not set.`
   Although this environment variable needed by GREAT-ER (specifying the GREAT-ER scenario directory) is set by the set-up program, it is now missing (maybe deleted manually). A following dialog enables you to specify the home directory for the current GREAT-ER session but it is recommended to set the variable permanently with the system settings.

3. `No unit information available. Unit is set to [mg/L]. Please check your system / scenario parameters!`
   For some reason the automatic unit conversion has failed. The simulator output is [mg/L] so it is assumed that the loaded data is in this unit. Please check this assumption. This message also appears when no release of the substance has been specified (e.g. a catchment with only industrial discharges and no site-specific release).

4. `GREAT-ER menu not found.`
   The GREAT-ER menu structure seems to be corrupt. This can happen by modifying the structure in the Expert Mode. A rough solution is to leave GREAT-ER without saving anything. If you want to save your scenario data you have to restore the menu structure: See the ArcView manual for customising a project. Check the menus for the View Doc. Rename the one which contains the usual GREAT-ER commands back to "`&GREAT-ER`".

5. `Exit item not found.`
   The GREAT-ER menu structure seems to be corrupted. This could happen by modifying the structure in the Expert Mode. A rough solution is to leave GREAT-ER. You may save your scenarios before leaving. An alternative is to restore the menu structure: See the ArcView manual for customising a project. Look in the GREAT-ER menu for the 'View Doc'. Scan through the menu items and find the item with the click script Exit GREAT-ER.ave Rename it to "`Exit`".

6. `Not able to fully delete the scenario. The scenario may now be invalid. Possible reason is access violation.`
   Because of some file access limitations, GREAT-ER was not able to delete the scenario data completely. One of the files in the directory may be being accessed by another program. Please close the file and remove remaining scenario data by deleting the scenario directory manually.

7. `Creation of export file xxx failed.`
   Due to some access limitations, the automatic generation of the export file is not possible. You might try to change the access restrictions and export again or to export the scenario manually: as all scenario data are stored in the related directory under the GREAT-ER scenario directory the export file is a zip archive of this subdirectory. You can create this archive with you favourite zip tool.

8. `Importing of file xxx failed.`
   Because of some access limitations the automatic unpacking of the export file is not possible. You might try to change the access restrictions and import again or to import the scenario manually: as all scenario data are stored in the related directory under the GREAT-ER scenario directory the export file is a zip archive of this subdirectory. You can unpack this archive with you favourite unzip tool to the scenario directory.

9. `Neither CAS nor Name specified.`
   The last changes have been lost because the data set has no CAS number or name, which are the minimum requirements to identify a substance data set.

10. `Not able to open database - keeping previous.`
    Two reasons are possible here: Either, due to access limitations, the database is not accessible or the database has somehow been deleted, which should not normally be the case.

11. `River network theme missing. Function not available.`

    The river network theme cannot be found, which means it is no longer a theme of the active view or it has been renamed. The easy-to-use way to fix both is to save and close the scenario and reopen it. When using the expert mode the problem can be solved by adding the river network theme to the active view or by renaming it to "River Net" in the Theme/Properties window.

12. `Discharge sites theme missing. Function not available.`

    The discharge site theme can not found, which means it is no longer a theme of the active view or it was renamed. The easy-to-use mode way to fix both is to save and close the scenario and reopen it. When using the expert mode the problem can be solved by adding the rivernet theme to the active view or by renaming it again to "River Net" in the *Theme/Properties window*.

13. `Discharge table is not editable.`

    This is due to access restrictions. To enable the discharge table to become editable the access rights need to be changed.

14. `xxx : can not be opened for writing.`

    This is due to access restrictions and can be solved by changing them. This "warning" involves no loss of data.

15. `The table of simulation results is not editable. Calculation of background concentration xxx aborted.`

    This is due to access restrictions and can be solved by changing them.

16. `Csim theme feature table has errors.`

    One of the fields QMean, Reallength, VMean or PECintMean is missing in the theme's feature table, probably due to the fields having been renamed manually. This edit need to be undone. A second possibility may be that the field is hidden. This can be fixed by ‘unhiding’ the field within the Expert mode.

17. `The table of simulation results is not editable. Calculation of xxx-percentile aborted.`

    This is due to access restrictions and can be solved by changing them.

18. `The theme's legend is not as required for PEC's. Profile plotting aborted.`

    The current legend classification is based on more than one field. This is not possible for profile plotting. Switch to the one field which should be used for plotting the profile.

19. `Background data table not found.`

    The table that contains information about additional background data can not be found. This indicates that the catchment installation routine did not work correctly or the table has been deleted or renamed manually. The file *`backgroundlst.dbf`* needs to be in the directory

`%GHOME%\catchments\<CATCHMENT>`.

20. `Background data list could not be created.`
    This is an internal AVENUE error which should not normally occur. Nothing has to be done and no data will be lost. Just try to reload the background data.

21. `DCW coverage can not be opened.`
    One or more of the coverages pppoly, pppoint, rdline, rrline can not be opened. Check whether the coverages are in the directory `%GHOME%\overview\<COUNTRY>`. This may be the case if a scenario with a catchment from a new country has been included. In this case the DCW data need to be included in the directory `%GHOME%\overview\<COUNTRY>`.

22. `Your scenario data is incomplete: no model parameters.`
    You have to edit the model parameters to specify all necessary ones, This warning is caused by cancelling the model parameter dialog during the creation of a new scenario.

23. `Picture of xxx (yyy) not found.`
    The image file of the picture can not be found. It may be deleted or renamed. Go into the expert mode and check the database by loading the attribute table of the Site Pictures theme (via *Themes/Table...*) and then looking whether the image file name corresponds to a file in the directory `%GHOME%\graphics\sitepics`. If there are some inconsistencies, eliminate them.

24. `Not able to save scenario in xxx - directory already exists.`
    As saving is not possible to a directory of another scenario, go back to the "Save As" dialog and specify a nonexisting directory. It will be created automatically.

25. `Not able to create directory`
    This is due to access restrictions and can be solved by changing them.

## 4.4 ERRORS

Errors indicate that something fundamental has gone wrong. An error may cause serious consequences, especially loss of data. But usually an error message indicates that something previous has failed or was deleted. Hence a GREAT-ER error message is caused by an earlier error.

1. `Banner file xxx/graphics/greater.gif not found!`
   This is usually caused by an impossible setting for the system variable %**GHOME**%. Check if %**GHOME**% is pointing to your GREAT-ER installation (by using the system settings); if not, set it correctly.

2. `The scenario directory named by GSCENARIOS (xxx) does not exist!`
   `Please create the directory and restart GREAT-ER.`

Create the directory pointed to by %**GSCENARIOS**% (as indicated in the system settings) and restart GREAT-ER.

3. `Cannot get file xxx!`

   Without this file the execution of GREAT-ER is not possible. The problem may in some cases be solved by changing access restrictions. Otherwise the file can be read from the CD by extracting it from the file *`greater.zip`* on the CD into the directory `%GHOME%\ave`. This message also arises when the set-up has been performed manually using an old version of ZIP that cuts the filenames to the old 8.3 convention. In this case, use the set-up program (recommended) or a newer version of ZIP.

4. `Cannot get script load procedure! This makes it impossible to launch GREAT-ER.`

   This indicates that the script *`ReloadScript.ave`* is not loadable. The problem may in some cases be solved by changing access restrictions. Otherwise *`ReloadScript.ave`* can be read from the CD by extracting it from the file *`greater.zip`* on the CD into the directory `%GHOME%\ave`. This message also arises when the set-up has been performed manually using an old version of ZIP that cuts the filenames to the old 8.3 convention. In this case, use the set-up program (recommended) or a newer version of ZIP.

5. `Cannot compile load procedure! This makes it impossible to launch GREAT-ER.`

   This indicates that the script has errors, i.e. it has somehow been modified. It needs to be reinstalled by either reinstalling the whole GREAT-ER software or by installing, i.e. extracting, only the scripts that contain errors from the file *`greater.zip`* on the CD into the directory `%GHOME%\ave`.

6. `Error occurred opening script file xxx!`

   The script could not be opened. The problem may in some cases be solved by changing access restrictions. Otherwise *`ReloadScript.ave`* can be read from the CD by extracting it from the file *`greater.zip`* on the CD into the directory `%GHOME%\ave`. This message also arises when the set-up has been performed manually using an old version of ZIP that cuts the filenames to the old 8.3 convention. In this case, use the set-up program (recommended) or a newer version of ZIP.

7. `Error occurred compiling script xxx!`

   This indicates that the script has errors, i.e. it has somehow been modified. It needs to be reinstalled by either reinstalling the whole GREAT-ER software or by installing, i.e. extracting, only the scripts that contain errors from the file *`greater.zip`* on the CD into the directory `%GHOME%\ave`.

8. `No catchment database found!`

The essential file `catchments.dbf` is missing. You have to reinstall GREAT-ER or only the file by extracting it from the file `greater.zip`, stored on the CD, to the directory `%GHOME%\catchments`.

9. `Internal Error: StretchID field missing!`
   The field to identify river stretches in the simulation result table is missing. Either the field name has been changed manually (it has to be 'stretchid') or the data is seriously corrupt. You should start a new simulation using the same parameters.

