**Simcat 15.7**

**The SIMCAT Manual**

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| --- |
| **Author’s notes:** |
| Items coloured ...... need attention ... |
| Items coloured ...... or ...... etc are new ... |

# AN INTRODUCTION TO SIMCAT

## A brief description

### SIMCAT is a mathematical model that calculates the quality of river water throughout a catchment. You can use SIMCAT to assess threats to water quality and to plan action to improve or protect water quality.

Increasingly the data files for SIMCAT are being produced by data bases and mapping systems such as SAGIS[[1]](#footnote-1).

### SIMCAT calculates summary statistics of water quality such as annual means and percentiles. It deals properly with the need to use standards defined as such statistics[[2]](#footnote-2).

### SIMCAT also calculates the effect of the statistical uncertainties associated with data, and it assesses compliance with standards.

### At any points in the catchment SIMCAT breaks down the pollution into contributions from all the different types and from any or all of the upstream discharges and sub-catchments. This helps decide where to act in order to protect water quality.

### SIMCAT has a feature, gap-filling[[3]](#footnote-3), which calculates the amount of pollution not accounted for. But few people use this.

### Chapter §**B** describes SIMCAT's data and how these are arranged in a data file. You will need this if you want to use a text editor to change the data.

### Background details are provided in the following chapters:

|  |
| --- |
| §**Q** (page 136) describes how SIMCAT works |
| §**R** (page 144) gives details about river chemistry |
| §**S** (page 147) discusses correlation |
| §**T** (page 148) deals with confidence limits |
| §**U** (page 150) is a brief background to the SIMCAT software |

### You do not need to read these appendices in order to use SIMCAT.

### §**V** (page151) is a copy of a SIMCAT data file and §**W** (page 162) gives copies of some of the shorter output files. (You can generate the copies of the longer output files by running SIMCAT with one of the data files provided for you when SIMCAT is loaded).

## Running SIMCAT

### When SIMCAT is first loaded it will, by default, finish up in a folder called C:\PROGRAM FILES\SIMCAT. The SIMCAT executable is called SIMCAT157.EXE. You can run SIMCAT by clicking on this.

### It is best to set up an icon (a “shortcut”) on the computer screen and to create special folders for your SIMCAT data and output.

### To run SIMCAT you "click-on" the SIMCAT icon. The first SIMCAT window is then displayed. To use a data file, you have already set up, click-on RUN THE SIMCAT MODEL on SIMCAT’s menu bar.



### You then select what you want SIMCAT to do. To do this click-on “BASIC Run” on SIMCAT’s menu bar. You can then “browse” to the folder you want and click-on a SIMCAT data-file.

### (When you install SIMCAT on your computer, you can get examples of sets of data such as EG.DAT).

### 

### You will then see the output scrolling up the screen.

### SIMCAT will also send messages to the screen and place them in its output files (§**W**) if it thinks there might be mistakes in your data-file.

### When the run has finished, you can return to the main SIMCAT window. You might then want to inspect the results in one or more of SIMCAT's output files.

### The SCN file is a good place to start. You can print the files or display them onscreen using things like NOTEPAD.

### You can "click-on" REPORTS on SIMCAT’s main menu and print the output as customised reports (§9). SIMCAT’s standard output files (§4) can also be printed from the menu under REPORTS, by clicking on PRINT TEXT FILE.

### You might want to click-on GRAPHS on SIMCAT’s main menu and display the output as plots of water quality along the river length. SIMCAT also creates files that can be picked up and worked on by EXCEL. You might prefer this option as a way of displaying results.

### A copy of a data-file is at §**V**. This is the file called EG.DAT. It is provided with your copy of SIMCAT or can be sent to you by e-mail. You will see that the file contains lines of text explain­ing the data.

EG.DAT was created from a make-believe river as a device set up to illustrate SIMCAT’s types of data.

You will want to create data-files for your own rivers. You can use a text editor to change EG.DAT (or any other SIMCAT data files you can get hold of. Hundreds exist).

Increasingly the larger data files for SIMCAT are being produced by data bases and mapping systems such as SAGIS[[4]](#footnote-4).

## Run Types 0 to 9

### Usually, for the first run with a new data-file, you will use Run Type 0 to test that the data have been assembled correctly. You may then need repeated runs (with Run Type 0) in order to complete a process of calibration (§5).

### There are other Run Types. These are:

|  |  |
| --- | --- |
| 0 | Basic run |
| 1 | Gap-filling for river flows |
| 2 | Use the gap-filled flows |
| 3 | Gap-filling for river quality |
| 4 | Use the gap-filled flows and quality |
| 5 | Perform Run Types 1 and 3 in sequence |
| 6 | Perform Run Types 1, 3 and 4 in sequence |
|  | BACKWARD calculations: |
| 7 | Set discharge standards to meet river targets |
| 8 | As 7 but with aspects of no deterioration |
| 9 | As 8 but assuming upstream quality is related to a classification system |

### SIMCAT stores the adjustments calculated by its own Gap-filling (Run Types 1, and 3) in two files called *filename*.FCL and *filename*.QCL. For the *What-If* Simulations (of Run Types 2, 4, 7, 8 or 9), the adjustments in these files are picked up and applied if the files exist. Otherwise the simulations will run without the Gap-filling adjustments.

## SIMCAT’s output

### The names of some of the files are shown below. The full set is listed at (§**W**). The term 'filename' is part of the name of the data-file. For the test data, EG.DAT, the output files will be called EG.OUT, EG.SCN, etc. Files of the type, CSV (comma-separated values), are those that can be imported into data-bases and spreadsheets such as EXCEL.

### These files will be created in the folder that holds as your SIMCAT data file.

|  |  |
| --- | --- |
| a copy of the output displayed on the screen | *filename* .SCN |
| the detailed output | *filename* .OUT |
| a shorter version of the detailed output | *filename* .OWT |
| a report on effluents | *filename* .EFF |
| a report on loads | *filename* .LOD |
| sources and sinks of pollution | *filename* .SUM |
| compliance with river quality targets | *filename* .TGT |
| apportionment of loads from discharges | *filename* .ALD |
| apportionment of loads from sub-catchments | *filename* .ALC |
| apportionment of contributions to concentrations | *filename .*ACD |
| apportionment of contributions to concentrations | *filename .*ACC |
| data that can be taken up into a Geographical Information System and used to display SIMCAT’s results as maps | *filename-GIS1* .CSV |
| natural purification and diffuse pollution | *filename* .PUR |
| errors or peculiarities in data uncovered by SIMCAT | *filename* .ERR |
| classification of river water quality | *filename* .WFD |
| a copy of the input data | *filename* .INP |
| data on effluents and controls needed to meet river targets | *filename*-EFF*.*CSV |
| data on determinand 1 | *filename*-*D1.*CSV |
| data on determinand 2 ... etc | *filename*-*D2.*CSV |
| apportionment for determinand 1 ... etc | *filename*-*P1.*CSV |

## Calibration

### Having completed a successful run under Run Type 0, you might look at places where SIMCAT compares its calculations of river flow with estimates based on measurements made at gauging stations or estimated from mathematical models.

