

# **GREAT-ER Preprocessing Manual**

**:: for version 2.0 ::**

**Geo-referenced Regional Exposure Assessment Tool for European Rivers**

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# 1 Introduction

The GREAT-ER pre-processing is a script-based routine to prepare a GREAT-ER catchment dataset from raw data in a pre-defined text format.

This document intends to enable the reader to prepare catchments for use with the GREAT-ER simulation system. The process as a whole is described as well as technical details on how the procedure works and on how to apply the associated software tools that actually perform the processing. The commented source code itself (released as Free Software) completes the documentation on all details.

Current information, all source codes, documentation and a mailing list can be found at the GREAT-ER development homepage:

<http://great-er.intevation.org/>

## 1.1 History

The pre-processing routines originate from the GREAT-ER 1 project as a script collection and have been further improved since then.

The major changes from GREAT-ER version 1.0 to version 2.0 are:

- Availability as Free Software.
- Independency from proprietary software (especially ArcInfo which was a major drawback due to its high license costs).
- Replacement of ArcInfo coverage format by ESRI Shapefile format for all geographic data.

The detailed changes of the present version are listed in the file `Changes.txt` of the pre-processing software package.

## 1.2 Requirements

Applying the GREAT-ER pre-processing requires experience with Unix-like systems; principle programming skills are helpful.

The basic requirements are

- a usual Unix-like system including the standard GNU software tools (recommended is a GNU/Linux system).
- The programming language Python which is usually available on such systems, but they may not be updated to Python version 2.0 as required for the pre-processing.
- The special tools `gen2shp`, `txt2dbf` and `dbf2txt`.

Details, e.g. on specific versions on the required tools are given in the Howto-section (see below).

## 2 How-To

### 2.1 Software Requirements

- Python  $\geq$  2.0
- GNU Awk  $\geq$  3.1.0
- gen2shp  $\geq$  0.3.0  
(<http://intevation.de/~jan/gen2shp/>)
- txt2dbf  $\geq$  1.0.2
- dbf2txt  $\geq$  0.5.2  
(<http://www.usf.uos.de/~fkoorman/software/dbftools.en.html>)
- GNU textutils (sort, join, cut, paste)  $\geq$  2.0
- GNU fileutils (rm)  $\geq$  4.1
- GNU sed version  $\geq$  3.02
- GNU sh-utils (echo)  $\geq$  2.0.11 (the programs must be somewhere in your search path)

### 2.2 Prerequisites

As a first step you have to copy `greater-pre-processing.py` somewhere into your `PATH` or extend the `PATH` to where you have installed the `greater-pre-processing` package:

```
cp greater-pre-processing.py /some/where/in/your/search/path
```

OR

```
export PATH=$PATH:/some/where/greater-pre-processing
```

Next, set this environment variable that points to where you have installed the `greater-pre-processing` package:

```
export GREATER_PRE_PROC=/some/where/greater-pre-processing
```

You then are able to execute

```
greater-pre-processing.py
```

in a directory with the pre-defined files for your catchment (you will be given further info on how to use the program).

## 2.3 Running the Data Preprocessing

```
$ greater-pre-processing.py help
greater-pre-processing 1.1.0
```

```
Found 'catchment.desc':
```

```
  ID           = went
  Name         = Catchment of River Went
  Description   = The Went catchment is a small, rural area in Yorkshire, UK.
  Format version src   = 1.0
  Format version result = 1.0
description complete.
```

```
greater-pre-processing [check|help|run]
  help  print this text
  check test for completeness and correct syntax of source files
  run   execute catchment pre-processing
```



## 3 Catchment Source Files Formats

*Note:* This new format slightly differs from the original GREAT-ER 1 format and is therefore not fully compatible. See the file *Changes.txt* of the software package for details.

All 6 catchment source files have to be collected in one directory.

All files are text based and use the character set ISO 8859-1 (ISO Latin 1). The format is line-oriented; each line starts with a '#' (comment line) and all empty lines have no meaning for the processing and can be inserted anywhere.

All coordinates are given in the same projection: "geographic projection" with unit "dd" (decimal degrees). A point, rather than a comma, is used as decimal point. Numbers are not allowed to contain any other delimiters. Exponential representation uses the letter 'E' or 'e'.

### 3.1 Info File, File 'catchment.desc'

This file contains general information. Example:

```
ID=went
NAME=Catchment of River Went
DESCRIPTION=The Went catchment is a small, rural area in Yorkshire, UK.
IN-VERSION=1.0
OUT-VERSION=1.0
```

**ID** is the basename for the actual data source files suffixed with .drn, .rna, .dsd, .cbp and .bgd.

**IN-VERSION** defines the format for the all catchment source files.

**OUT-VERSION** defines the output format.

### 3.2 Digital River Network, File 'ID.drn'

IN-VERSION = 1.0

The river network attributes are stored in a simple tabular structure. Columns are separated by commas. The following example illustrates the order of the columns:

```
7421
-1.399004,53.718807
-1.374895,53.730835
```

```
-1.368942,53.734528  
-1.364163,53.736794  
-1.363446,53.738102  
6787  
-1.399046,53.717968  
-1.399043,53.718178  
[...]
```

In this example no information is available for flow velocity and depth and hence the corresponding columns are left empty.

### 3.3 River Network Attributes, File 'ID.rna'

IN-VERSION = 1.0

The river network attributes are stored in a simple tabular structure. Columns are separated by commas. The following example illustrates the order of the columns:

```
# Aire/Calder Catchment, Yorkshire  
# StretchID,Qmean(m^3/s),Q5(m^3/s),vmean(m/s),v5(m/s),  
# ... RealLength(m),depthmean(m),depth5(m),Name  
26954,34.751000,12.280656,,,2491.655000,,,Unnamed  
22954,0.009000,0.002359,,,1648.222000,,,Unnamed  
7333,34.739000,12.276415,,,1629.885000,,,Unnamed  
22932,0.005000,0.001088,,,540.190000,,,Unnamed  
26950,34.731000,12.274977,,,2336.740000,,,Unnamed  
22923,0.017000,0.002167,,,2447.520000,,,Unnamed  
[...]
```

In this example no information is available for flow velocity and depth and hence the corresponding columns are left empty.

### 3.4 Discharge Site Data, File 'ID.dsd'

IN-VERSION = 1.0

Each line defines one discharge. The first column is its unique ID, followed by the coordinate pair and the attributes. The order of the columns is shown in this example:

```
# ID,X,Y,Pop,DWF(m^3/d),Flow(m^3/d),Type,StretchID,Name  
41,-1.390494,53.422081,422677,130000,180000,AS,26842,Blackburn STW  
42,-1.349155,53.369724,95750,21800,24506,AS,26843,Woodhouse Mill STW  
43,-1.326922,53.445114,107203,31250,32410,AS,26841,Aldwarke STW
```

### 3.5 Catchment Boundary Polygon, File 'ID.cbp'

IN-VERSION = 1.0

The polygon is described linewise by single coordinate pairs (x,y). The following example illustrates the format:

```
-2.052912,53.683811  
-2.060483,53.683807  
-2.060477,53.679314  
-2.068047,53.679310  
[...]  
-2.045346,53.688309  
-2.045342,53.683804  
-2.052912,53.683811
```

This example also shows that the polygon must be closed, cf. the last and the first point must be identical.