10. `Catchment CCC can not be opened!`
    The basic catchment data or parts of it are missing. There are three possibilities for this:

    a. You imported a scenario for a catchment you do not have the data for. Check your installation and contact the party from which you obtained the scenario to update your catchment database;

    b. Your catchment database (under your GREAT-ER installation in the directory 'catchments' and its sub-directories) has the wrong read access restrictions. Change these settings by yourself if possible or ask your system administrator;

    c. Your catchment database has been seriously corrupted. Try to restore the catchment data by reinstalling GREAT-ER over your existing installation.

    The essential basic catchment coverages are: catchbound, disch_river, rivernet, discharges.

11. `Not able to get information about scenario!`
    The communication between this dialog and the GREAT-ER core application has failed. ArcView has run into an unstable mode. It is recommended to leave GREAT-ER immediately without saving and to restart it.

12. `Substance not found! Database seems to be corrupt!`
    Although the substance you have selected is listed in the database there seems to be no data for it. This suggests that the substance's data set, or more generally the substance database itself, is damaged.

13. `The result theme data structure seems to be corrupt!`
    The result theme data structure seems to be corrupted. You should try to recreate the scenario and restart the same simulation. If the problem should occur again, one of the needed idfields are missing ...

14. `Can not open 'scenario.odb'!`
    The basic scenario settings are not accessible. This may be caused by the wrong access restrictions, which can be fixed by changing them to read/write permission, or by a loss of data. In

the latter case you need to reconstruct the scenario and save it again.

15. `Wrong number of items in 'scenario.odb'!`
    The basic scenario settings seem to be damaged. This may imply a loss of data. You need to reconstruct the scenario and save it again, preferably using a different name.

16. `No view for active scenario!`
    This problem should not normally occur. It indicates that the system has become unstable. You should therefore leave GREAT-ER without saving.

17. `Active scenario not found!`
    This problem should not normally occur. It indicates that the system has become unstable. You should therefore leave GREAT-ER without saving. Simulation results are stored under your scenario directory in the files 'pec.dbf' and 'pecstp.dbf'.

18. `Scenario data seems to be corrupt!`
    The scenario data structure would appear to have been seriously corrupted. Saving is no longer possible. Simulation results which you might want to keep are stored under your scenario directory in the files 'pec.dbf' and 'pecstp.dbf'. Exit the scenario without saving.

19. `No catchment database found!`
    The essential file *`catchments.dbf`* is missing. You have to reinstall GREAT-ER or only the file by extracting it from the file *`greater.zip`*, stored on the CD, to the directory `%GHOME%\catchments`.

20. `xxx table fields missing! Function not available.`
    The table seems to be corrupt or has been edited manually. You have to reinstall it by extracting it (a *.dbf file) from the file *`greater.zip`*, stored on the CD, to the appropriate location in your installation (see *Table/Properties* for the correct location).

21. `QueryString for xxx table has errors!`
    A wrong query string suggests impossible field names and therefore a corrupt table. You have to reinstall the table by extracting it (a *.dbf file) from the file *`greater.zip`*, stored on the CD, to the appropriate location in your installation (see *Table/Properties* for the correct location).

22. `More than one entry for WWTP! WWTP data table seems to be corrupt.`
    The query to obtain the wwtp data from the database resulted in more than one data record for one wwtp. It may be fixed by manually deleting one of the entries, i.e. by editing the table WWTP data in the Expert mode.

23. `Can not find field fff in xxx table! Simulation aborted.`
    The table seems to be corrupt or has been edited manually. You have to reinstall it by extracting it (a *.dbf file) from the file *`greater.zip`*, stored on the CD, to the appropriate location in your

installation (see *Table/Properties* for the correct location).

24. `Required parameter ppp not found in xxx dataset! Simulation aborted.`
    The dataset seems to be corrupt or has been edited manually. You have to reinstall it by extracting it from the file *`greater.zip`*, stored on the CD, to the appropriate location in your installation.

25. `Simulation results: the Csim xxx field was not found!`
    This error should never occur. It suggests that the simulation table has an incorrect structure. If this happens, just delete these simulation results, save the scenario and restart GREAT-ER to repeat your simulation.

26. `Csim theme feature table not found!`
    This error should never occur. It suggests that the simulation table has an incorrect structure. If this happens, just delete these simulation results, save the scenario and restart GREAT-ER to repeat your simulation.

27. `Can not find table with STP Csims!`
    The scenario data structure seems to be corrupt. This might have been caused by a loss of data or by renaming the result tables. You can check this by looking to see whether the file *`CsimSTP.dbf`* is in the scenario's directory. The easiest way to fix this is to repeat the simulation.

28. `Discharge record not found!`
    The database seems to be corrupt or has been changed manually. You have to reinstall it by extracting it from the file *`greater.zip`*, stored on the CD, to the appropriate location in your installation.

29. `Background data table seems to be corrupt!`
    One of the essential fields "Name", "MapName", "Type", "Legend" has not been found. This means the installation is either corrupt or was changed manually. A reinstallation from the CD is necessary.

30. `Necessary script for data set xxx not found!`
    The background data table indicates a special script to be used for displaying the selected data. The script is not loadable, i.e the selected background data can not be displayed. The necessary script is given in the file *`backgroundlst.dbf`* in the catchment-specific subdirectory of the *`overview`* directory. The table can be added in the Expert mode to look (and then search for) the script.

31. `Error occurred compiling display script xxx!`
    The background data table indicates a special script to be used for displaying the selected data. The script seems to have some errors hence compiling (which is previous to executing) has failed. This makes it impossible to visualise the selected background data automatically. The file must be

edited by an AVENUE programmer to fix the error.

32. `Background data information not complete!`

    The background information table *`backgroundlst.dbf`* is not complete. Refer to the technical manual for the required structure, and then look to see whether this is the same for the table which is stored in the catchment-specific subdirectory of the *`overview`* directory.

33. `Unsupported background data format!`

    The background data is of a type not considered in the current implementation. The data can therefore not be displayed. Supported types are point, arc, polygon, shape, grid and image.

34. `Cannot make xxx theme!`

    The background theme could not be loaded. Check whether the name and the path given in the background information table *`backgroundlst.dbf`* are valid. If not, change them (in the Expert-mode) or, more easily, make a complete reinstallation. First, check whether you have read access to the data.

35. `Background data not loadable!`

    ODB: either access problems, or a file is missing or corrupt.

    Parts of the background data you selected are missing or unreadable. First check if data is available and change access restrictions if necessary. If the data is missing, try to reinstall GREAT-ER over your existing installation to restore the data. If the data is not part of the original GREAT-ER package, contact the party you received the data from.

36. `xxx table not editable! Analysis aborted.`

    This is usually due to access restrictions. You require write access in the directory named by your <**TEMP**> system variable.

37. `Picture theme missing! Function not available.`

    The picture theme is not in the scenario dictionary structure. This implies a corrupt scenario. Create a new scenario using the same catchment. If the error persists, you need to reinstall GREAT-ER over your old installation.

38. `Picture theme seems to be corrupt! Function not available.`

    Essential fields are missing, due to corrupt or manually changed data. If the catchment was part of the CD, reinstall GREAT-ER over your old installation. If not, contact the catchment's data provider to enquire how to proceed.

39. `Not able to save scenario.odb`

    This is caused by a missing write access in your scenario directory, i.e. a subdirectory under the directory named by your <**GSCENARIOS**> system variable.

40. `Not able to write xxx. Scenario may be corrupt now!`

This is caused by a missing write access. It may have caused a loss of data.

41. `No subcatchment selected in the active scenario.`
Although the flags report a sub-catchment for the active scenario the required information can not be found in the data structures. This suggests the scenario data are damaged. Try to recreate the scenario using a new name.

# APPENDIX A. CHEMICAL FATE SIMULATOR AND MODELS

## A.1 CHEMICAL FATE SIMULATOR

### Description

A detailed description of the geo-referenced chemical fate simulation methodology used in GREAT-ER was published in Boeije *et al*. (1997).

To deal with statistically distributed inputs and outputs, a hybrid simulation approach is used, 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 distributed 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 analyzed, to obtain distributed results as simulation output.

For reasons of model and data set simplicity and computation performance, only steady-state model formulations are applied. Hence, a number of fundamental assumptions are made: (1) constant chemical emissions: diurnal patterns in product and water consumption are disregarded, as well as variations between different days of the week; (2) constant flows within each steady-state model calculation run; (3) constant environmental properties.

To allow a straightforward mass-balancing approach, all determinands (chemical levels, water flows) are expressed as fluxes. Chemical mass fluxes $\Phi$ *(mass/time)* are applied to describe chemical loads. Water flows are expressed as volumetric fluxes $Q$ *(volume/time)*. In the models, chemical concentrations $C$ *(mass/volume)* are not used, because they are not independent of water flows, and they do not describe chemical transport. Chemical mass fluxes, on the other hand, are independent of dilution or flow (unless this dependency is implicitly included in the models which are used to calculate chemical mass fluxes). When concentrations are explicitly required, they are derived from the chemical mass fluxes and the hydrological volumetric fluxes: $C = \Phi / Q$.