### You might look also at places where SIMCAT compares its calculations of river quality with results recorded at monitoring stations. These checks may indicate errors and omissions like misplaced tributaries or discharges. It may also point to gaps in knowledge about the sources of flow or pollution.

### Having corrected any errors, you might want to introduce diffuse inputs or losses of flow in order to secure a better match between SIMCAT's results and the data based on the measurements made at river flow gauges (§32). Ideally you should continue with this process of calibration until you have good agreement.

### Having secured agreement with river flows you should turn your attention to river water quality, looking to match data recorded at monitoring stations. You might want to introduce natural purification or add diffuse gains of pollution.

### SIMCAT calculates the statistical confidence that its results match those recorded at monitoring points. These will eventually affect the confidence that particular types of action will provide particular improvements to water quality.

The process of calibration can be time-consuming, especially for big catchments. The discovery of a late error in an upstream part of the model may mean you have to repeat much of the process all over again.

But it is important to secure agreement with the recorded data on flow and quality in order to avoid errors in making decisions on how to protect water quality. To help with the process of calibration, SIMCAT provides a form of automatic calibration, Gap-filling.

## Gap-filling

### Run Types 1-4 automatically invent or remove flows or pollution so that perfect agreement is secured with the data recorded for flow gauges and monitoring stations (or anywhere else). The added and removed loads are displayed with the contributions of things like sewage works and diffuse pollution. This means that they display the implications of such uncertainties in identifying action to clean up rivers.

Gap-Filling is also helpful if you do not need to quantify gaps and surpluses of load implied by the contents of your data-file and if you need quick or preliminary results. And the information may help track down the causes of such gaps and excesses.

Gap-filling is not a replacement for calibration so much as a check on its success. It is a process for showing the extent to which SIMCAT’s results show a complete picture for all sources and sinks of flow and quality. It is foolish to report, for example, that 50% of pollution is from industry in cases where large sources and sinks remain unaccounted for.

Gap-filling is also limited to adding sources and sinks to the section of river you have defined as a Reach in SIMCAT’s data (§32) – the section of river that contains the values of flow and quality you wish to see reproduced.

### Once you are happy with your results from Run Type 0 you might want to use Run Type 1 (Gap-filling for river flows). To do this you repeat the run but choose Run Type 1. SIMCAT then invents whatever sources and sinks of river flow are needed to achieve perfect agreement with the results obtained at sites like gauging stations (§32).

### Once you are happy with the calculations of river flow you would use Run Type 2 (Use the Gap-filled flows) to inspect once again places (in *filename*.SCN, or graphically) where SIMCAT compares its calculations of river quality with measurements made at water quality monitoring stations (§152). These checks will indicate errors and gaps in the quality data.

In the process of Gap-filling the additions and losses of flow are restricted to the Reach in SIMCAT that contains the point whose flow you wish to estimate.

### Next you might want to introduce natural purification or diffuse gains of pollution or dilution. Do this within Run Type 2. You might do this in order to secure a better match between SIMCAT's results and the data based on the measurements made at Monitoring Stations (§152).

### Next you might want to use Run Type 3 (Gap-filling for river quality). Under Run Type 3 SIMCAT invents the sources and sinks of river quality which are needed to achieve perfect agreement with, say, the results obtained at Monitoring Stations (§152).

### After this it is then a good idea to use Run Type 4 and to inspect once again places (in *filename*.SCN, or graphically) where SIMCAT compares its calculations of river quality with measurements made at monitoring stations. These checks may also indicate errors and gaps in the data.

In its subsequent outputs on apportionment of sources of pollution SIMCAT lists separately those added by SIMCAT’s automatic Gap-filling. It is important to take these gaps into account when deciding action to improve water quality. It can be foolish report that 70% of the load in the river is due to discharges if, within this, you have made no estimate of the “gaps”.

### Run Type 6 executes Run Types 1, 3 and 4, in sequence. It is risky to do this on a new model until you have gone through the above steps one at a time.

### SIMCAT stores the adjustments calculated by Gap-filling (Run Types 1, and 3) in two files called *filename*.FCL and *filename*.QCL. For the *What-If* Simulations (of Run Types 2, 4, 7, 8 0r 8), the adjustments in these files are picked up and applied. Otherwise they will run without the Gap-filling adjustments.

## What-if

### Once you are happy that your model is adequately calibrated, you can start to forecast the effects of possible fu­ture developments like new laws, and changes to discharges and abstractions. You do this by altering some of the data (discharge quality, for example) and repeating Run Types 0 or 4.

Run Types 7, 8 and 9 calculate automatically the actions to meet river targets specified in your data file. This can include the calculation of legal targets for effluent discharges that are needed to meet river quality standards. (§57 and §58).

### Run Type 7 constrains a discharge standard within values you define as “Best” and “Worst” (§57 and §58). Run Types 8 and 9 do not allow the calculated standard to exceed the current quality of the discharge.

### Type 9 is the same as 8 but replaces SIMCAT’s calculated upstream river quality with a value set at a point within the target class for, say, the Water Framework Directive. The target class is defined as part of the Reach data (§77).

### In mode 9, the default point in the class is the lower limit for the class plus 50% of the class width. This value of 50% can be changed within the General Data (§77).

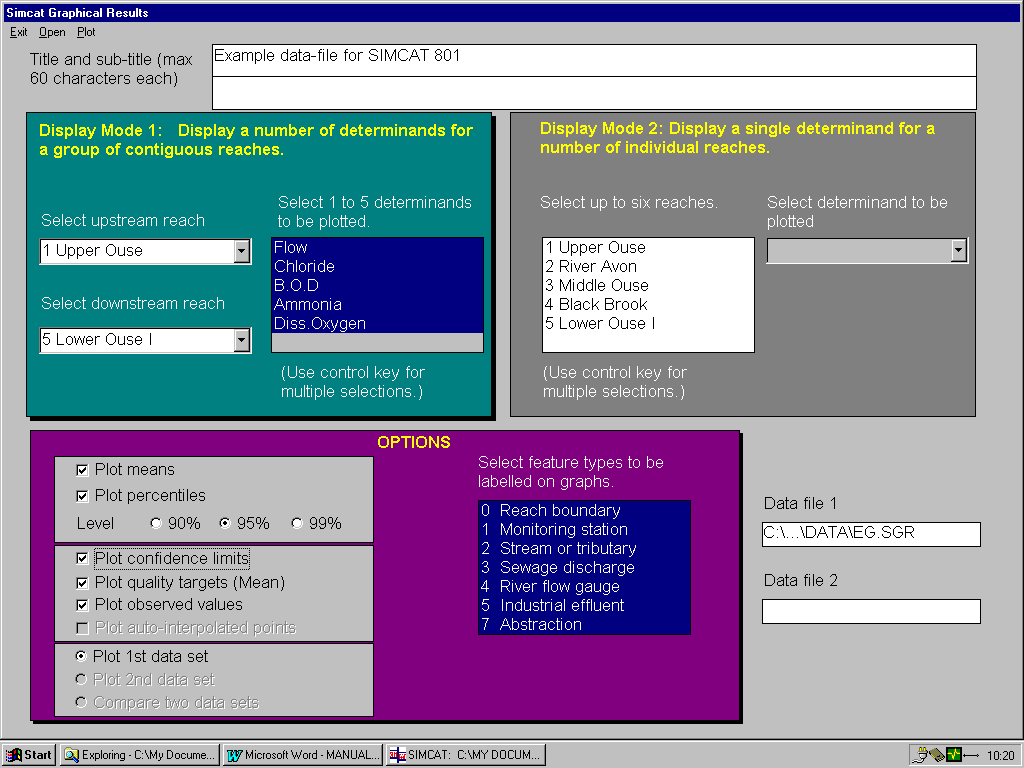
### SIMCAT stores the adjustments calculated by Gap-filling (Run Types 1, and 3) in two files called *filename*.FCL and *filename*.QCL. For the *What-If* Simulations (of Run Types 2, 4, 7, 8 or 9), the adjustments in these files are picked up and applied. Otherwise they will run without the Gap-filling adjustments.