### 3.6 Lakes, File 'ID.lks'

IN-VERSION = 1.0

A list of stretch IDs which actually are lakes. Example:

```
# StretchID  
345  
2256
```

This file can be empty, but must exist.

### 3.7 Pictures, File 'ID.pic'

IN-VERSION = 1.0

If pictures are available for the catchment, location and picture files can be specified:

```
# ID,X,Y,File,Name  
1,6.860403,51.157661,mgmuendung.gif,Confluence to the Rhine  
3,6.872726,51.158089,mgddorf.gif,in Duesseldorf  
4,6.897292,51.159611,uhilden1.gif,Below STP Hilden  
5,6.899222,51.159081,uhilden2.gif,Below STP Hilden
```

This file can be empty, but must exist.

## 3.8 Background Data, File '.bgd'

IN-VERSION = 1.0

To support the user with a quick and easy access to geographic background information, a list of background data sets can be defined for each catchment.

In the ".bgd" file names of additional background data that are to be loaded by the menu entry "Display/Add Background Data" are specified. The data can be given in two ways. In a simple case, a background data set is only a geographic data set that ArcView can load as a theme, i.e. anArcInfo Coverage, an image, a grid or a shapefile. This case is indicated by the value "yes" in the field "ctch\_flg" (see below). In the more complex case a background data set consists of a set of geographic data, indicated by the value 'no' in the field 'ctch\_flg'. In this case, instead of the name of the data set an ID for a script that knows how to load the geo-data sets is specified.

### Name

This is the name for the corresponding background data. It is used for user selections in the GREAT-ER system.

### Mapname

In the case of a simple background data set, this is the file name of the coverage, image or shapefile that contains the data. Otherwise this field contains the script which can load the background data sets.

### Type

In the case of a simple background data set, this is its feature type. Valid entries are "point", "line", "polygon", "shape", "image" and "grid". Otherwise the field is left empty.

### Legendfile

In the case of a simple background data set, this is the name of an optional ArcView legend file. Otherwise this field can contain (optional) parameters for the script specified in the field "Mapname".

### ctch\_flg

This is a boolean field that contains either "yes" or "no". "yes" indicates that this background data set consists of one theme that does not need a special script to load into the active view of GREAT-ER. "no" means that a special Avenue script has been developed by the user which runs within GREAT-ER and loads the background data set into the active view.

There is one special case: The DCW data (Digital Chart of the World, a variant of VMAPL0) are incorporated in the GREAT-ER project for the whole of Europe. For this incorporation specific

scripts loading the DCW data in dependence of the viewed country are developed. If the DCW data are to be a background data set for a catchment, the following line needs to be inserted into the file:

```
DCW data,,,,
```

If a user installs the DCW data for countries that have not yet been included, e.g. France, Spain or Denmark, these data need to be installed analogous to the included countries.

### **Example ".bgd" file**

This example file describes background information for the River Itter (Germany):

```
#River Itter background data
#Name,Mapname,Type,Legendfile,ctch_fl
Cities,itter\cities,polygon,itter\cities.avl,yes
Tk25,itter\tk25tiffz.tif,image,,yes
Rhein,itter\rhein,polygon,itter\rhein.avl,yes
DCW data,,,,no
```

## 4 Catchment Result Files Formats

Currently two versions of the results files can be created:

OUT-VERSION = 1.0: creates catchment datasets compatible with GREAT-ER 1.

OUT-VERSION = 2.0: creates catchment datasets compatible with GREAT-ER 2. The difference is additional columns down1 and down2 in river.dbf.

## 5 Preprocessing Basics

Besides the environmental model itself, the availability and quality of environmental data mainly determine the validity of simulation results. This and the following sections introduce general aspects and problems of spatial data for environmental exposure assessment. A proposed procedure is described for how to deal with the collection, processing and quality assessment of data considering also the origin and purpose of readily available data. The technical aspects will be focused on but it must also be stressed that obtaining spatial data in the EU reveals serious coordination and authorization problems.

An example of the proposed procedure is given in which the digital river network is the backbone of the spatial data set for "down-the-drain" exposure assessment. The example is given for GREAT-ER but the methodology is equally applicable for similar systems.

The data required for the regional geo-referenced exposure assessment is characterized by its complexity and inhomogeneity. This is partly due to the fact that there are large amounts of single data. But another fact plays an important role: the composition of such data is not readily available. It is typically scattered among several competent authorities and other data owners. In the past those different parties had seldom experienced the necessity to harmonize their data and hence it is to be expected that all obtainable data are in several digital formats and/or geographical resolutions. Inconsistent ID reference systems are likely to be faced as well. The approach to regional geo-referenced exposure assessment has created a need for the coordination and composition of base data which are, though collected and applied for various topics, nothing more than *raw* data in respect to the new task.

The reason for this lies also in the way in which most geographic data are used: for mapping purposes where structural integrity is much less important than visual appearance.

The data composition for exposure assessment in river networks reveals many problem-specific aspects. When one would set up a very special recipe for certain data sources or data origins, this task would lack re-use capabilities and also would not be considered adequate for other comparable tasks. In the framework of a simulation system for a growing number of catchments, re-use capabilities require special attention to ensure the efficient creation of many digital river network data sets. The solution for data composition must be simple and open enough to offer quick understanding, general applicability and also to enable technical solutions to be adapted.

The usual steps of data composition and processing as a GIS task are typically single manual steps of applying geographic methods and routines. The required quality and structure of the final geographic data (i.e. maps) is approached in a straight-forward manner. The data sources and intermediate stages are often eliminated as soon as the latest version passes a quality control. It

is unusual for GIS users to automate the processing steps because each new job reveals other aspects of processing which can not all be foreseen. To make the results transparent and to avoid later wrong use, all processing steps must be documented very carefully. This is especially important when results are not only used for reporting purposes but also for further processing and comparison with other data sets processed in a similar way.

A well defined intermediate stage of the data is a general approach to separate the specific problems of raw data from the actual data preparation. Setting up this intermediate state on text-based formats increases transparency. A set of pre-defined files requests data at an adequate level of simplicity while at the same time being able to grant some aspects of quality and completeness. Furthermore, a high degree of automation can be created starting from pre-defined text files.