Simulations can be performed for different scenarios (i.e., evaluations of different chemicals and chemical consumption patterns). The simulation input consists of a scenario-independent and a scenario-dependent data set. These data are expressed as statistical frequency distributions, incorporating seasonality and parameter uncertainty. Environmental characteristics are constant, and hence non-scenario-dependent. These include the river network structure, flow and flow velocity distributions, discharge point locations, treatment plant information, emission data, properties of sewers and small surface waters, etc. Chemical-specific information is scenario-dependent: chemical properties (i.e., biological, chemical and physical properties, specific process rates,...), and chemical market data (i.e., per capita product consumption rates). Market data are geo-referenced in the same way as the waste water information (i.e., related to waste water discharge points).

The simulation input data are expressed as statistical frequency distributions. This allows to include both seasonality effects and parameter variability and/or uncertainty into the simulation input. For river flows and flow velocities, the lognormal distribution is used (after NRA, 1995). For hydrological information this distribution is described by the mean and the 5$^{th}$ percentile. In the case of flows, there is a 95% probability that the 5$^{th}$ percentile low flow (also referred to as *Q95*) is exceeded: $P(Q>Q95) = 0.95$.

The simulation results are frequency distributions of chemical concentrations, incorporating temporal variability. For risk assessment purposes, these can be expressed as lognormal 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. For the calculation of the latter, specific algorithms have to be provided in the deterministic models.

**Simulation Output**

The output of a simulation consists of a geo-referenced set of predicted concentrations in the aquatic environment. For each river stretch, the following results are obtained:

■ RIVER

| | |
|---|---|
| $C_{SIM,start}$ | predicted concentration at the beginning of the stretch |
| $C_{SIM,internal}$ | average predicted concentration in the entire stretch |
| $C_{SIM,end}$ | predicted concentration at the end of the stretch |

| | |
|---|---|
| ■ WWTP | (only if a waste water emission occurs in the considered stretch) |
| $C_{SIM,influent}$ | predicted WWTP influent concentration |
| $C_{SIM,effluent}$ | predicted WWTP effluent concentration |

## A.2 CHEMICAL FATE MODELS

Three ‘complexity modes’ are available. At higher ‘complexity modes’, more detailed models are used.

*General Fate Pathway Structure*

The general structure of the aquatic fate pathway within one segment (without a waste water emission point) is shown in Figure A.1. For a segment which contains an emission, it is given in Figure A.2. The treated sewer flow fraction (which enters the WWTP) is given in the geo-referenced parameter set for each waste water emission point.

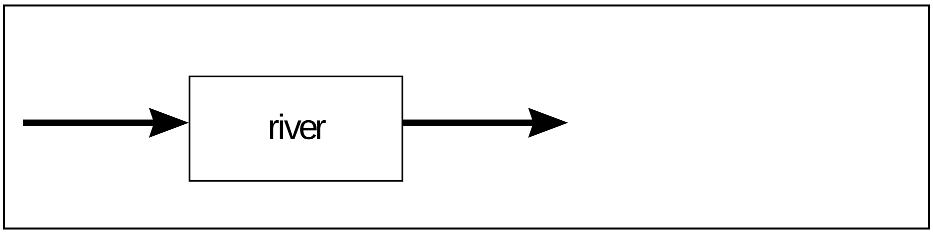


Figure A.1: *Fate pathway structure - without emission*

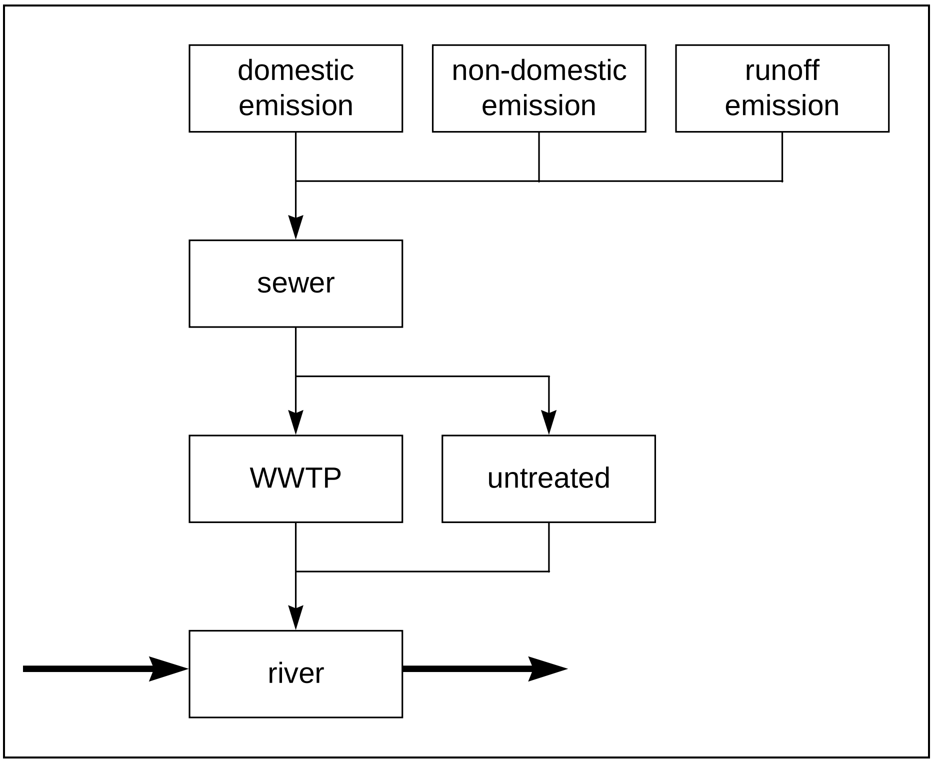


Figure A.2: *Fate pathway structure - with emission*

**Emission**

The emission models are identical in all complexity modes. Domestic emission fluxes are calculated from population numbers, market data and water consumption. For other emissions (non-domestic and runoff), the chemical mass fluxes are taken directly from the emission data. The flows are taken directly from the geo-referenced parameter set.

**Transport / Conversion**

***Complexity Mode 1***

Complexity Mode 1 allows GREAT-ER simulations with a minimal geographically referenced and chemical input data set. No in-sewer removal is assumed to occur. Chemical elimination in a WWTP is described by a fixed removal efficiency, which depends on the type of treatment. Chemical elimination in rivers is described by first-order in-stream removal, assuming a fixed rate coefficient.

***Complexity Mode 2***

Complexity Mode 2 allows GREAT-ER simulations with a minimal geographically referenced input data set for rivers. However, for WWTPs a detailed data set is needed, as well as a detailed chemical parameters set.

In-sewer removal is assumed to be a fixed percentage, and is taken directly from the chemical parameter set. Chemical elimination in a WWTP is described by mechanistic mathematical models for primary settling and for activated sludge (derived from *SimpleTreat* 3.0, Struijs, 1996). For trickling filter treatment, a simple percent removal model is used. Like in mode 1, chemical elimination in rivers is described by first-order in-stream removal, but here sorption equilibrium is taken into account. The different sub-processes (degradation, volatilization, sorption-sedimentation) are dealt with by fixed removal rate coefficients.

***Complexity Mode 3***

Complexity Mode 3 requires detailed parameters for rivers, for WWTPs and for the simulated chemical.

In-sewer removal is assumed to be a fixed percentage, and is taken directly from the chemical parameter set (identical to mode 2). Chemical elimination in primary and activated sludge WWTPs is described by models derived from *SimpleTreat* 3.0 (Struijs, 1996). For trickling filters, it is described by a fixed removal efficiency (identical to mode 1). The separated individual river fate processes are described by means of mechanistic models (cf. Trapp and Matthies, 1996), and degradation is further split up into three sub-processes (biodegradation, hydrolysis, photolysis). The chemical's water solubility is also taken into account.

# APPENDIX B. HYDROLOGICAL MODELLING WITHIN GREAT-ER

## B.1 INTRODUCTION

Estimates of the magnitude and variability of river flow and flow velocities at ungauged river reaches are an essential component of GREAT-ER. There is a considerable variation in river flow behaviour across Europe over both space and time. The seasonal flow regime of a Mediterranean catchment, with its winter high flows, dry periods in summer and frequent flash floods, is very different from that of an English lowland chalk stream, where flows show little variation over the year. Both have a very different seasonal regime from a catchment in the Alps where maximum flows follow the spring snowmelt. At the broadest European scale, river flow regimes are dependent on rainfall, temperature and evaporation. At a finer scale, the detailed effects of a particular climate on river flows are controlled by the physical properties of the catchment. River flow regimes are also affected directly and indirectly by human activities such as reservoir impoundment, abstraction of water and effluent discharges. Taking the UK as an example of a member state with a mature river gauging network, less than one percent of reaches mapped at a scale of 1:50,000 are gauged and, furthermore, less than 20% of gauged catchments can be regarded as being natural. The development and application of steady state hydrological models by the Institute of Hydrology for predicting flow statistics and flow velocities at ungauged river reaches are presented in this appendix. Central to the models is the use of a digital river network and thematic digital grids of relevant catchment characteristics. The structure of the digital river network facilitates the estimation of catchment boundaries, catchment characteristics and indexing of artificial influences (abstractions, discharges and impounding reservoirs), the influence of which are incorporated into the model. The flow models are incorporated into an Institute of Hydrology PC based software product which has been in operational use since 1991 within all of the environmental protection agencies within the UK.