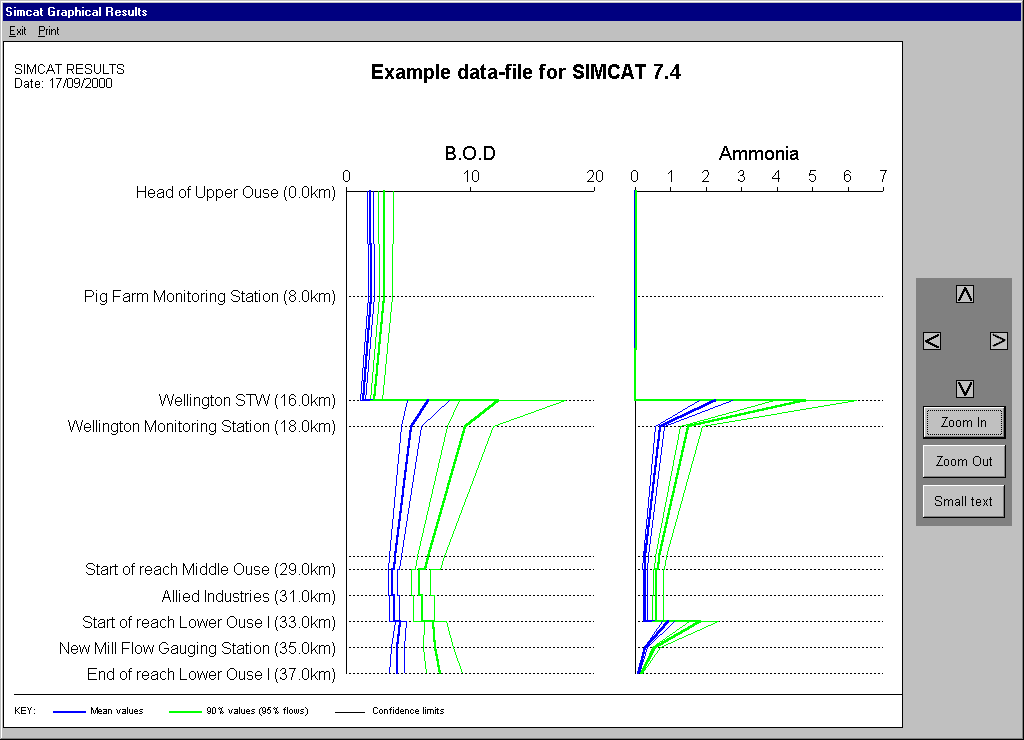
## Graphical output

### Once the model has been run, graphical output can be selected using Graphs on the menu bar of the Start-up Screen. (You may prefer to upload SIMCAT’s output into devices such as EXCEL).

### There are options to display the 90, 95 or 99 percentile concentrations, as well as loads and river quality standards.

### Often you will want to set up duplicates of a SIMCAT data file and change one of them in order to display graphs that compare, for example, river quality before and after changes to discharges.





## Reports

### Once you have run the model, you can look and print the output files produced by SIMCAT using systems such as WORDPAD.

### You can also obtain items using Reports on the menu bar of the SIMCAT. This deals with three types of report:

* output, selected by you, that is sent to the printer (by selecting ‘Print’ on the menu bar)
* output, selected by you, that is sent to a Comma Separated Variable (CSV) file. This is suitable for reading into a spreadsheet such as EXCEL. You take this option by selecting ‘Spreadsheet file’ on the menu bar. The will be given the name *filename*.CSV for a SIMCAT data file *filename*.DAT

### 

### The options for customising the report are similar to those available for graphs and you must select what you want before selecting the ‘Print’ or ‘Spreadsheet file’ options. The options define the number of columns and rows that will be displayed on your report. The columns are defined from the options shown below:

* all or a selected set of the determinands
* the mean, 90, 95, 99 percentile values
* the upper and lower confidence limits
* the observed values
* the quality targets

### As you select or deselect options you will see an indication on the screen of whether the report will be printed in Portrait or Landscape or whether the number of columns you have selected makes the output too wide to print. (Note that, if you select the ‘Spreadsheet file’, any number of columns can be selected.)

### You define the rows from the options:

* show all or a selected subset of the reaches
* show the results upstream of each feature (the default is just downstream).

### If the ‘Upstream’ option is not selected, there will be one line of output per feature and reach start or end; otherwise there will be two lines of output.

## Back-tracking

### At points in the catchment SIMCAT calculates the load of pollution and breaks it down into contributions from different types of pollution. It also breaks the total load down into the contributions from all and any of the upstream discharges.

A parallel feature breaks the total load into contributions from any and all of the upstream sub-catchments. This includes the contributions from discharges and diffuse pollutions within each sub-catchment.

Such a breakdown of the total load indicates the important sources of risk or damage but a breakdown of load may not tie in exactly with breakdowns of the contributions to failed standards that are expressed as concentrations. This is especially the case for intermittent additions of pollution or standards expressed as 95 or 99-percentiles.

Certain types of breakdowns of contributions to failed concentrations can now be done in SIMCAT. These devices provide improved estimates of where to act in order to protect water quality.

## Running lots of models in one go – Batch Runs

### There is an option by which any number of models can be run as a set, one after the other. This is called Batch Mode. You can use Batch Mode through a menu item on SIMCAT’s Start-up Screen. This is titled “Batch Run” (§**P**).

## Preparing data for SIMCAT

### Details the structure of a data-file, and instructions for its assembly, are given in §**B**.

### You will need to have a stab at defining the upstream and downstream boundaries of your catchment. At the same time, you should list the significant inputs of pollution.

### You will also need estimates of the mean, standard deviation and number of samples for the quality of rivers and discharges. And you will need estimates of the mean river flow and 5-percentile low river flow at points in the catchment such as river flow gauges.

### Get a map of your catchment. Mark the positions of the discharges (and other developments) which may affect river quality. Mark the **upstream boundaries** of the river and its tributaries. Fix these upstream of the discharges that you have already marked on the map.

### The **upstream boundaries** should be placed either where data on river flow and quality exist or where they can be assumed or calculated.

### Next, define the **downstream boundary**. Then mark any tributaries which receive no discharge from any of your marked discharges.