As an alternative intermediate state a pre-defined database management system (DBMS) can also serve the task of separation. Such an approach creates further needs in software requirements and skills to handle them. Depending on the frequency of usage, the DBMS solution, once set up and tested, can be more efficient than the solution based on simple text files. The advantages arise from the DBMS environment which offers support for distributed systems (including Internet applications) and high performance in handling large data sets. With its higher level of sophistication such a solution loses self-explaining transparency which needs to be compensated by comprehensive usage documentation and/or by dedicating a human operator. Proving its principle operability with the text files as an intermediate stage is a recommended step before setting up a DBMS solution. The two-step approach is therefore chosen for the GREAT-ER data processing.

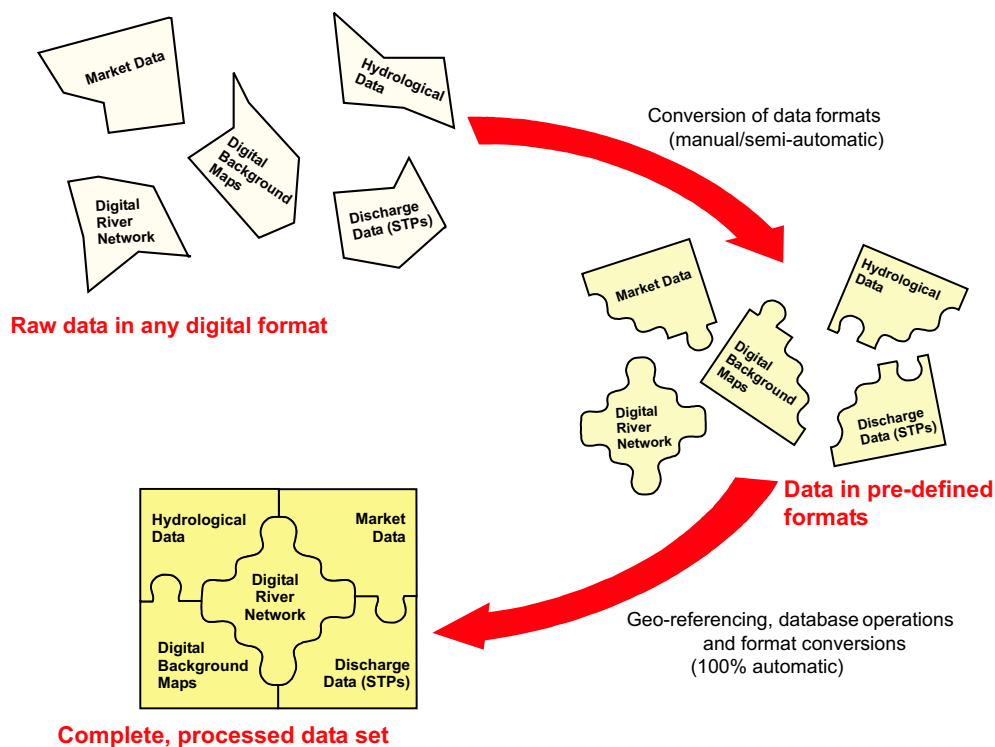


Figure 5.1: *Two steps of data processing*



Inventing an intermediate stage for data consequently results in two steps of data processing. In a first step, collected raw data are transformed into the pre-defined intermediate form. A second and independent step then creates final ready-to-use data from the intermediate stage.

The initial data processing is very much determined by the gap between demanded data quality and formats and the present state of the raw data. The required files have to be produced manually from the original raw data or with special routines which probably have to be developed anew.

The final data processing is a well defined task, provided that all required data are collected and fit the demands of pre-defined formats. Of course, the final environment of the geo-referenced exposure assessment tool must also be defined precisely to make the data processing fully automatable. In this context, the simulation method determines the structural shape and order of the data while the user interface and data management modules determine the actual formats of files.

The two steps of data processing are illustrated in figure 4.1. An example is given for an exposure assessment tool for river networks. Three main states of the five data groups are shown. These data groups cover any information that is related to space in one way or another. For example, physico-chemical data of a substance are excluded but the substance's market data are included as regionally resolved information.

Another view of the finally produced data sets is shown in figure 4.2. The data groups form layers which build the visual interface available to the user.

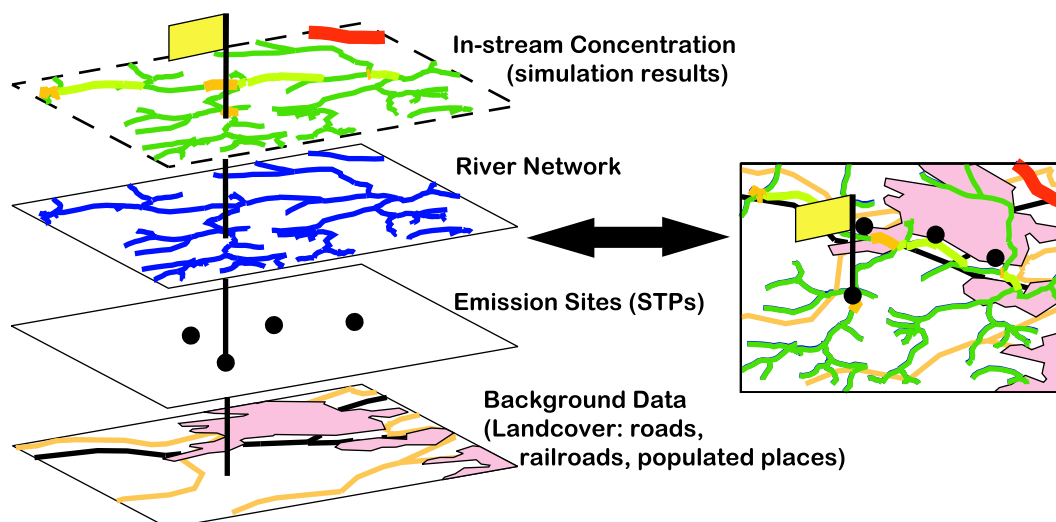


Figure 5.2: *Layered view of data groups*

## 5.1 Data requirements and composition

### 5.1.1 Digital river network

#### General overview

The digital river network describes the structure of the river network in question. At the very bottom it consists of lines (also referred to as 'polylines' or 'arcs'), each of which represents a river segment. Furthermore, it consists of nodes which represent the point of connection of two segments. Lines are expressed as a sequence of at least two coordinate pairs, nodes are expressed as exactly one coordinate pair (figure 4.3b).

Lines have to be considered as vectors; the first point of the sequence is the starting point and the last is the end point. The vector direction is used to represent the flow direction (figure 4.3c). The length of a segment can be computed from the coordinates.

Each transition from one segment to a subsequent one (sequence, confluence or bifurcation) is defined by a node which contains the information 'from' and 'to'. The ID's of the upstream ('from') and the downstream ('to') segments are stored. The geographic position of a node is uniquely defined with the last point of the upstream and the first point of the downstream segment. If these two points are not identical, the two stretches are not connected and no corresponding node exists.

Besides the persistent Arc-Node geometry model, a second, flexible segmentation can be set on top of it. The two-dimensional geometry model lacks the ability to precisely locate sites along the lines between two given coordinates. This can be solved by introducing a one-dimensional measuring system with only starting and ending information.