The steady state hydrological models applied within the UK Pilot Study catchments to generate reach based estimates of both the natural and artificially influenced flow regimes using catchment characteristic based regional flow models are also described. The use of this type of model is recommended by the Institute of Hydrology for use within GREAT-ER. The models are intensive in terms of the spatial data and sample set of gauged data required, but once developed they can be applied within any catchment described by the spatial data, in this case the UK.

Section three describes the hydrological model developed for the Lambro pilot study catchment. In this case traditional hydrological techniques were used to harmonise the gauged data associated with five gauged locations within the catchment. These data were used to statistically describe the flow regimes. The flow statistics were then extrapolated to the ungauged river sites within the network using the river network based modelling framework as that used in the UK Pilot study catchments.

## B.2 THE UK MODELS AND THE RIVER NETWORK BASED MODEL FRAMEWORK

The first major UK study of the relationships between low flow regimes and physiographic and climatic catchment characteristics and associated hydrological models was published by the Institute of Hydrology as the 1980 Low Flow Studies Report (NERC, 1980). The techniques for estimating annual and monthly low flow statistics are summarised in the following sections.

**Annual Flow Statistics**

The models used to estimate annual flow statistics are based on a simple conceptual water balance model for estimating mean flow (MF), and a statistical multivariate model for estimating the Q95 statistic (i.e. the flow equalled or exceeded for 95% of the time) from the hydrological response of soil types. The mean and Q95 flow statistics estimated from catchment characteristics are used to determine the flow duration curve (FDC) for an ungauged catchment. The overall estimation procedure is presented as a flow diagram in Figure B.1. The individual stages are briefly summarised here. A more detailed description of the models is presented in Gustard *et al* (1992).

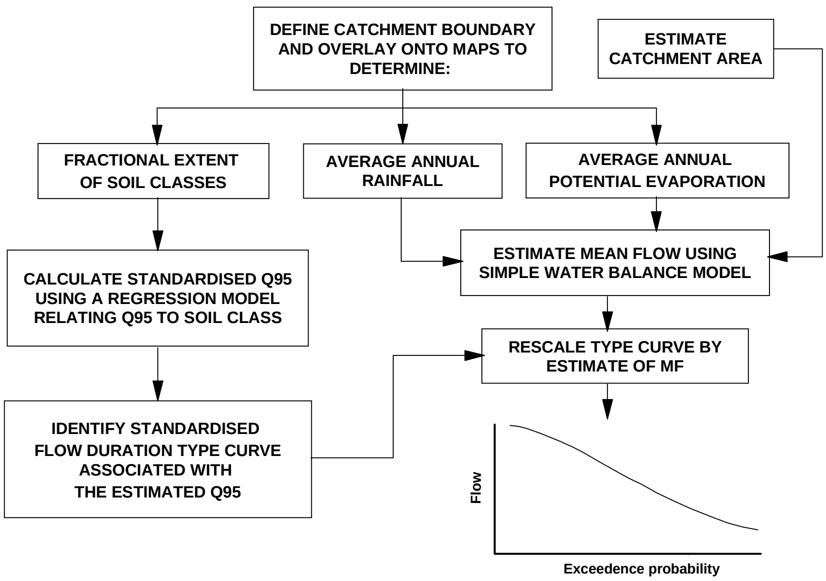


Figure B.1: *Procedure for Estimating Natural Annual Flow Statistics*

*Annual mean flow*

The mean flow at an ungauged site is estimated using a simple conceptual water balance model in which mean flow is estimated from catchment average values of long term annual rainfall (SAAR) and potential evaporation (PE). The average annual runoff depth is derived using a simple water balance given by:

AARD = SAAR - (r x PE)

where r = (0.00061 x SAAR) + 0.475 for SAAR < 850mm/yr
r = 1 for SAAR > 850mm/yr

The actual evaporation is equal to the potential evaporation in catchments with annual average rainfall in excess of 850mm where evapotranspiration rates are rarely limited by soil moisture deficit. The adjustment factor (r) reflects the impact of soil moisture deficit and associated reductions in transpiration rates observed in low rainfall catchments. The regression model for r used climatic data and gauged runoff data from 687 catchments within the UK. The long-term mean flow is then estimated by rescaling AARD by catchment area.

*Annual flow duration curve*

The flow duration curve represents the complement of the cumulative distribution of daily mean flows over a specific period. Using the FDC it is possible to identify the percentage of time that any given flow is equalled or exceeded. Studies have demonstrated (NERC, 1980) that in the temperate Europe the gradient of a FDC (or variance of a flow distribution) is principally controlled by the catchment low flow response, which in turn is strongly related to the hydrogeology of the catchment. The key low flow statistic used within the model to characterise the low flow regime is the annual Q95 flow, standardised by the mean flow to minimise the influence climatic controls. Analysis of UK gauged flow records has demonstrated a strong relationship between this Q95 statistic and the gradient of the FDC.

A statistical multivariate regression model has been derived which relates the standardised Q95 statistic to the hydrological characteristics of soils within gauged catchments. The distribution of these hydrological soil groupings in Yorkshire is presented in Figure B.2. The regression model relating Q95 to the factional extent of LFHGs was again derived from data relating to 687 UK catchments. The model is applied within a catchment by identifying the fractional extents of individual LFHGs within the catchment and taking an average of the parameter estimates for each group weighted by the fractional extent.

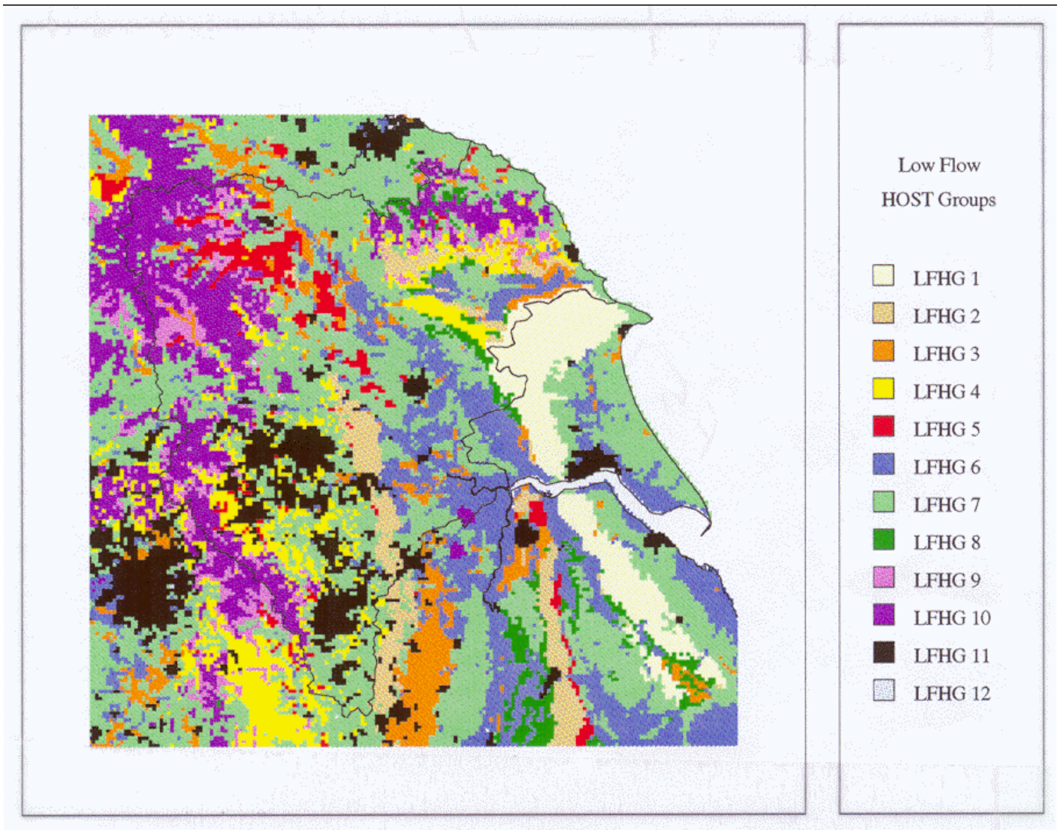


Figure B.2: *Distribution of Low Flow Host Groups across the Yorkshire Region*

The procedure for deriving the long term flow duration curve at an ungauged site utilises natural long-term annual Q95 (as described above) to select a flow duration curve from a family of type curves (standardised by the mean flow) (Gustard *et al*, 1992). These type curves are illustrated in Figure B.3. The type curves adjacent to the estimated value of Q95 are identified and an FDC that coincides with the predicted value of Q95 is generated by linearly interpolating between these curves. The final step in the estimation procedure is to re-scale the flow duration statistics by the estimated value of mean flow.