### All these assignments are provisional. It is simple to change them later. You can add extra discharges and extra tributaries if you decide later that they are significant.

## Automatic production of data for SIMCAT by SAGIS

### Increasingly data files for SIMCAT can be produced using GIS systems such as SAGIS. It may be that someone else has already created data files for the catchment you wish to model.

# SIMCAT DATA FILES

### When you set up the data for SIMCAT you create a **SIMCAT data-file**. We shall use a simple example of a data-file called *EG.DAT*. A version of something like this is usually delivered with the version of SIMCAT that was set up for your computer or can be sent to you via e-mail. A copy of this file starts at §**V**.

### It can be wasteful to seek high precision in all the data. It is best to work up a mix of what is to hand, estimate the rest and start to run SIMCAT to produce results. The results will help show where more precision will help and where it is not needed.

## Defining the reaches

### A key part in setting up data is the defining of what SIMCAT defines as **Reaches**. These are lengths of river that have the sources of pollution you are interested in. Such sources, along with other items such as monitoring stations, discharges, abstractions and flow gauges are referred to by SIMCAT as **Features** (§16).

### Mark an upstream boundary on your river and trace downstream until you come to a confluence with another river. Check whether the new river has any discharges or other significant features that you may want to model to improve downstream river quality. If there are none, carry on downstream to a con­fluence with a river that does have such significant features. Mark this con­fluence. The length between the marks is a **SIMCAT Reach**.

### Proceed downstream in the same way, defining more Reaches as the lengths of river between successive confluences. Then go back to any other upstream boundaries and repeat the exercise. For the time being you can ignore tributaries which have no marked discharges. You might want to model these as **Features** (§16).

### At this stage you could sketch a map of the catchment. Mark the Reaches and the discharges. You will need to obtain the length of each Reach.

### Give each Reach a code name that you will be able to recognise in SIMCAT's output (use up to 16 characters). The picture below (§15) illustrates a catchment with five Reaches.

## Reaches in a Catchment



## Features

### The next stage is to get lists of all the discharges, flow gauges and monitoring points. These types of things are called **Features**.

### A **Feature** is a point on a river which affects or which is in­fluenced by river flow or river quality. Some of the types of Feature in­cluded in SIMCAT are listed below but the details are discussed in §**K**:

* river quality monitoring points
* streams
* continuous point discharges
* intermittent discharges
* mine waters
* river flow gauges
* abstractions
* river flow regulation points
* upstream river boundaries
* bifurcations
* start points for many forms of diffuse pollution
* end points for these forms of diffuse pollution

### In the above, **Streams** are rivers which are not important enough to be classed as **Reaches** (perhaps because they receive no significant discharges).

### You must place your Features on the Reaches in the correct geographical sequence. Work out the distance to each Feature from the head of its Reach. Give each Feature a name that you will recognise in SIMCAT's output (use up to 40 characters).

### The information on Reaches and Features can be shown as a diagram (§15) or as a table (§17). These define the structure of the catchment. You will need to augment this with data on water flow and quality. These are described later.

## Reaches and Features in the Example Catchment

|  |  |  |
| --- | --- | --- |
| (a) Reaches | | |
| Code Number | Name of Reach | Length (km) |
| 1 | Upper Ouse | 14.0 |
| 2 | River Avon | 10.0 |
| 3 | Middle Ouse | 2.0 |
| 4 | Black Brook | 10.0 |
| 5 | Lower Ouse | 4.0 |
| (b) Features | | |
| Reach Code Number | Name of Feature | Distance from Head of Reach (km) |
| 1 | Head of River Ouse | 0.0 |
| 1 | Pig Farm Gauging Station | 4.0 |
| 1 | Pig Farm Monitoring Point | 6.0 |
| 1 | Ouse Stream | 8.0 |
| 1 | Wellington Sewage Treatment Works | 9.0 |
| 1 | Wellington Monitoring Point | 9.0 |
| 2 | Middle Ouse Monitoring Point | 14.0 |
| 2 | Head of River Avon | 0.0 |
| 2 | Brickton Sewage Treatment Works (old) | 3.0 |
| 2 | Brickton Sewage Treatment Works(new) | 2.0 |
| 2 | Valley Bottom Monitoring Point | 9.0 |
| 2 | Valley Bottom Gauging Station | 9.0 |
| 3 | Allied Industries' Discharge | 1.0 |
| 4 | Head of Black Brook | 0.0 |
| 4 | Black Brook Monitoring Point | 2.0 |
| 4 | Appleford Sewage Treatment Works | 3.0 |
| 5 | New Mill Monitoring Point | 1.0 |
| 5 | New Mill Flow Gauging Station | 1.0 |
| 5 | Tenply Monitoring Point | 6.0 |
|  |  |  |

## Setting up the data-file

It is often simplest to start with an existing data-file and change it using a text editor. Data-files such as EG.DAT contain information that will help with this. It may be that your data-file can be produced automatically from a GIS mapping system such as SAGIS.

## Using the Text Editor to Set up Data

### The data-file consists of Sections. Each Section and all the data within it are described below. Each Section is said to be a Data-set.

|  |  |
| --- | --- |
| General | §**D** (page 26) |
| Determinands | §**E** (page 34) |
| Reaches | §**F** (page 43) |
| River Flow | §**G** (page 51) |
| River Quality | §**H** (page 60) |
| Discharge Flow & Quality | §**I**  (page 69) |
| River Quality Targets | §**J** (page 77) |
| Features | §**K** (page 80) |

### You should start with the section on **Reaches** (§**F**). A schematic map or table should provide most of the information (§15 or §17). At this stage, the values required in some of the columns, such as a number that identifies sets of data on flow or quality can be marked as some sort of code such as a question mark and filled in later.

### Next you should work on the **Features** (§**K**). Here too, the values required in some of the columns can be marked as some sort of code.

### After this you could start to work on the data-sets for the flow and quality of rivers and discharges. (These data-sets consist, for example, of summary statistics like the mean and the standard deviation).

### As each data-set is entered you can give it a code number and re­place a question mark in the data for the Reach or Feature with this code. Gradually, you will replace all the question marks with numbers.

### You might want to enter River Quality Targets for Features. Finally, fill in the General Section (§**D**).

### The SIMCAT data-file allows you to enter comments at any point (§20). The option to add comments can be used to enter notes and reminders, or to give details of the source of data and any assumptions you have made.

# STRUCTURE OF THE DATA FILE

### The first few lines of the Example Data File are shown at the end of this section (§**C**). The full data-file is at §**V**.

## Comment Lines

### The table at §**C** illustrates the use of **Comment Lines**. These are lines which begin with ====. Any text which follows ==== is an ex­planatory note. Comment lines do not affect the running of SIMCAT. Only lines without the ==== are genuine SIMCAT data.

### You will see that the Example Data File has lots of comments. These are provided so that the data-file comes with instructions defining the meaning of the variables. You should find this helpful if you opt to use your Text Editor to create or change a data-file. You can delete the comments if they get in the way.

## Sections

### The SIMCAT data-file is split into **Sections**. The sequence in which the Sections are assembled is up to you. A procedure was suggested above.