These one-dimensional geometric objects are called 'routes'. For digital river networks, each river is a 'route'; the whole network constitutes a 'route system'. Any site along the rivers in a route system can be referenced by the route name and the distance from the route start (e.g. River Rhine at kilometer 744 which is at Düsseldorf, Germany). The start and end of routes are a matter of definition. In Germany, the distance reference of rivers that lead into the ocean begin at the source. The distance reference of tributaries begins at the point of confluence in reverse flow direction. Standard GI Systems offer methods to create route systems from an arc-node model. This must be a two-step routine where a raw route system is first created based only on the information contained in the arc-node representation (figure 4.3d). The raw route system requires two further adjustments. First, the digitized rivers do not necessarily start at the actual source and hence the starting points of the routes must be set to the correct value for later consistent referencing. Second, the length computed from the digitized lines depends on the resolution and hence is always lower than the actual river length. A remeasurement routine that is provided with the actual length of a route, is to be performed to gain revised coordinates for any event along the stream. The route system approach for exposure assessment was applied for intermediates in the River Rhine catchment (Koormann, 1997 and Koorman et al. 1998) and for a small tributary of the Rhine, the Itter catchment (Schulze, 1998 and Schulze et al., 1999).

Fundamental to the creation of a digital river network are maps of the corresponding area. Traditional printed maps can be used as a basis but usually such maps now exist in digital format.

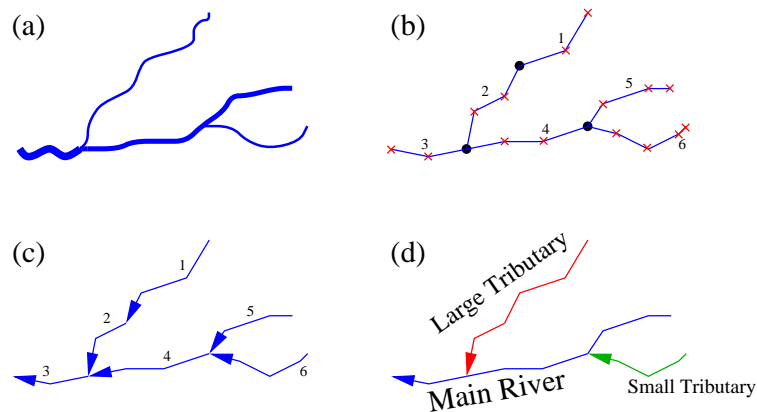


Figure 5.3: *Steps of creating a digital river network: (a) Reality (i.e. aerial photo or comparable basis). (b) Digitized network (crosses and dots = coordinates, dots = nodes, numbers = IDs of lines). (c) Direction of lines (vectors). (d) Representation as route system.*

Digital maps can be created in two ways, either by collecting coordinates directly with a Global Positioning System (GPS) or from aerial photographs. While GPS data are naturally already geographic objects in vector format, pictures taken from planes or satellites offer information in a raster format. I.e., surface waters consist of single points (squares) and hence do not contain information about e.g. flow direction, but on the other hand may offer information about areal aspects (e.g. width of rivers, shape and size of lakes) and possibly further properties (temperature, depth). The raster information must be converted to vector data to gain a digital river network as described above. This conversion can partially be automated but manual reworking by human experts is unavoidable for quality assurance.

### Solution for GREAT-ER

As a requirement for data, the arc-node model is preferred rather than the route model. This is because, especially for more detailed river networks, an assignment of river names and remeasurement become problematic and time-consuming.

In summary, the following demands for a digital river network have been defined:

- Only the coordinate sequences for the river segments are to be given. No extra node specification is required.
- Should two segments be connected, it is necessary that the end point of the upstream and the starting point of the downstream segment are identical. This also means that for confluences or bifurcations the upper segment(s) always end at that point and one (or two) new segments start from the same point.
- All river segments must be directed downstream.
- All segments must have a unique ID.

Only confluences and bifurcations enforce the beginning of new stretches. Sequences like segments 1 and 2 in figure 4.3 have no topological meaning for the network. Splitting up segments into a sequence of two or more stretches becomes important for the semantic purposes the digital river network has to serve. Simulation models using digital river networks may need to simplify river segments by assuming stretches to be homogeneous in a hydrological sense. In this case flow data would be attributed to river stretches and hence long segments need to be split up according to the required resolution or available knowledge about hydrological changes. Additionally, for visualization purposes the level of segmentation also determines the capabilities to graphically display stretch-specific information. Hence, when setting up the digital river network the later purpose of these data should already be considered at this point and segmentation should be performed. This task can also be undertaken automatically provided that the single coordinates of the lines are more or less equidistant.

### 5.1.2 River network attributes

Depending on the needs of an applied exposure simulation model, information about certain properties of the river network are required. Usually these are floating point numbers (e.g. flow in  $[m^3/s]$  or flow velocity in  $[m/s]$ ). Further attributes such as boolean (shipable [yes|no]) and others are conceivable. Most of the traditionally measured data are expressed as statistics due to natural fluctuations and seasonal variation. For example, flow data are usually expressed as log-normal distributions characterised by the mean and standard deviation (or mean and low, e.g. 5th, percentile).

However, all discrete attributes (in space) have in common that they correspond with a certain river segment. A set of discrete parameters for a river network can hence be given in tabular style. Continuous parameters (in space) are more difficult to attach to digital river networks, and applications using such data also reach a level of complexity which is seldom acceptable for actual environmental simulations. Usually distribution curves are derived from temporal data series which are then applied for a specific task.

Depending on the purpose for which the river attributes are needed, in some cases the variation of each river segment is of importance and for other parameters variations are only of interest for entire rivers or river networks. Furthermore, decisions regarding the stretch-wise resolution of parameters are influenced by data availability. Consequently, a task-specific separation of parameters is helpful and can be solved by defining river classes and associating each river segment to a river class.

Parameters that are semantically important and presumably different for each segment are directly associated to river segments. For many parameters the reasons for actual availability at high resolution represents the opportunity not only to measure but also to interpolate between measurements or to estimate them from other attributes. Hence, again depending on the semantic context, not all parameters are obligatory. A flexible (interpolating, estimating) system of optional parameter specification is possible.

The methods of chemical exposure assessment are organized in a tiered approach in terms of physico-chemical processes. Lumped transport and elimination processes will be applied first and if it is not capable of explaining monitored behavior, refined substance-specific processes will be

added (e.g. photodegradation). Any refinement increases data demands, uncertainties and, on a very practical side, expense and time.

The counterpart of the lumped parameters for chemicals (transport and elimination) are hydraulics and geometry of rivers. These basically determine the dilution and dispersion of chemical loads. Accompanied by length and name, these were chosen as direct attributes. All other parameters are assembled in river classes. This choice reflects the data requirement of the simulation software incorporated in GREAT-ER (Boeije, 1999). The concept of the intermediate data stage still allows us to consider data requirements of any comparable simulation model by providing corresponding automatic data processing routines for the second step (figure 4.1).