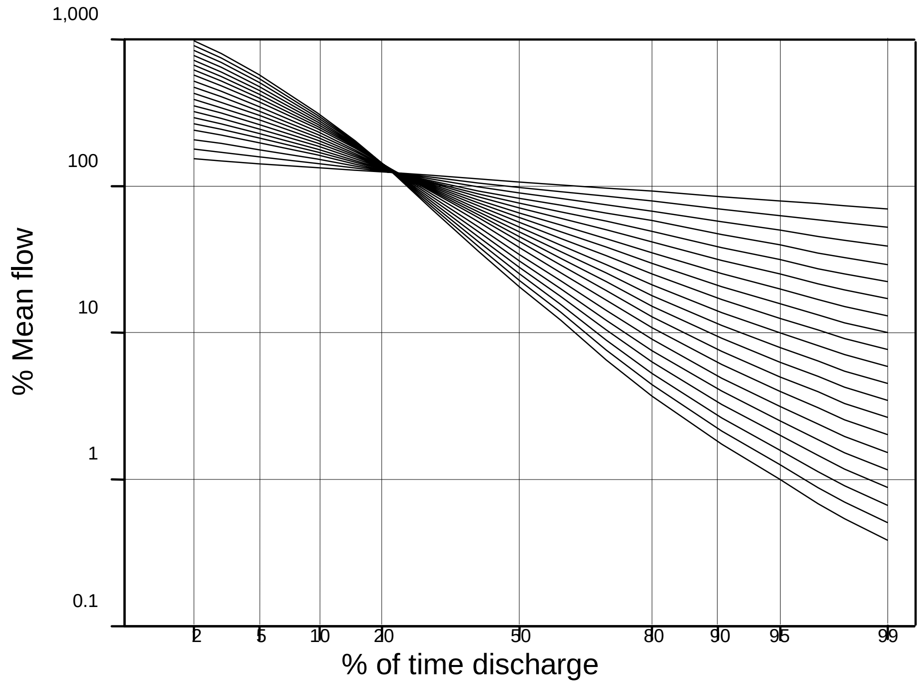


Figure B.3: *Annual flow duration type curves*

**Monthly Flow Statistics**

The estimation of monthly flow duration curves is an essential step in incorporating the impacts of artificial influences into the estimates of annual MF and Q95. The overall estimation procedure for monthly statistics is summarised in Figure B.4 and the individual steps in the estimation procedures are briefly discussed in the following sections. In common with the long term flow statistics and the key monthly statistics that need to be determined are the mean flow, the annual Q95 and the FDC.

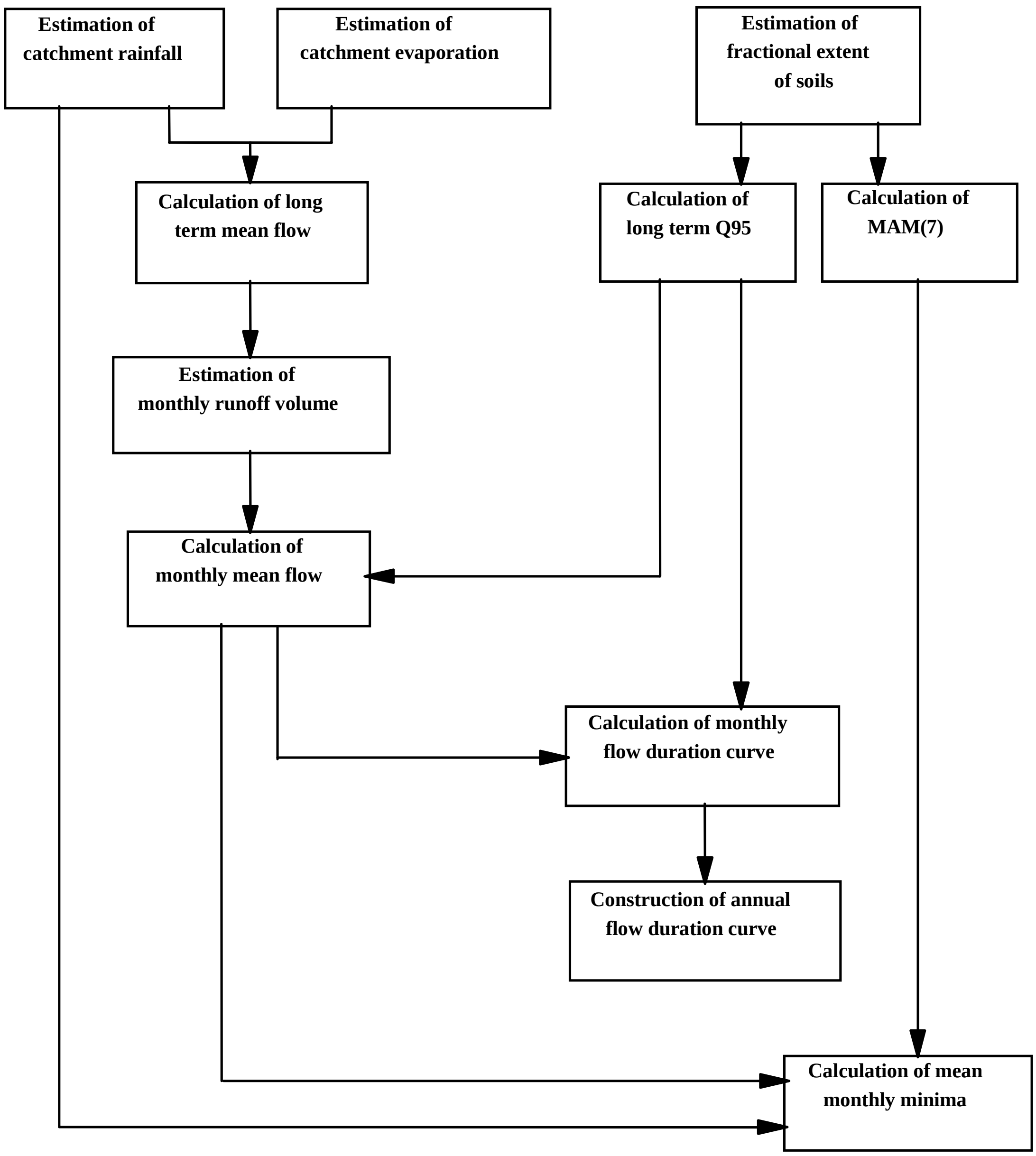


Figure B.4: *Procedure for estimating natural monthly flow statistics*

*Monthly Mean Flows*

The derived monthly FDCs are dimensionless curves expressed as a percentage of the monthly mean flow. In order to express this curve in units of flow it is necessary to re-scale the FDC by an estimate of the monthly mean flow. The variability of Monthly Runoff Volume (MRV) can be linked to the magnitude of the standardised Q95 statistic (i.e. the permeability of the catchment) (Bullock *et al*, 1994). In Great Britain, the more impermeable catchments (i.e. those with Q95 values of less than 30 % of the mean flow) demonstrate significant regional as well as seasonal variations in the partitioning of annual mean runoff between calendar months. Using multivariate interpolation techniques grids of the variation in monthly runoff as a function of catchment permeability (as represented by the standardised Q95 value) have been derived. In application the partitioning of the annual mean flow between calendar months is achieved by identifying the appropriate set of grids using the estimated Q95 values and deriving catchment average values of the variation monthly runoff .

*Monthly Flow duration curves*

The seasonal variations of the flow regime are lost when the flows are represented using the long-term annual FDC. However, Bullock *et al* (1994) identified that the family of type curves used for estimating the annual FDC at an ungauged site can also be used to represent the variation in monthly curves, when expressed as a percentage of the monthly mean flow.

In common with the annual FDC, the estimation of the standardised monthly FDCs requires the estimated natural annual Q95 which is used to identify the appropriate type curves for the individual months based upon a selection matrix.

## IMPLEMENTATION OF THE NATURAL LOW FLOW ESTIMATION MODELS WITHIN THE MICRO LOW FLOWS SOFTWARE

### Estimating Catchment Characteristics

Within the Micro LOW FLOWS software a digital river network for hydrometric regions within the UK is archived, based on the 1:50 000 scale Ordnance Survey maps. Using the river network, catchment characteristics are automatically calculated through the generation of a synthetic boundary for the catchment above every stretch (Sekulin *et al*, 1992). The synthetic catchment area is determined by the number of grid cells, with a resolution of 0.5 km x 0.5 km, above each stretch. The grid cells are assigned to each stretch based on a shortest distance algorithm and constrained by digitised coastlines, hydrometric and catchment boundaries.

Digital databases of SAAR and PE are archived within the software as well as a grid of standardised

Q95 derived derived from the regression model relating this statistic to UK soils (LFHGs). All catchment characteristic grids are held at a resolution of 1 km x 1 km. Every cell assigned to each river stretch has an associated value of SAAR, PE and Q95. Catchment average values of these climate and low flow characteristics can be determined by accumulating the number of squares above a given stretch and taking the average of the individual grid square values. These catchment average values form the input into the models described in the preceding sections. The river networks for Yorkshire and the reach scale natural estimates of Q95 derived using Micro LOW FLOWS are presented in Figure B.5.