### The eight **Sections** in the data-file are listed above (§19) and are discussed in detail later in this document.

### A line beginning with \*\*\*\* is used to mark the **end of a Section**. The only section where this is not used is the first or **General Section**.

## Text and Numbers

### You can see that **Text data** like the names of Determinands, Reaches and Features are always contained within single quotes, as in:

### 'Wellington STW '

### (You should avoid using single quotes as part of the names you give to Determinands, Reaches and Features).

### For data expressed as numbers the data-file must leave at least one blank space to separate different entries, as in the following four num­bers:

0 0 10.0 50.00

### **Integers** are whole numbers written without any decimal point, as in the four values:

11 14 18 -45

### All the values which are written as integers in the Example Data File are required as integers for SIMCAT. You should try to keep them as integers in your data files.

## Initial Comment Lines from the Example Data File

**======================================================================0**

**======= Test data file for SIMCAT: EG.DAT (25/11/18) =====0**

**======================================================================0**

**======= Lines beginning with '====' are notes explaining the data 0**

**======= Such lines are not used by SIMCAT and may be removed from 0**

**======= the data-file without affecting the calculations ... 0**

**======================================================================0**

**======= The following sets of data (Data-Sets) are required: 0**

**======= [1] General 0**

**======= [2] Determinands 0**

**======= [3] Reaches 0**

**======= [4] River Flow 0**

**======= [5] River Quality 0**

**======= [6] Effluent Flow and Quality 0**

**======= [7] River Quality Targets 0**

**======= [8] Intermittent Discharges 0**

**======= [9] Features 0**

**======================================================================0**

**======= For sets [4],[5] and [6] extra data will needed if the more 0**

**======= unusual distributions are selected. These will take the form 0**

**======= of extra data files called ANYNAME.NPD. 0**

**======= 0**

**======= In the following notes the term, River Chemistry, refers to 0**

**======= the effect of the fixed set of Rate Constants defined below 0**

**======= in the Data-Sets for Determinands and Reaches. These can be 0**

**======= used with the equations written into SIMCAT to model changes 0**

**======= in river quality. 0**

**======================================================================0**

**======= A descriptive title follows ... 0**

**======================================================================0**

# GENERAL DATA

### The General Section is mainly a set of parameters which you use to control the running of SIMCAT. The Section from the Example Data File is given at the end of §**D**. Most of it is comments. The eleven lines of actual data are in **bold** type. We shall now go through each of these lines in turn.

## Description

### Remember that lines beginning with ==== are comments and will not be treated as data by SIMCAT:

|  |
| --- |
| ===== A descriptive title follows . . . |

### You can use a descriptive title to identify the catchment or the reason for using SIMCAT. For example, in §44:

|  |
| --- |
| River Ouse ... set up by Tony Warn |

### In this and in later descriptions of data, each line of SIMCAT's data is encased in a yellow box, as in:

|  |
| --- |
| This is a line of SIMCAT's data . . . . |

## Switch for the Use of Monthly Data

### SIMCAT includes options to define separate data for each month in the year. Monthly results are also produced in the output

### The options date from times when certain types of data were available for each month and some users wished them to be part of SIMCAT’s data. Usually such data were loads of pollution from agricultural sources.

### In terms of the overall calculation, monthly data are seldom necessary. The full variability is fully and better represented by sets of annual data and the correlations between them.

Problems also occur when some data are assigned monthly structures but others are left with only their annual descriptions. In such cases SIMCAT can attempt to construct a monthly structure for river flows (§88) using assumed sets of hard-wired data on the relation between annual and monthly summary statistics. To impose this requirement set the following item to 1.

|  |
| --- |
| **1** …set to 1 to add the monthly structure to all annual flow data |

The monthly shapes will then be imposed even if there are no sets of monthly data (Types 5 or 8). This done by scaling annual mean flows by the following numbers:

|  |  |  |  |
| --- | --- | --- | --- |
| January | 1.9 | July | 0.3 |
| February | 1.6 | August | 0.4 |
| March | 1.4 | September | 0.4 |
| April | 1.2 | October | 0.8 |
| May | 0.6 | November | 1.2 |
| June | 0.5 | December | 1.8 |

The ratio of annual mean to annual 95-percentile low flow is preserved for each month.

Set to zero for this scaling not to happen. The value will be reset to 1 if data types 5 or 8 are subsequently detected in sets of data for flows or quality.

Set to a value of 2 to prevent scaling happening even if data types 5 or 8 are present.

## Set percentage of class limits for use in Mode 9

### Mode 9 is an option for Backward calculations. It calculates the discharge quality needed to achieve a downstream target (§3)

### Mode 9 also sets upstream quality equal to the percentage of the range between the upper and lower limits that define the target class. By default, this is 50%. To change this set a value between zero and 100 at this point in the DAT file.

|  |
| --- |
| **0** … percentage of class used in Mode 9 (the default is 50) |

## Switch for the Control of Output

### You can also exclude output to certain files from all Features which are not discharges:

|  |
| --- |
| **0** … set to 1 to exclude o/p for non-discharge Features |

## Switch for Mode (0 to 9)

### The next line defines whether SIMCAT will run in **Mean Mode**, **95-percentile Mode**, **90-percentile Mode** or **99-percentile Mode**. The Mode affects the output displayed on the screen while SIMCAT is running. Within SIMCAT itself all the summary statistics will tend to be calculated and written to SIMCAT’s output files.

|  |
| --- |
| **0** … set to 1 for Mean Mode; 0 for 95%ile; 2 for 90%tile; 3 for 99%tile |

### If your DAT file sets no definitions of the summary statistics used as standards for determinands then the Mean Mode is used to define one.

## Number of shots

### The next line of the data-file is used to define the Number of Shots to be used in Monte Carlo Simulation. You can use only 10 or 20 shots during the initial runs of a new data-file. This will speed up the detection of any errors you might have made in assembling the data. Later you can increase to a value of 500, up to maximum of 5,000.

|  |
| --- |
| **500**  … number of Shots (minimum is 5; maximum is 5000) |

If SIMCAT data contains type 5 or type 8 data for river or effluent flow or quality it will check whether the number of shots is a multiple of 365. If it is not the number is changed to a multiple of 365 (§85-§88).

## Temperature

### We shall see later that SIMCAT can be used to simulate river temperature directly. This option is often unnecessary and where not used a default value entered here is used instead.

### Tem­perature is used to adjust the rate of Natural Purification. The data entered here should correspond to the period of time used for other data on river quality, perhaps a period of three years.

Enter the mean, standard deviation and the correlation coefficient for the variation of temperature with river flow.

|  |
| --- |
| **11.2** **3 -0.6** … river temperature - mean, SD, correlation coefficient with river flow |

You can also just enter the mean. In this case, SIMCAT defaults to a standard deviation of 3.0 and a correlation coefficient of –0.6.

|  |
| --- |
| **11.2** … mean temperature of river water |

## Units of Flow

### This allows you to describe the units of flow as 4 characters enclosed in single quotes. You should then use the same units for all the flow data for rivers and discharges in the catchment.

|  |  |
| --- | --- |
| **'Ml/d'** … units of river and discharge flow (4 characters in quotes) |  |

## Switch for Diffuse Inputs of River Flow to Reaches

### If you set this variable to **1** you will switch into the calculations any diffuse input of river flow that you have defined for individual Reaches (§**F**). You will specify the amounts of flow added to individual Reaches in Section 69. The quality of the inflows made to each Reach will be specified in Section §70.