## Flow, Velocity, Depth and Width

**Overview of interrelation** For a sufficient period of time, the flow passing the full extent of a river segment can be assumed as constant in space and time. In this case the continuity equation 5.1 is true.

$$Q = vA \quad (5.1)$$

where  $Q$  = flow,  $v$  = velocity and  $A$  = cross-sectional area.

Rivers have no rectangular cross-section and hence  $A$  can not simply be substituted by the product of depth and width. Depth and width have a correlation with the flow within certain ranges. A set of power equations 5.2 can express the interrelation of velocity ( $v$ ), width ( $w$ ), depth ( $d$ ) and flow (Leopold & Maddock, 1953).

$$v = aQ^\alpha \quad ; \quad d = bQ^\beta \quad ; \quad w = cQ^\gamma \quad (5.2)$$

where both  $\alpha + \beta + \gamma$  and  $a \cdot b \cdot c$  must be equal to 1.

Compared to velocity and depth, width is generally less variable (in space) for most rivers (Chapra, 1997). Especially when dealing with one-dimensional models, width is of less semantic importance. In contrast, depth is important, i.e. for chemical volatilization processes. In this approach width is hence dropped from the list of required river properties. It should of course be taken note of when considering transversal dispersion (two-dimensional river models).

Site-specific measurements and site-specific regression functions are optimal to gain most adequate information on river properties. In the absense of such data, and this is true for most sites, literature or new field studies need to be undertaken.

Numerous studies were conducted to obtain values for parameters  $a, b, c$  and  $\alpha, \beta, \gamma$  which vary with different climatic location and degree of artificial influences on the river networks.

It has also been shown that the hydraulic geometry can alternatively be obtained from the corresponding watershed size: Based on a strong correlation of bankfull flow and watershed area, a geometric relationship was shown and extrapolated for all river segments (Miller et al., 1997). Another method is based on the hortonian stream order for river networks. This ordering method attaches the order of 1 to all source stretches. The order of any other stretch is the maximum order

of the directly connected upstream stretches plus 1. A good correlation of the hortonian order and the river geometry has been proved for a watershed in Arizona, U.S.A. (Miller et al., 1996).

Besides the statistical approaches described above, mechanistic techniques can be applied. The best known method is the Manning equation (5.3) (Chapra, 1997).

$$v = \frac{R^{2/3} S^{1/2}}{n} \quad (5.3)$$

where  $n$  = Manning's roughness coefficient [-]  
 $R$  = hydraulic radius (equal to  $A/P$ ) [m]  
 $P$  = wetted perimeter [m]  
 $S$  = energy slope (here equal to geological slope) [-]

Substitution into the continuity equation results in the approach of Manning-Strickler (equation 5.4) (Dyck & Peschke, 1989).

$$Q = \frac{AR^{2/3} S^{1/2}}{n} \quad (5.4)$$

Besides flow and velocity, the depth can also be obtained based on the Manning equation. The depth is the root of equation 5.5 (Chapra, 1997).

$$f(y) = \frac{1}{n} \frac{[(w_0 + sy)y]^{5/3}}{(w_0 + 2y\sqrt{s^2 + 1})^{2/3}} S^{1/2} - Q \quad (5.5)$$

where  $s$  = side slope and  $w_0$  = bottom width.

For the GREAT-ER project a new study has been undertaken to estimate the velocity of any river reach in the UK (Round et al., 1998). A statistical approach was chosen based on hydrological databases for the UK. The quality of the velocity estimation model (equation 5.6) was not significantly reduced in terms of performance by excluding the hydraulic radius. The error analysis showed that with 68% confidence the true velocity lies within a factor of 1.59.

$$v = 10^{-0.583} Q_{mean}^{0.283} \left( \frac{Q}{Q_{mean}} \right)^{0.495} \quad (5.6)$$

To obtain average depth values, variations in three dimensions have to be made. First, depth can vary in transversal and longitudinal extent of the river bed and next, it changes in time due to flow variation. For unknown geometry and known flow an application of the Regime Theory provides equations 5.7 and 5.8 (Simons & Albertson, 1960).

$$w = 6.175\sqrt{Q} + 0.305 \quad (5.7)$$

$$d = \begin{cases} 0.610 + 0.93r & : r > 2.13 \\ 1.21r & : r \leq 2.13 \end{cases} \quad (5.8)$$

where  $r = 0.57Q^{0.36}$ .

**Selection of values and methods** Literature review has shown examples of the ability to estimate the interrelated river properties flow, velocity, depth and width from each other in several ways. Also area and mathematical topology can be included for estimations. The latter can even be applied when no stretch specific properties are known.

In general, higher efforts are required to measure the geometry of river segments while flows are easier to obtain: In most European countries a system of gauging stations is in operation, delivering flow statistics for some sites. Usually interpolation equations can easily be set up or are even readily available for ungauged sites between two gauging stations. Ungauged headwaters are more complicated to establish flow estimation. The flows can be computed from geo-morphology and other information, i.e. MicroLowFlows additionally applies soil type and precipitation information for this task (Gustard et al., 1992).

For the methodology introduced in this chapter, flow data are chosen as obligatory, and velocity and depth are optional parameters. Optional parameters will be estimated during the data processing. Consistency checks based on the literature can be integrated in the final processing.

Most estimation equations derived from statistical studies are associated with several limitations concerning the environmental framework of the investigated river network (natural/regulated, arid/humid, lowland/highland, etc.). If estimation equations are available which were set up for the same or a similar type of river these should be preferred and the resulting values should be used. Automatic selection of estimation routines can not decide adequately compared to human judgement. This is due to the fact that much general information on a river network is required and this information can not easily be formalized.

One important property of the discussed parameters is variation in time, which means that these parameters usually consist of three subparameters describing their statistical distribution (i.e. distribution type, mean, standard deviation). This must be kept in mind when dealing with corresponding data collection and estimation.

## Length

In conjunction with velocity, the length basically determines the transport of a (chemical) load. The process of transport in terms of chemical exposure modeling is a relatively fast process and hence the travel distance should be given as accurately (feasibly) as possible.

Obtaining the actual length of rivers should in general not pose a serious problem because it is relatively easy to measure. For some countries, canoeing guides offer this information in great detail, i.e. for Germany (Deutscher Kanu-Verband, 1985).

In theory, there are of course no problems in calculating the length of each segment based on coordinates. These values are naturally (sometimes much) lower than the real length of the river segments. These differences become obvious when taking into account that even detailed digitizing (e.g. one point every 300m) can not reflect the actual shape of a very curvy river. Additionally, the digitizing itself reveals uncertainties.

## **Name**

Names for each river segment are not meant to identify stretches in terms of database operations. Obviously one river can be split up in very high numbers of stretches and therefore unique name specification does not make sense. The names are required rather for identification and orientation purposes in the final simulation tool. Names of rivers can hence be associated with other site names or any information that is felt to be helpful to users.