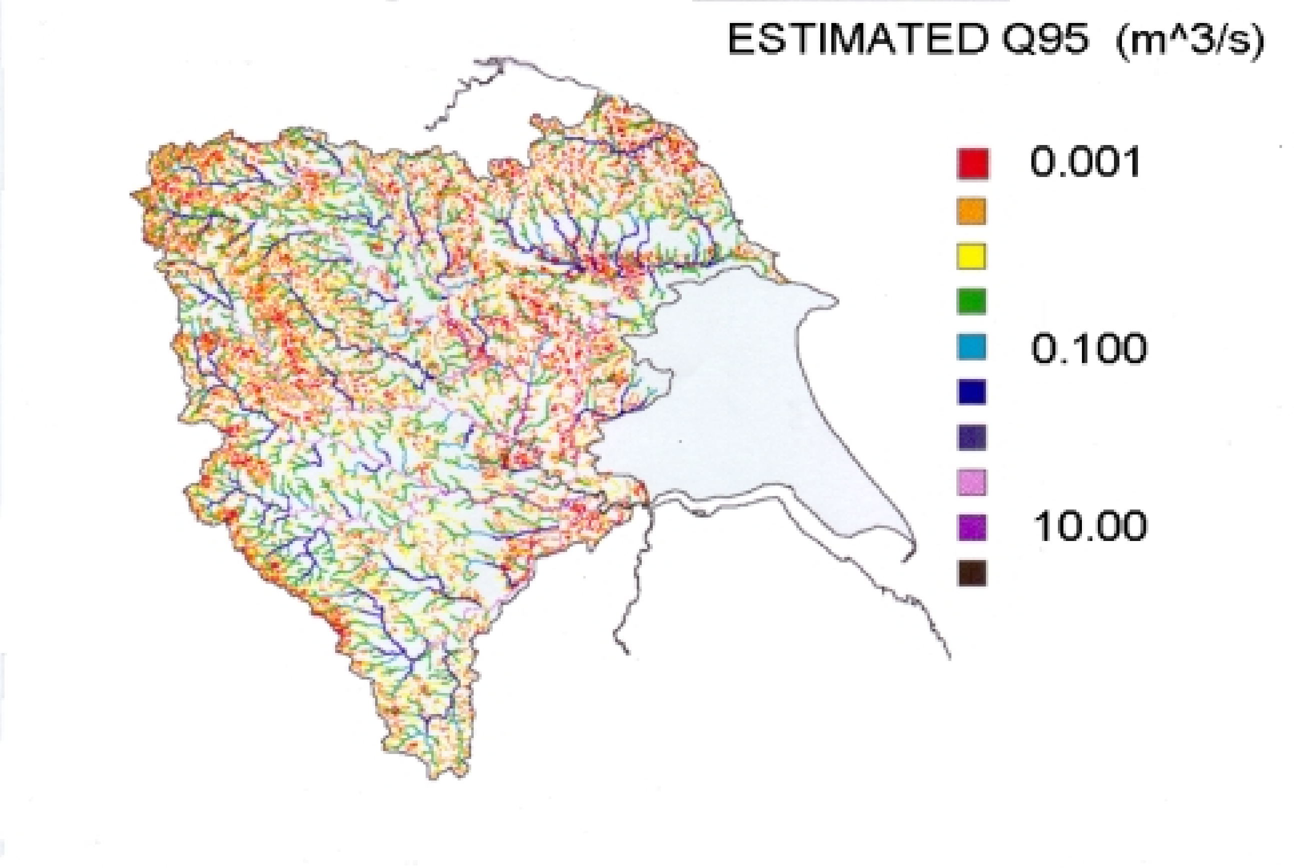


Figure B.5: *Natural Q95 estimates for the Yorkshire rivers*

**Incorporating Artificial Influences**

The software incorporates databases of gauging stations, licensed abstractions, consented discharges, impounding reservoirs and spot gauging information. Sites associated with these features are geographically located by grid reference and are automatically assigned to the closest river stretch. Within the existing framework of the commercial version of Micro LOW FLOWS, the information relating to gauging stations and spot current meter readings are held for information only. The impacts of abstractions, discharges and reservoirs on the downstream flow regimes are automatically incorporated into the natural flow estimation procedures. Artificial influence sites are quantified in terms of a typical monthly volume for each calendar month within the year. Reservoirs are single-site features whilst abstraction licences and, to a lesser extent discharge consents, may be multi-site features. In the case of abstraction licence and discharge consents the monthly volumes relate to water that is either abstracted or discharged however the situation is more complex for reservoirs. The monthly profiles for reservoirs represent a combination of estimates of spill volumes and compensation releases for each month minus the natural monthly flow duration curves estimated for the catchment upstream of the dam site. If an abstraction licence relate to groundwater abstractions an estimate of the impact of an abstraction profile on the nearest river reach is derived using an algorithm based upon a modified version of the Jenkins superposition method (Jenkins, 1970). This is applied to the Theis analytical solution for predicting the impact of a groundwater abstraction from a phreatic aquifer (Theis, 1941). The algorithm requires the user to define values for aquifer transmissivity and storativity. The distance of the abstraction site from the nearest stream is calculated automatically using the grid reference of the site in conjunction with the digital river network. The derivation of these monthly volumes is presented in the context of the Aire and Calder catchments in the Yorkshire Pilot Study.

When estimating the flow regime at a site the software uses the river network to identify all upstream influence feature sites, discounting those that lie above impounding reservoirs. The individual monthly profiles for each upstream site are then accumulated into a total monthly influence profile for each influence feature type. The monthly profiles for discharge sites then added to the estimated natural monthly mean flows and the accumulated monthly influence profile for abstractions is subtracted from the natural monthly mean flows to derive influenced monthly mean flow estimates. These influenced estimates are then used to scale the appropriate monthly flow duration curves which are subsequently combined to yield an influenced annual flow duration curve.

***The Catchment Characteristics and Water Use of The Aire and Calder Catchments***

The headwaters of the River Aire drain from the carboniferous limestone on the edge of the Pennines, through Skipton, Keighly and the Leeds/Bradford conurbation, to its confluence with the River Ouse near Goole, an overall distance of 148 km. The area of the Aire sub-catchment is 1100 $km^2$, excluding the Calder catchment (NRA, 1993). The River Calder flows from the Pennine Moors eastwards to its confluence with the River Aire at Castleford, a distance of 109 km (NRA, 1995) and drains a total area of 957 $km^2$.

The Calder catchment is heavily industrialised, including textile manufacturers, chemical plants and dye works. The catchment has been a traditional mining area. Some groundwater is abstracted for industrial purposes, although some parts of the Millstone Grit are also exploited to provide some water for public water supply. There are a total of 66 reservoirs/dams within the catchment. There are 39 impounding reservoirs operated by Yorkshire Water Services Ltd (YWS) who are licensed to provide water for public supply. Another 4 impounding reservoirs supply water to the canals reservoirs and there are 23 primary sewage treatment works supporting a population of 790, 000.

Within the Aire catchment water, is abstracted from reservoirs and rivers for public water supply and industrial use including cooling water for two large power stations and fish farms. Abstractions from the carboniferous limestone are predominantly used for industrial purposes. Water for public water supply is taken from the Sherwood Sandstone aquifers near Selby, Goole, Askern and Pontefract.

Within the Aire catchment there are 18 impounding reservoirs used for public water supply and one for supporting the Leeds/Liverpool Canal. In contrast to the Calder catchment, a significant amount of water is transferred into the catchment from the Wharfe, Ouse and Derwent catchments for public water supply (Tattersall, 1980). There are also 12 reservoirs which are not are not used for public supply. Within the major river catchments, many of the reservoirs are linked together in conjunctive use schemes and are often located in pairs. In these pairs, the upper reservoirs are often used for supply and the lower reservoir used for releasing compensation flows.

The overall impact of the transfer of potable water and subsequent discharging of treated effluent is that the actual low flows in the river within these catchments are significantly higher than the natural flows.

***Data used within the Study to Characterise Water Usage within the Aire and Calder Catchments***

*Abstraction data*

The Environment Agency provided information for 547 licenced abstractions within the Aire and Calder catchments. For each licence the data consisted of details relating to the number and location of abstraction sites covered by the licence, abstraction purposes, licensed quantities for purposes, licenced season for each purpose and time series of actual annual abstraction volumes for the past 10 years. These are provided by abstractors to comply with Section 201 of the 1991 Water Resources Act and the previous 1963 Act. Using the actual abstraction volumes, an average annual abstraction volume was calculated for each purpose and site.

Within Micro LOW FLOWS the techniques for incorporating artificial influences require the identification of net monthly influence profiles upstream of a stretch. To construct abstraction profiles for each licenced site the annual abstraction rate for each purpose at the site was distributed over the twelve months according to the season specified on the licence for the purpose. Where the seasonal period was not available a season was inferred based on existing knowledge of typical profiles for different abstraction purposes (Bullock *et al* 1994). The distributed abstraction profiles for individual purposes at an abstraction site were then summed to give a total abstraction profile for each site.

*Discharge data*

The 28 primary waste water treatment plants in the Aire and Calder catchments have been characterised in GREAT-ER and were included within the hydrological model. These were characterised by estimates of the foul sewage component of the discharge. It should be noted that there where many consents for small works that were not considered in this study, furthermore there was no attempt to quantify the discharge non-YWS consents. The reason for this was that the majority of non-YWS consents did not hold information related to volumetric limits, with volumetric checks not forming part of consent compliance checks within the catchments.