### You can also use this facility to build in diffuse losses of flow along the length of a Reach. The losses are modelled as if they were leaks through the bed of the river, and not as caused by evaporation. This means that river quality is unchanged when flow is lost (though the reduced flow will mean less dilution for downstream discharges).

### In the early stages of setting up the data you will find it in­structive to keep this variable at **0**. This will suppress the addi­tion of diffuse inflows to Reaches and show you the size of any shortfall in flow. You will then be better placed to check for er­rors in flow data for rivers and discharges and to decide the scale of any diffuse inflows.

### You will see later that you can also use **Features** to make SIMCAT add extra diffuse sources of flow and **pollution** to the river (§173). These latter additions will be superimposed on the types of inflows we are discussing here and they are not controlled by the Diffuse Sources Switch. (Any diffuse inflows entered as Features are not controlled by the Switch).

### Also, when you run SIMCAT you will see that you can let SIMCAT set up some or all of the diffuse sources in such a way that the river flows calculated by SIMCAT agree perfectly with the data recorded at flow gauging stations. This is **Gap-filling**.

### Gap-filling is superimposed on any diffuse inflows you specify through the use of the Diffuse Sources Switch and through the use of Features. With the Switch set to zero you can allow Gap-filling to account for all diffuse sources (or losses) not defined as Feature. With the Switch set to one, Gap-filling will only top up the diffuse sources already specified by the Switch and through Fea­tures.

## River Chemistry Switch

### Often you will need to assume that river quality improves because of something like **Natural Purification**.

### If you set this Switch to **1** you will make SIMCAT engage a set of equations within SIMCAT that describe Natural Purification. The parameters which define the effect of Natural Purification will be specified for individual Determinands later (§52); and there are options to set up parameters for individual Reaches. If you set this switch to zero, none of these defined parameters, nor any of the equations in SIMCAT will be applied.

|  |
| --- |
| **0** …set to 1 to include River Chemistry |

### In the early stages of setting up the data you should set this variable to **0**. This will suppress the application of River Chemistry and show you the size of any shortfall or surplus of pollution load. You will then be better placed to check for errors in data and to decide the scale of any Natural Purification.

### You will see later that you can let SIMCAT set up some or all of the Natural Purification in such a way that the river quality agrees perfectly with the data recorded at monitoring stations. This is **Gap-filling**.

### Gap-filling is superimposed on top of any River Chemistry you specify through the use of this Switch. With the Switch set to zero you can allow Gap-filling to invent all the sources or sinks of pollution needed to force SIMCAT's calculations to agree with the quality observed at Monitoring Stations. With the Switch set to one, Gap-filling will only mop up what is left after the application of River Chemistry already specified by the Switch.

## Switch for Interpolation

### In the early stages of setting up the data you should also keep this variable at **0**. The variable is used to produce more detail, especially for graphs.

### If the value is **0**, SIMCAT will calculate and output flow and quality only at Features. If the value is **1**, flow and quality is also calculated between your Features.

|  |
| --- |
| **0** …set to 1 for Auto-interpolation |

### This is done by automatically inserting hidden Plotting Points into your data. Interpolation can also be introduced by directly inserting Features called Plotting Points into your data-file (§162).

## SWITCHES.GPD – changing SIMCAT’s hard-wired switches

### The remainder of section §**D** can probably be skipped if you are new to SIMCAT.

### Some changes are available by the use of a special data file called SWICHES.GPD. If SIMCAT finds that this file exists in the same folder as your DAT file, SIMCAT reads it and “switches in” a variety of changes.

### The file is set out below. Each of the “switches” is then described below.

1 set up a master set of data based on the first run in a batch

0 force in the flow gap-filling against the flow data entered for the feature when set to 1

0 produce the huge GIS output files when set to 0 (over-write by global policy data)

0 produce full output if set to 0

0 no longer used

1 exclude BOD from classification if set to 1

0 exclude Phosphate from classification if set to 1

1 exclude Ammonia from classification if set to 1

1 exclude Dissolved Oxygen from classification if set to 1

1 apply corrections to bad data if set to 1

1.0 percentage impact used to remove a discharge from back-tracking

### These switches are examples that can be developed to provide other ways of managing SIMCAT more efficiently.

## Switch in master set of data in a batch run

The first entry in SWITCHES.GPD is useful if you are running a batch run of lots of DAT files and wish to see summaries of results across all of these. If this switch is set to 1, the first DAT file creates a master set of information that ensures consistency across all the others.

The purpose of this is to remove the need to edit dozens of DAT files to make them consistent. It was developed to provide national summaries for 50,000 kilometres across 20 regions.

## Switch to force in gap-filling of river flow

### The second entry in SWITCHES.GPD is a switch forces SIMCAT to calibrate river flows to match the sets of data specified at flow gauges even if the there is no separate request to do so in the actual data on Features in the .DAT file.

### For example, for Pig Farm Gauging Station, you may have specified that the set of river flow data is given by the value 7 in the following line of data for the Feature:

|  |
| --- |
| 'Pig Farm Gauging Station ' 4 1 2.0 **7** 0 0 0 0 |

### You may also request that SIMCAT use gap-filling to fit flow data at this feature to match that represented by data set number 7. To do this you may specify that the set of river flow data used to obtain a fit is given by a second value of 7 in the line of data for the Feature. (All this is set out in Section §154).

|  |
| --- |
| 'Pig Farm Gauging Station ' 4 1 2.0 7 0  **7** 0 0 |

### The switch described here forces in gap-filling even if the second value of “7” is not entered and the value of “0” left in its place.

## Switch to produce GIS output

### You may wish to suppress the formation of these huge files. Do this with this switch.

## Switch to produce full and detailed output

### Similarly, you can request that SIMCAT’s output files are made smaller.

## Switch no longer used

### No longer used.

## Switches to exclude determinands from classification

### Use this, for example, where you want the classification limited to include only Phosphate or Ammonia.

## Switch to correct bad or strange data

### With this switch SIMCAT looks for cases where water quality has been specified as a mean but with a zero standard deviation. A value is set for the standard deviation based on typical data.

### Similarly, cases are corrected where a 95-percentile low flow is set as bigger than the mean.

### A record of such changes is written to the file called *filename*.ERR (§**W**).

## Switch to change the number of back-tracked discharges

### This switch will be useful for huge models with thousands of discharges. It imposes a cut-off point for discharges that are to be back-tracked in terms of their impact throughout the entire catchment.

### This value is a percentage. It expresses the contribution of a discharge to the load represented the river quality target that applies at the point the discharge enters the system. So, if a value of 1.0 per cent is entered, SIMCAT excludes from back-tracking, a discharge which contributes less than 1 per cent of the river load that would be present if river quality were equal to the water quality standard.