## **River Classes**

The composition of the river class parameters is to be selected dependent on the semantic purpose of the simulation models. This way, the number of properties can be reduced to a minimum to retain low complexity and an easy overview.

The methodology presented in this chapter takes the river class composition as used for the simulation software in GREAT-ER (Boeije, 1999). Included are typical water quality parameters, i.e. suspended solids, dissolved oxygen, biological oxygen demand and pH. All these parameters are only used in higher model complexity modes, i.e. not applying lumped degradation rates. Among the biochemical properties, the type of segment is also described (river or lake).

### **5.1.3 Catchment boundary**

The catchment of a river network is defined by the most downstream point, i.e. the most downstream segment. The catchment boundary represents the natural drainage area. Any point in that area will drain to that most downstream segment. The catchment boundary must always be a closed polygon.

The introduced data composition additionally enables several separated river networks to be joined. This helps users to deal with e.g. flat coastal regions, entire islands or even whole countries. In such cases the catchment boundary should be the union of all single subcatchments.

Information about the actual border of a catchment serves two purposes. First, it supports geographic methods, e.g. spatial selection routines. Second, within the final tool the user is given further support for orientation and interpretation.

In regions where water management has a long tradition, watershed boundaries should be readily available. Any new or re-calculation applying a GIS will require digital elevation data. This computation is often performed and several technologies are available, partly already built into a GIS.

### **5.1.4 Discharge data**

The discharge data, in this context, are a set of points through which substances are released into the river networks, e.g. sewage treatment plants. The discharge information will not be able to express diffuse input (unless it is made discrete as a series of point inputs). Diffuse input is not focused in the presented methods because a different class of simulation models would be required.



Discharge points with geographical reference define an area where any release will pass this point travelling "down-the-drain". Such areas are scale-independent geographical units interconnected by a network topology (figure 4.3). This scale independency allows us to flexibly *refine* or *aggregate* (parts of) the geographic data where required. Refinement on the one hand offers dynamic, problem-oriented geographical resolution to avoid unnecessary data collection and helps to deal adequately with data gaps and to zoom into areas of special interest. Aggregation on the other hand enables us to reduce complexity, to compare regions by abstracting data and to calibrate actually needed scales of data.

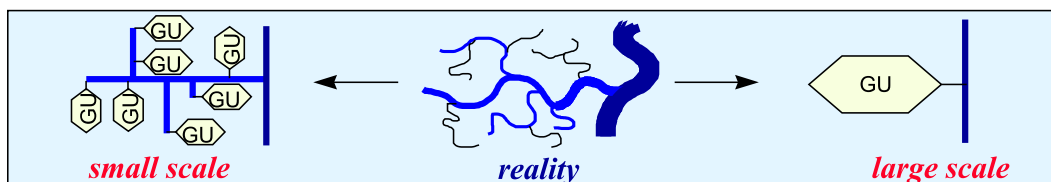


Figure 5.4: *Geographic units (GU): scale independent*

**Coordinates** The coordinates of a discharge site are obligatory. In the case of treatment works they describe the position of the actual plant and not the point at which the emission enters the river. The connection to the river will be established by explicit specification of the corresponding river segment. This enables provision of location information to the user who is supported in interpretation by offering the distance of the plant to the river and whether the emission takes place on the left or right bank.

**Population** For simulations of chemical ingredients in consumer products, the per capita consumption is usually available in mass per time. To properly estimate the release, the actual real population connected to a discharge is required. These numbers should be readily available from responsible environmental protection authorities, water authorities or water supply companies. For purely industrial discharges the population is zero.

It is not feasible to use population equivalents, because these numbers include industrial emissions based on a special selection and weighting of water quality parameters. For example, in Germany a per capita emission of 200 liters of waste water with an equivalent load of 60 g of biological oxygen demand (BOD) is assumed. Based on this, several population equivalent types are defined (DIN 4045 (12/1985); Römpp, 1997): Equivalents based on BOD (EGWB60), based on waster water emission (EGWW200), resulting sludge volume (EGWS2,0) and resulting dry sludge (EGWTS80). Across Europe several national standards are to be expected; for some countries variations between water authorities are even possible (e.g. in the U.K.). For most consumer substances no correlation with the standard water quality properties exists and hence population equivalents may reveal helpful background information, but are not required for chemical exposure assessment.

**Flows** Flows within the waste water and associated paths are measured and defined in several ways across Europe. For the data requirement definition a most common and practical selection is

presented here. Above all the most important value is the flow leaving the plant and entering the river network. The actual daily flow (ADF) will mean the average (measured) emission of a plant in  $m^3/d$ .

In many cases consented maximum emissions are available. Such values are only variable with the consenting interval and do not necessarily represent the real emissions. For those sites for which no ADF is available the consented daily flow (CDF) is the best approximation, since the operators of waste water treatment facilities usually try to fill the consented flow.

The inflow of a treatment plant consists of three components: Runoff, non-domestic and domestic flow.

**Discharge Type** The type of a discharge is considered in the simulation with specific models to estimate removal efficiency. Usually the technological type of the corresponding waste water treatment plant is required (i.e. trickling filter plant, activated sludge plant), but the discharge type can be "direct discharge" (no chemical removal) as well.

Some sewage treatment plants are actually a combination of different technologies. A specific modeling of such situations is not feasible. A conservative simplification choosing the less efficient type is recommended, but for transparency the situation should be noted (see the *Name* below).

**River connection** Discharges are connected to the first point of the given segment which is to be specified with its ID. For an optimal representation of the actual river entry point, the river network digitizing or segmentation should already consider these points.

In principle, GIS routines (distance measures) can be applied to find out the most reasonable stretches. These methods are automatic but always require human plausibility control.

**Name** The only purpose of the names is to support user orientation and interpretation as well as reporting. The names need not to be unique and should contain further information or hints when necessary.

### 5.1.5 Background maps

Though not used in the simulation models, background information is important for the final end user system. They allow visual orientation and plausibility control as well as aiding interpretation of simulation results, which is carried out by the user.

Different types of background information can be provided: raster landcover maps, vectorized information (geographic objects) on e.g. soil types and land use. Additionally, semantically related (temporal) information can be prepared such as monitoring sites with attached measured time series.

## 5.2 Final automatic data processing

The final data processing requires syntactically and semantically correct source files of the files ".drn", ".rna", ".dsd", ".cbp" and ".bgd" as described above. The whole processing with its subsequent steps is managed by the main program *greater-pre-processing.py*.

This part of the data processing is, in principle, not dependent on the required simulation system, though it does simplify the simulation system and user environment developed within the framework of GREAT-ER. The simple tabular structures allow the easy extension of the data files for adaptation to any other comparable simulation system.

The data to be generated can be divided into two groups: geographic data and the corresponding attribute data. The geographic data form the basis for visualization and geo-referenced data processing. These elements (cf. points, lines and polygons) are associated with attribute data via unique ID's. Their interconnection is based on the same ID reference.