*Reservoir release profiles*

The primary source of the data used for quantifying reservoir releases was the Institute of Hydrology Report 99 "A study of compensation flows in the UK" (Gustard *et al*, 1987). Within this Report reservoirs with a capacity greater than 500ML or a catchment area greater than $5km^2$ were listed including information on the amount of compensation release and/or the release policy from the reservoirs. Where multiple reservoirs were linked in a system of supply only and compensation reservoirs, the lowest reservoir (usually compensation only) was taken to represent the whole system. In Micro LOW FLOWS influence features lying upstream of an impounding reservoir are ignored in the calculation of downstream flow estimates. For this reason, in the majority of cases, the upper reservoirs were not represented within the software. In total 37 reservoirs where included within the software.

***Calibration of the Impacts of the artificial Influence***

Once the artificial influence data were loaded the final stage of the procedure was to calibrate the representation of the artificial influences to account for incorrectly characterised, or missing influence features. This latter point is particularly pertinent to the representation of discharges. The calibration procedure was based on minimising the differences between the gauged mean flow and predicted influenced mean flow at all gauging stations.

Having undertaken the initial data load the influenced mean flows were compared with the gauged mean flows for the selected stations and were found to be systematically and significantly smaller with negative mean flows observed at many stations. This is a direct consequence of the omission of cooling water returns and other industrial discharges and the omission of the smaller waste water treatment plants. To address these issues a global percentage return factor was introduced for each purpose type. At each abstraction site the purpose monthly profiles were rescaled by the relevant global percentage return. A percentage return of zero for a particular purpose indicates that the purpose is entirely consumptive with the water being lost from the system. Spray irrigation is an example of a highly consumptive water use. A percentage return of 100% indicates that that most of the water that is abstracted from the system is returned, for example low temperature cooling water from power stations. Automated procedure was developed for optimising the global percentage return figures for individual purposes. This procedure was based upon minimising the standardised sum of squared differences between the estimated influenced mean flows at a gauged reach and the gauged (influenced) mean flows across all gauging stations. The use of a standardised sum of squares gave equal weight to the fit at each gauging station. The optimised return factors for individual purposes derived in this way are presented in Table B.1.

Table B.1 shows that 98 percent of the water abstracted for cooling water is returned to the river. Similarly, fish farming can be considered as a non-consumptive purpose, with only 2% of the abstracted volume being lost from the system. By comparison, it is assumed that all of the water abstracted for spray irrigation is lost through evaporation. The final calibrated fit of the model for the Aire/Calder catchments at gauging stations within the catchment is summarised in Figure B.6 and Figure B.7 for Q95 and Mean Flow, respectively.

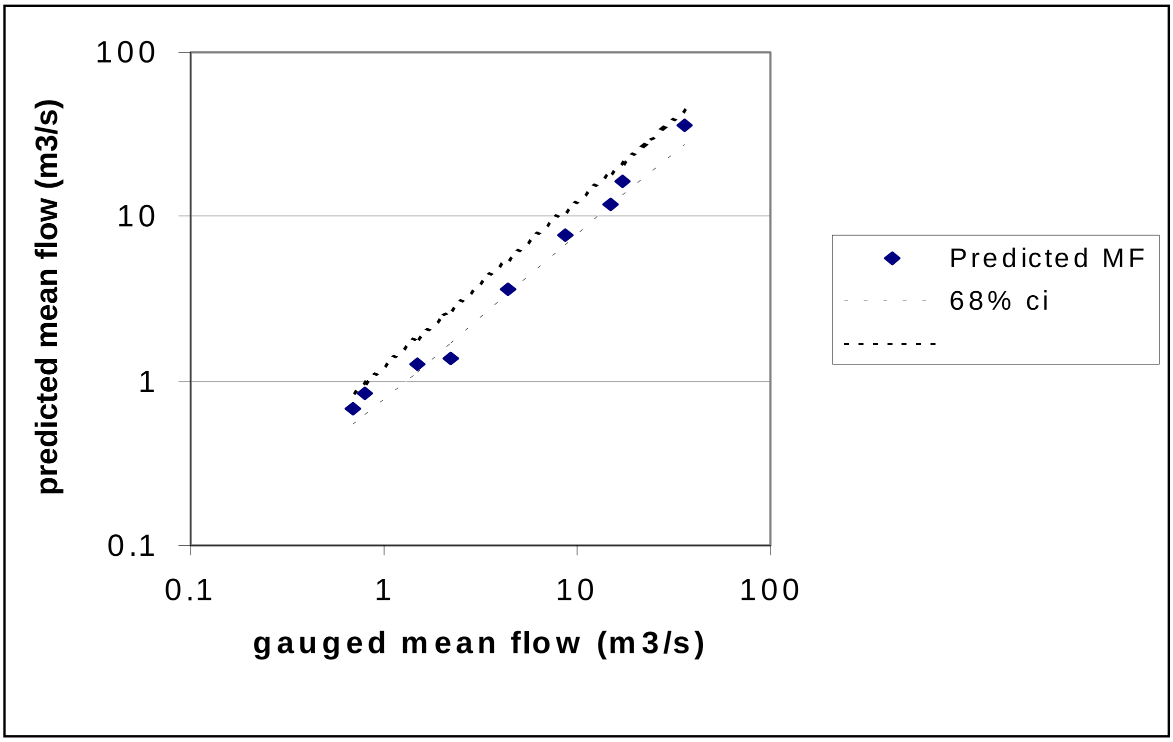


Figure B.6: *Final calibrated influenced estimates of mean flow at gauging stations*

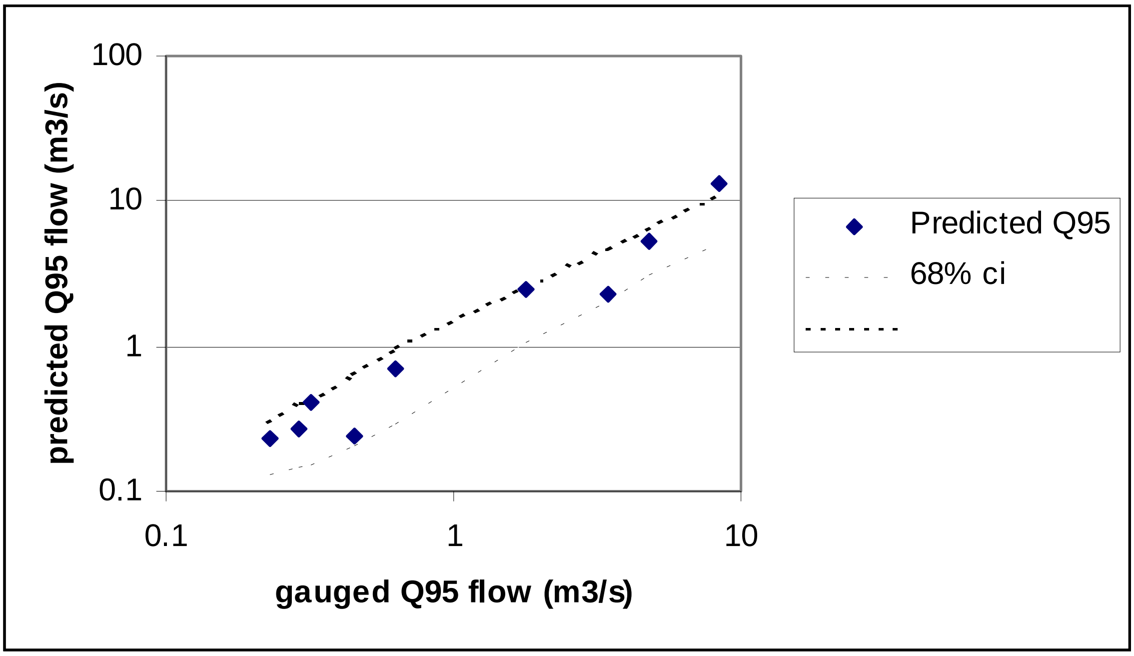


Figure B.7: *Final calibrated influenced estimates of Q95 flow at gauging stations*

## B.3 THE HYDROLOGY OF THE LAMBRO PILOT STUDY

The Pilot Study in the Lambro catchment represents a typical traditional analysis of the low flow hydrology of a catchment in a data poor region where it is not practicable to construct a statistical model of the form described for the Yorkshire pilot study. The sparse data and simple methodology adopted in this study could be compared to the complex techniques employed using Micro LOW FLOWS within the Yorkshire catchments.

**Catchment Details and Water Use**

The headwaters of the river Lambro lie in the Pre-Alps at approximately 1450m above sea level (a.s.l.) between the southern arms of Lake Como in northern Italy. The river flows southwards approximately 130km to its confluence with the River Po at approximately 50m a.s.l. The Pilot Study focussed on the portion of the Lambro catchment to the north of the city of Milano with an approximate catchment area of 465km$^2$. Average annual rainfall for the catchment varies between 900mm and 1500mm.

The Lambro catchment north of Milan contains two main topographical zones; the Pre-Alp mountainous region adjacent to Lake Como and the flatter undulating lands to the north of Milan. The headwaters of the catchment discharge into a natural glacial lake, Lake Pusiano, which then discharges to from the upper reaches of the Lambro south of the town of Erba. The headwaters of the Lambro, upstream of Lake Pusiano, consist of steep slopes with impermeable soils underlain by dolomite geology.