### Where there are lots of determinands, the highest value is used to check for exclusion.

### SIMCAT produces warning messages if discharges are excluded and, at the end of the run, prints out a message if the maximum number of back-tracked discharges exceeds the value hard-wired into SIMCAT. It also displays the required value of the hard-wired limit. On receiving such a message, you can increase the percentage listed in SWITCHES.GPD to constrain the back-tracking.

## General Section of the Data-file

**======================================================================0**

**======= Test data file for SIMCAT: EG.DAT (25/11/18) =====0**

**======================================================================0**

**======= Lines beginning with '====' are notes explaining the data 0**

**======= Such lines are not used by SIMCAT and may be removed from 0**

**======= the data-file without affecting the calculations ... 0**

**======================================================================0**

**======= The following sets of data (Data-Sets) are required: 0**

**======= [1] General 0**

**======= [2] Determinands 0**

**======= [3] Reaches 0**

**======= [4] River Flow 0**

**======= [5] River Quality 0**

**======= [6] Effluent Flow and Quality 0**

**======= [7] River Quality Targets 0**

**======= [8] Intermittent Discharges 0**

**======= [9] Features 0**

**======================================================================0**

**======= For sets [4], [5] and [6] extra data will be needed if the 0**

**======= more unusual distributions are selected. These will take the 0**

**======= form of extra data files called ANYNAME.NPD. 0**

**======= 0**

**======= In the following notes the term, River Chemistry, refers to 0**

**======= the effect of the fixed set of Rate Constants defined below 0**

**======= in the Data-Sets for Determinands and Reaches. These can be 0**

**======= used with the equations written into SIMCAT to model changes 0**

**======= in river quality. 0**

**======================================================================0**

**======= A descriptive title follows ... 0**

**======================================================================0**

**Set of data to illustrate the SIMCAT User Manual ... EG.DAT**

**======================================================================1**

**========[1] General Data =============================================1**

**======================================================================1**

**1 Set to 1 to add monthly structure to all annual flow data 1**

**======= Set to zero otherwise. This will be reset to 1 if monthly 1**

**======= data (types 5 or 8) are entered. 1**

**======= Set to 2 never impose monthly structure on annual flow data 1**

**0 percentage of class used in Mode 9 (the default is 50) 1**

**0 set to 1 to exclude output for non-effluent features 1**

**======================================================================1**

**======= In Mean Mode the calculated values of the mean quality will 1**

**======= be output to the screen ... 1**

**======= In 95, 90 or 99-percentile Mode the calculated values of the 1**

**======= corresponding percentiles will be output to the screen 1**

**======= All any of these summary statistics are calculated by SIMCAT 1**

**======= can be plotted etc ... 1**

**======================================================================1**

**1 set to 1 for Mean Mode; 0 for 95-percentile mode; or set as 2 1**

**======= for 90-percentile mode; 3 for 90-percentile mode =============1**

**365 number of shots (minimum is 5; maximum is 5000) 1**

**11.2 3.0 -0.6 river water temperature ... mean, SD, correlation 1**

**'m3/d' units for river and effluent flow (4 characters in quotes) 1**

**======================================================================1**

**1 set to 1 to insert Diffuse Sources specified for Reaches 1**

**1 set to 1 to include River Chemistry 1**

**0 set to 1 for Auto-Interpolation between Features 1**

**======================================================================1**

# DETERMINANDS

## Number of Determinands

### Determinands are characteristics of water quality like the concentra­tions of phosphate, ammonia and copper. SIMCAT can simulate up to 9 different determinands (plus river flow). This section shows how these data are placed in the data file.

### If you want more than 9 determinands you can set up parallel data files for the same catchment. It may also be better to follow this approach where you have more than 5.

### The Determinand Section from the Example Data File is shown below. Most of it is comments. The actual data are in **bold** type. The comment lines describe the layout of the data. **GF** stands for Gap-filling.

### You will see at §63 that there is one line of data for each determinand. Each line has several items of data. We shall now go through these items in turn.

## Sequence of Determinands

### The SIMCAT data file does not require that you enter a special Code Number for each determinand. SIMCAT generates its own using the order in which the data for determinands are entered. Thus, in §63, *Chloride* is Determinand 1; *BOD* is Determinand 2, and so on.

### If you then decide not to use a determinand then you exclude it from the SIMCAT run by specifying 4 as the Determinand Type (§47). It is often efficient to set up a data-file which includes full data on 3-5 determinands and then to run these one at a time using “4” to exclude those to be left out.

|  |
| --- |
| **4** 'Chloride...' ' Cl' 'mg/l' 0.0 0.0 32.0 20.0 0.0 0.0 0.0 1 |

## Determinand Type

### The first number given for each determinand is the **Determinand Type**. It controls the way SIMCAT applies Natural Purification and Gap-filling.

### The types of determinand are listed below.

### Type 1: the determinand is **Conservative**, like Chloride; also, any adjustments calculated by Gap-filling will be applied along the river as a linear function of river length.

|  |
| --- |
| **1**  'Chloride...' ' Cl' 'mg/l' 0.0 0.0 32.0 20.0 0.0 0.0 0.0 1 |

### Type 2: the determinand is **Non-conservative** like the BOD and Ammonia; Natural Purification, if specified (§52) and switched in (§33), will be exponential with respect to river length or the time-of-travel.

### Any losses that are calculated by Gap-filling will be ap­plied as an exponential function of river length. Any gains will be linear.

|  |
| --- |
| **2**  'Ammonia....' ' Amm' 'mg/l' 22.0 0.0 0.0 0.0 32.0 2.0 10.0 1 |

### Type 3: the determinand is Dissolved Oxygen; the corrections calculated by Gap-filling are as for Type 2.

|  |
| --- |
| **3** 'Diss.Oxygen' ' DO' 'mg/l' 10.0 0.0 0.0 0.0 0.0 7.0 2.0 1 |

### Type 4: (or any other number) the determinand will be excluded from the run.

|  |
| --- |
| **4** 'Chloride...' ' Cl' 'mg/l' 0.0 0.0 32.0 20.0 0.0 0.0 0.0 1 |

## Determinand Name

### Next is the Determinand Name - 11 characters enclosed in single quotation marks, as in ‘Choride...’:

|  |
| --- |
| 1  **'Chloride...'** ' Cl' 'mg/l' 0.0 0.0 32.0 20.0 0.0 0.0 0.0 1 |

## Short Determinand Name

### This is 4 characters enclosed in single quotation marks, as in:

|  |
| --- |
| 1 'Chloride...' **' Cl'**  'mg/l' 0.0 0.0 32.0 20.0 0.0 0.0 0.0 1 |

### We have arranged that the following short determine names are treated identically. We did this mainly to ensure Batch Runs are consistent across a set of models.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Determinand | Short names now considered identical | | | | | |
| Chloride | CL |  |  |  |  |  |
| BOD | BOD |  |  |  |  |  |
| TOC | TOC |  |  |  |  |  |
| Ammonia | AMMN | NH4 | AMM | NH3 | NH3N | NH4+ |
| Dissolved Oxygen | DO | DOX | D.O. | D.O |  |  |
| Phosphate | PO4P | PO4 | TOTP | PHOS | SRP |  |
| Nitrate | NO3N | TON | NO3 |  |  |  |

## Parent and Daughter Substances

### This is a determinand (the “parent”) that converts into another (the “daughter”). The short determinand names are ‘PAR’ and ‘DAU’ for the parent and daughter respectively. The change does not apply to Gap-filling - changes to PAR are not applied to DAU.