Processing of the background data (".bgd" file) is not related with the main processing due to its special task to support the user. It is not discussed further in this document.

### 5.2.1 Geographic data

The establishment of geographic data consists of two processing steps (figure 4.5). First, the geographic elements (their ID's and coordinates) are extracted from the files in the pre-defined formats and converted into another format that can be handled directly by a GIS that handles the Shapefile format.

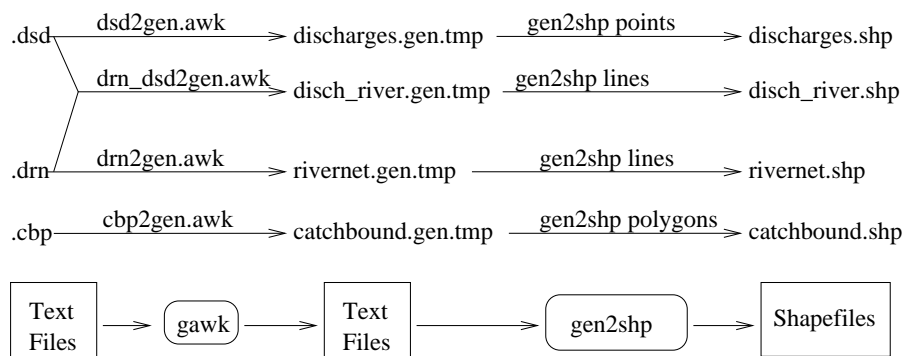


Figure 5.5: *Command sequence for automatic processing of geographic data*

A straightforward conversion is executed for the two digital maps: discharge sites (".discharges.shp") and river network (".rivernet.shp"). For the boundary of the catchment (".catchbound.shp") a further attribute is appended from the datafile "catchments.txt": the full name of the catchment.

The connection lines between discharges and corresponding river segments are computed using information from the ".dsd" and ".drn" files. A special shapefile is created (".disch\_river.shp"), which provides visual information on where the discharge is connected to the river network.

## 5.2.2 Attribute data

While the attribute data are being processed (figure 4.6), the three main data files (".dsd", ".rna" and ".drn") are first joined and then create the primary attribute files for river segments ("river.att") and discharges ("disch.att") as well as the secondary attribute files for treatment plant types ("wwtp.att") and river classes ("rivclass.att"). The two secondary files are (currently) static and basically describe generic treatment plants and rivers.

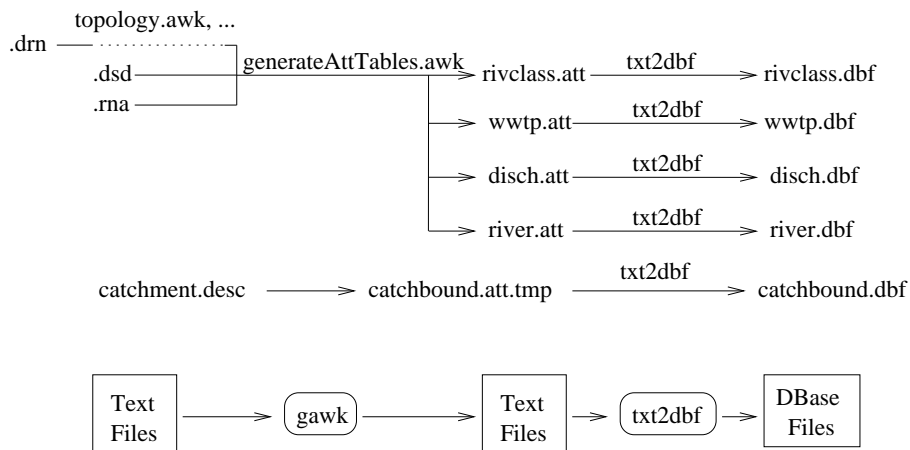


Figure 5.6: Command sequence for automatic preparation of attribute data

In the final processing step, text based tables are converted into DBase format. The purpose of this is to optimize data management within the visualization tool.

## 5.2.3 Core algorithms

Several data processing steps consist of simple routines (e.g. format conversions). They are not explicitly explained here. In this section the core problems of data processing are discussed.

### Creation of River Stretch Sequence

The information about the logic sequence of single river segments plays an essential role for simulation models. A simulation model must be able to *walk* down from any source to the final mouth. Hence, each stretch must offer information (the ID) about its successor. This purpose is served by a simple two-column table `fromStretchID, toStretchID`.

The ".drn" files, if semantically and syntactically created as described above, contain the topology information, but coded in the given coordinates. The arc-node model is used to convert the topology to the coding based on StretchIDs. Building the arc-node model from a ".drn" file associates all segments with IDs of the corresponding "from-node" and "to-node" to describe their direction. Consequently, the two-column tables `fnode, StretchID` and `tnode, StretchID` can be extracted directly from the arc-node model ("topology.awk"). Joining these two tables by the node ID and then omitting the node ID results in

the two-column table `fromStretchID, toStretchID`. In both columns IDs may now occur multiple times due to confluences and bifurcations. To create a table where the `fromStretchID` is a unique identifier, the `toStretchIDs` are joined up into a (space character divided) list. The resulting two-column table `fromStretchID, toStretchIDlist` is a straightforward representation of the downstream topology. Analogously, an upstream topology table `toStretchID, fromStretchIDlist` can be created starting with the `fromStretchID, toStretchID` table and exchanging the position of the two columns.

### Creation of Binary River Network Topology

Fast and straightforward access for any algorithm walking up or down the river network is realized using simple data tables. The minimum number of columns to describe any river network topology is four. Demanding one column being a unique segment ID and also allowing only exactly one ID in any field, virtual segments need to be added to grant topologic consistency (e.g. confluence of three streams at one point). An additional column finally describes the segment type (listed in table 3.1). This is needed to correctly interpret the content of the other columns. Extending the network by virtual segments will not increase but decrease the total table size because a further column would rarely be filled for natural networks where a confluence of two streams is usually the maximum. For artificial networks (e.g. sewer systems) the situation can be different.

Table 3.1 *Segment Types*

Type	Number of segments		Description
	Upstream	Downstream	
0	0	0,1,2	Source
1	1	1,2	Normal segment
2	2	0,1	Confluence
-2	1*	0,1,2	Bifurcation

\* which must be of type 1 with 2 downstream segments

Algorithms for walking on binary trees from the leaves to the root (cf. downstream) are typically implemented recursively starting with the root (cf. mouth). For exposure assessment in river networks the binary recursion has to be "post-order" which means performing an action for a segment after all upstream segments have already undertaken this action. Hence, the upstream direction is required for the two-column topology table.

The above-described tables for the river stretch sequence are the basis for building the binary topology. During the data loading routine, the highest segment ID is looked up. This is important to invent further ID's for virtual segments.