The undulating land between Lake Pusiano and Milan contains large areas of intensive industrial and residential landuse such as the city of Monza and the Brianza area, as well as large tracts of arable land. Permeable to very permeable gravels and sands characterise the lithology of this portion of the catchment. Current indications are that groundwater interactions begin in the vicinity of Monza at the downstream end of the catchment, (Gandolfi, pers. comm. 1998).

The flow regime in the catchment north of Milano is basically natural. However, the city of Monza, to the north east of Milano, represents an area where major discharges from sewerage works occur and other minor discharges and abstractions are likely to occur. The majority of the water supply for the city of Milano is drawn from groundwater aquifers that do not interact with the Lambro river system and it is likely that returns, in the form of sewerage effluent, occur downstream of the catchment considered. Accurate quantification of discharges and abstractions within the catchment was not possible due to a lack of data.

**Hydrologic and Climatic Data Sources**

The Pilot Study catchment north of Milan was divided into five sub-catchments at the location of flow gauging stations, see Table 2.

**Table 2**

| Guaging Station | Catchment Area ($km^2$) |
|---|---|
| Caslino | 53 |
| Colombaio | 40.2 |
| Lambrugo | 170 |
| Biassono | 270 |
| Parco Lambro | 465 |

Climatic data, including included temperature data on a monthly or daily basis, and rainfall data on a daily and monthly basis was available for seven stations within the catchment.

*Verification of data*

Detailed verification of the data and data sources was conducted prior to hydrologic analysis. This process enabled some inconsistencies to be rectified, appropriate rating curves to be developed to convert stage records into flow records, the most reliable data sources to be identified and the general hydrologic response of the catchment to be investigated.

**Methodology**

Traditional hydrologic analysis was used to derive spatially distributed flow statistics of mean flow and Q95 within the Lambro catchment. The detailed spatial data sets and gauging station data sets that were available for the Yorkshire catchments were not available for the Lambro catchment. The modelling is not as efficient, in terms of resources, as for the Yorkshire pilot study, as the Lambro model is catchment specific. The models developed and applied in the Yorkshire Pilot study are applicable to any UK catchment.

The primary problem associated with the data for the Lambro catchment was that common periods of flow records were not available for the limited flow gauge network and thus differences between the gauged locations will in part be a function of the climatic differences between gauged periods. In particular, the Lambrugo and Colombiao gauges ceased operation in the early 1970's. It was therefore necessary to develop techniques that would allow contemporary flow statistics to be produced.

*Mean Flow estimation*

Firstly long term climatic trends were investigated to ascertain whether mean flow statistics obtained from data in the 1970's were appropriate for use in a contemporary period (1980 to 1990). It was found that the contemporary climate represented a period of lower than average rainfall (approximately 10% lower than the long term average) and higher than average temperature. Hence it was not possible to adopt mean flow statistics derived from an earlier period of record and a technique for producing mean flow estimates for the period 1980 to 1990 were developed.

A simple statistical model IHACRES developed collaboratively by the Institute of Hydrology and the Centre of Resources and Environmental Studies at the Australian National University, Canberra, was to predict mean flow for the Lambrugo and Colombiao sub-catchments using contemporary rainfall and temperature data. This model accounts for all of the non-linearity observed between rainfall and runoff within a loss model and does not purport conceptualise the physical behaviour of soil moisture, Littlewood and Jakeman (1994). A verification period was available for the Lambrugo sub-catchment but not for the Colombiao. Comparisons of runoff accretion profiles were also used to verify the predicted flow estimates.

*Q95 estimation*

Flow distribution curves (FDCs), standardised by mean flow, were produced for all flow gauges from suitable periods of actual flow data. FDCs produced from different periods of time at the same gauging station were compared to allow the temporal consistency of the variability of flows to be investigated. Standardising the FDC from a period by the mean flow over the period identified that the form of the

FDC for each sub-catchment was independent of the period of record from which it was derived. Hence, the standardised Q95 statistic determined from actual data was used in combination with the contemporary estimate of mean flow to calculate an estimate of Q95 in flow units.

*Incorporation of artificial influences*

The information regarding artificial influences within the Lambro catchment could not be well quantified in terms of actual discharge/abstraction volumes or the location of these influences with respect to the river network. It was generally thought that the majority of influences would be discharges rather than abstractions, since abstractions for Milano's water supply were known to be outside the catchment area. This was confirmed by runoff accretion profiles which showed an increase incremental runoff between Monza and Milano. The only documented discharge in this area was that from the Monza sewer treatment plant. This artificial influence was included as a constant rate discharge, for lack of other information.

*Interpolation of flow statistics*

The low flow statistics of Q95 and MF for the five gauging stations in the Lambro catchment were interpolated throughout the digital river network by application of procedures modified from those established within the Micro LOW FLOWS software, (IH, 1996). The procedure involves estimating the Q95 or MF value at an ungauged river reach by taking a weighted average of the flow statistics calculated for the n nearest neighbour gauging stations. Nearest neighbour in this context is defined as adjacent but on a common flow path. The weight applied to a station was based upon the inverse distance in catchment area space between the target ungauged reach and gauging station. The discharges from the treatment plants within the catchment were incorporated into this interpolation procedure. The reach based estimates for mean flow in the Lambro catchment are presented in Figure B.8.

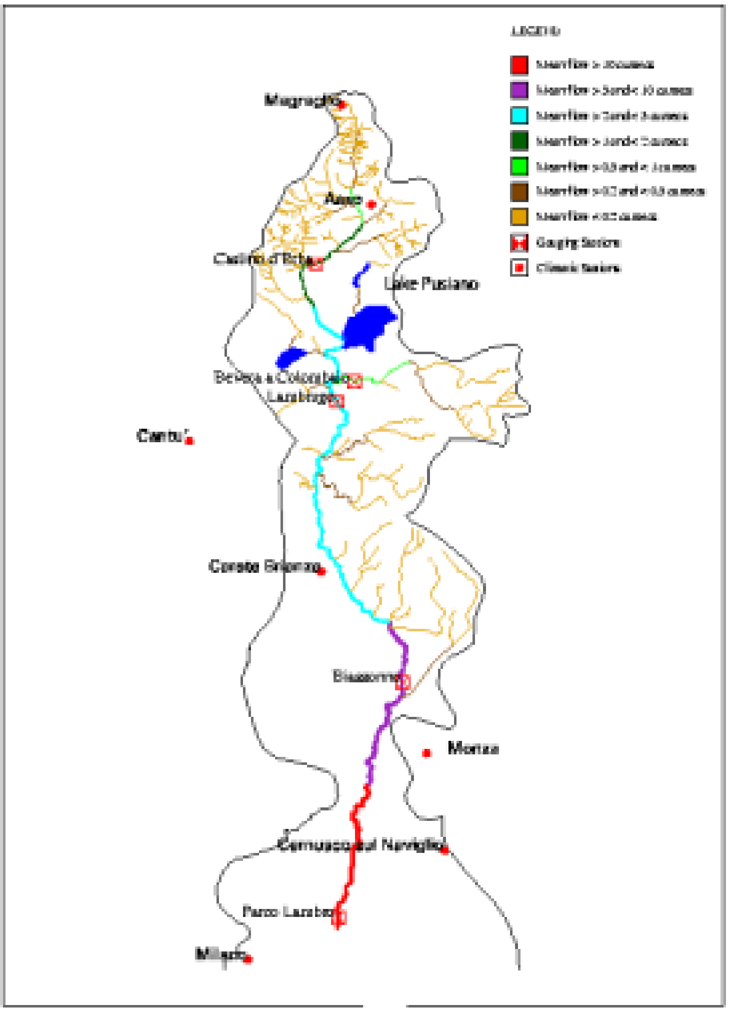


Figure B.8: *Reach based Mean Flow Estimates within the Lambro catchment*

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# MEMBERS OF THE TASK FORCE

| | |
|---|---|
| T. Feijtel | Procter and Gamble<br>B – Strombeek-Bever |
| G. Cassani | Condea Augusta<br>I – Padermo Dugnano |
| J. Ferrer | Petresa<br>E – San Roque |
| K. Fox | Unilever<br>UK – Bebington |
| C. Gandolfi | Università Degli Studi di Milano<br>I – Milano |
| C. Heidorn | European Chemicals Bureau<br>I – Ispra |
| V. Koch | Clariant<br>D – Frankfurt am Main |
| M. Matthies | Universität Osnabrück<br>D – Osnabrück |
| E. Matthijs | Procter and Gamble<br>B – Strombeek-Bever |
| G. Morris | Environment Agency<br>UK – Leeds |
| R. Murray-Smith | Zeneca<br>UK – Brixham |
| J. Rosenblom | Akzo Nobel<br>S – Stenungsund |
| D. Schowanek | Procter and Gamble<br>B – Strombeek-Bever |
| R. Schröder | Henkel<br>D – Düsseldorf |
| P. Vanrolleghem | Universiteit Gent<br>B – Gent |
| A. Young | Institute of Hydrology<br>UK – Wallingford |
| M. Holt | ECETOC<br>B – Brussels |

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# MEMBERS OF THE SCIENTIFIC COMMITTEE

(Peer Review Committee)

| | |
|---|---|
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