When all data are loaded, first bifurcation situations are searched for. The corresponding segments (type "-2") are associated with their neighboring segments. This is important in order to reduce the final topology processing to a one-pass computation (a single linear processing step). Next, the segment table is processed straightforwardly. Depending on the number of upstream and downstream segments, the type is then decided. Several special cases need further treatment i.e. insertion of virtual segments:

**(I) Confluence of three segments at one point** When exactly three segments are directed to the same point, a new (virtual) segment is inserted as shown in figure 4.7.

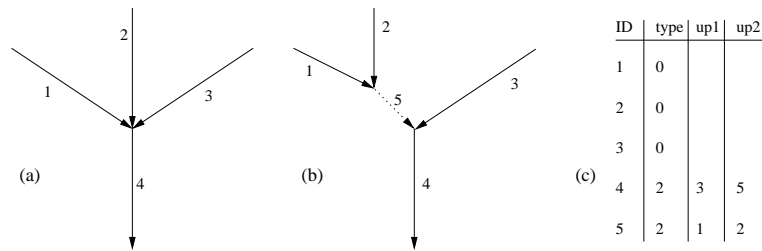


Figure 5.7: Resolving confluence of three segments (a) into binary representation (b). Numbers are stretch IDs. The table of binary network topology of (b) is (c).

The virtual segment obtains a length of 0. The ID does not appear in the geographic data of the river network and is neutral for the database operation "join". The simulation software must of course know how to treat segments with a length of 0: The results (e.g. chemical loads) must be transferred one-to-one to the next downstream segment.

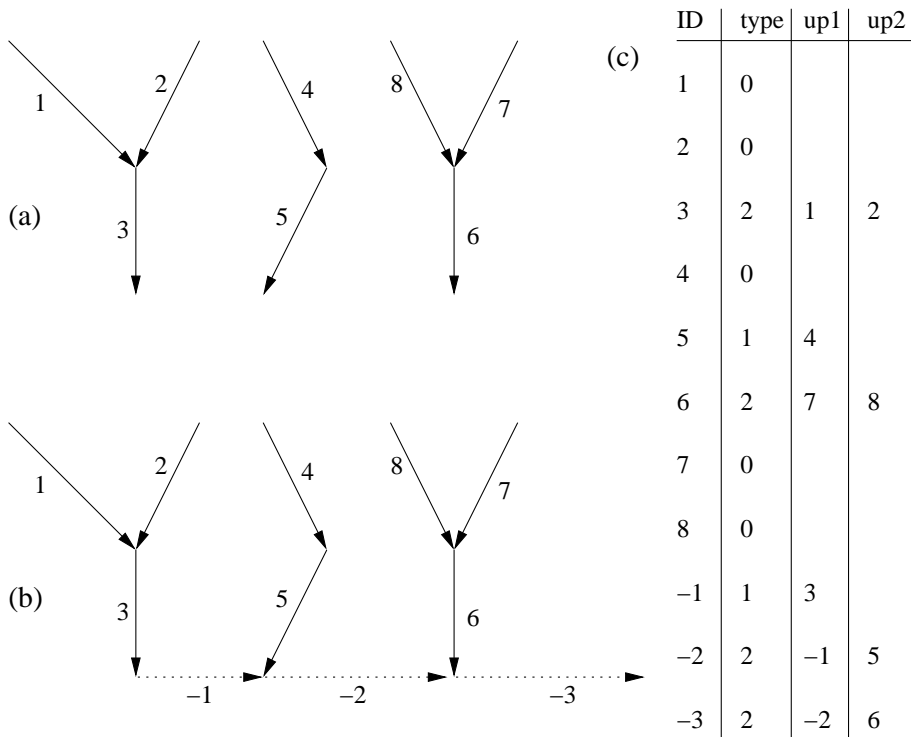


Figure 5.8: Resolving multiple end segments (multiple catchments) (a) into one catchment (b). Numbers are stretch IDs. Table of binary network topology of (b) is (c).

**(II) Several end segments** If several catchments are joined (e.g. to cover an entire island) the problem of multiple start segments (mouths) occurs and needs to be incorporated into the topology. The solution is a linear interconnection with virtual segments. By definition all "ocean segments" are attached with negative ID's.

In the example shown in figure 4.8, the lowest ID is -3 and it is the new starting segment for the resulting catchment. The ocean segments influence neither visualization nor simulation.

**(III) Bifurcation** For bifurcation situations both neighbours are of the type "Bifurcation" (figure 4.9). Field up1 will contain the ID of the upstream segment and field up2 will contain the ID of the neighboring segment.

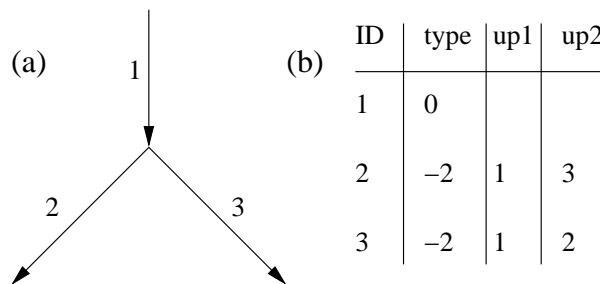


Figure 5.9: Handling of bifurcations (a) in the binary presentation (b).

**(IV) Unconsidered situations** Some situations may occur in the digital river network, but are unlikely to happen in reality for natural catchments. In practice it is more likely that wrong digitizing or another error may cause the situation. Such situations are not considered in the presented methodology though it is possible to resolve them with further virtual segments or additional definitions.

**(IV.a) Multiple confluence** More than three segments are directed to the same point (figure 4.10a). This situation could be managed similar to the confluence of three segments using virtual segments, but from a hydrologic point of view this situation is most unlikely and the chance of using wrong base data is much more probable.

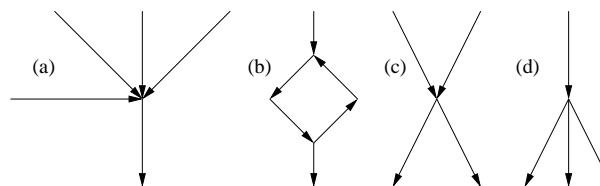


Figure 5.10: Unconsidered situations: Multiple confluence (a), crossing (b), circle (c) and multiple bifurcation (d).

**(IV.b) Crossing streams** Both, a confluence and a bifurcation take place at one point (figure 4.10c). Such a crossing is unlikely. Furthermore, a chemical fate model would need additional

information to adequately deal with such a situation (what fraction of which upstream segment goes into which downstream segment?).

**(IV.c) Circular flow** The segment sequence forms a ring (figure 4.10b). Building a ring, a river network is in topological terms not a directed graph. The applied simulation system is not capable of dealing with this situation. Such circles may occur, for example, in estuaries where the flow direction changes over time following a certain probability distribution.

**(IV.d) Multiple bifurcation** Flow separation of one segment into more than two segments (figure 4.10d). This situation is again unlikely from a hydrological point of view. An error in the base data is to be supposed.



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