### The “parent” and “daughter” can take any position in the list of determinands. If Parent is entered twice, the last one is used for all the entries for Daughter.

## Units of Measurement

### This is also 4 characters enclosed in single quotation marks, as in:

|  |
| --- |
| 1 'Chloride...' ' Cl'  **'mg/l'**  0.0 0.0 32.0 20.0 0.0 0.0 0.0 1 |

## Global Rate Constant

### If the River Chemistry Switch (§33) has been set to 1, the Global Rate Constants should be defined. These can be overwritten for in­dividual Reaches. If the determinand is Type 1, e.g. Chloride, no decay occurs and, therefore, a zero rate is assumed.

|  |
| --- |
| 1 'Chloride...' ' Cl' 'mg/l' **0.0** 0.0 32.0 20.0 0.0 0.0 0.0 1 |

### If the determinand is Type 2, e.g. Ammonia, the constant is en­tered in units of reciprocal days.

|  |
| --- |
| 2  'Ammonia....' ' Amm' 'mg/l'  **22.0** 0.0 0.0 0.0 32.0 2.0 10.0 3 |

### For Dissolved Oxygen, Determinand Type 3, a **Re-aeration rate** is required. The units are reciprocal days.

|  |
| --- |
| 3 'Diss.Oxygen ' ' DO' 'mg/l'  **10.0** 0.0 0.0 0.0 0.0 7.0 2.0 5 |

### Initially, it is best to suppress the Global Rate Constants using the Switch for River Chemistry (§33). Later you may want to find the best values for your catchment by a process of trial-and-error.

## Minimum Values of River Quality

### Quality cannot have negative concentrations. Often a sensible minimum value is greater than zero. An example is BOD where it is rare for values to decay to zero. A more sensible min­imum value might be 1.0. This variable ensures that values below this limit are never generated within SIMCAT.

|  |
| --- |
| 1 'Chloride...' ' Cl' 'mg/l' 0.0  **0.0** 32.0 20.0 0.0 0.0 0.0 1 |

## Quality of Diffuse Flows added by Gap-filling

### During the Gap-filling of river flows, extra river flow may be added. This column of data gives the concentration in any added flow. In the case below it is 32.0 mg/l.

|  |
| --- |
| 1 'Chloride...' ' Cl' 'mg/l' 0.0 0.0  **32.0** 20.0 0.0 0.0 0.0 1 |

## Best River Quality from Gap-filling

### During Gap-filling, the upstream effects can be extrapolated downstream. In some circumstances, this could lead to a river quality which unrealistically good. The value entered here specifies the lower bound for the extrapolation. You might want to specify the value for pristine river water within the catchment. In the case below it is 20.0 mg/l.

|  |
| --- |
| 1 'Chloride...' ' Cl' 'mg/l' 0.0 0.0 32.0 **20.0** 0.0 0.0 0.0 1 |

## Discharge Quality

### The next three variables are used in different ways in Run Types 7, 8 and 9. These Run Types deal with the calculation of the discharge standards needed to achieve River Targets. The values are described below.

## Worst Permissible Discharge Quality

### In Run Types 7, 8 or 9, SIMCAT calculates the discharge quality needed to meet river targets (§7). Type 7 constrains a discharge standard within values defined as “Worst” and “Best” (§58). Types 8 and 9 do not allow the calculated standard to exceed the current quality.

### This variable defines the worst annual mean quality which will be allowed to result from the calculation of the discharge quality needed to meet river targets. The value will reflect policy on discharges that have a trivial impact on river water quality or it might reflect the quality of an un­treated discharge. In the case below the concentration is 12.0 mg/l. SIMCAT presumes a coefficient of variation of 0.6 for all determinands.

|  |
| --- |
| 2  'Ammonia....' ' Amm' 'mg/l' 22.0 0.0 0.0 0.0  **12.0**  2.0 10.0 3 |

### If zero is entered the value is over-written by SIMCAT as a large number for certain determinands to the following:

* Chloride 500
* BOD 24
* Nitrate 15
* Phosphate 8
* Ammonia 20

## Best Available Discharge Quality

### In Run Types 7, 8 or 9, SIMCAT calculates the discharge quality needed to meet river targets (§7). Type 7 stops a discharge standard being set values better than defined as “Best”.

### This variable defines the best annual mean quality that can result from this calculation. The value may reflect current policy or the limits of the technology for discharge treatment. In the case illustrated below the concentration is 1.0 mg/l. SIMCAT presumes a coefficient of variation of 0.6 for all determinands.

|  |
| --- |
| 2 'Ammonia....' ' Amm' 'mg/l' 22.0 0.0 0.0 0.0 32.0 **1.0** 10.0 3 |

## Good Discharge Quality

### In Run Types 7, 8 and 9, SIMCAT sets the discharge quality needed to meet river targets (§7). This variable defines an annual mean of good discharge quality which can be imposed in cases where the current quality is worse than this and river target cannot be achieved even if the discharge had zero concentration of pollutant (often because the river is too polluted upstream).

### In Run Type 8 this quality is also imposed in cases where the river target is met with the current effluent quality. If the annual mean of the current discharger quality is worse than that defined as the Good Discharge Quality then the latter will be imposed.

### In the case below the Good Discharge Quality is 4.0 mg/l. SIMCAT presumes a coefficient of variation of 0.6 for all determinands.

|  |
| --- |
| 2 'Ammonia...' ' Amm ' 'mg/l' 22.0 0.0 0.0 0.0 32.0 2.0 **4.0**  3 |

## Suppress the Backward Calculation

### If the value expressed as Good Discharge Quality is set as a negative value, this will be taken as a sign that this determinand is not to be subject to the backward calculation (Modes 7, 8 or 9) when discharge quality is calculated as that which meets a downstream standard.

|  |
| --- |
| 2 'Ammonia...' ' Amm ' 'mg/l' 22.0 0.0 0.0 0.0 32.0 2.0 **-9.9**  3 |

## Code for the Summary Statistic for River Quality Targets

### There are output files covering compliance with river quality targets. These are named FILENAME.TGT. There is a code to define the summary statistics for the river quality targets. These codes are: 1, mean; 2, 95-percentile; 3, 90-percentile; 4, 5-percentile; 5, 10-percentile; 9, 99-percentile.

|  |
| --- |
| 2 'Ammonia....' ' Amm' 'mg/l' 22.0 0.0 0.0 0.0 32.02.0 10.0 **3** |

## Partitioned determinands

### Certain chemicals split between two or more forms. For example, there is interplay between dissolved lead and the lead absorbed or combined with solid matter suspended in river water. We say that the “total lead” is partitioned between its dissolved and solid forms.

### It may be that we measure the “total lead” discharged to a river but that the standard for river water quality is expressed as dissolved lead.

### It is customary to express the proportions of dissolved and solid lead as a Partition Coefficient. This is the logarithm (to the base of 10) of the value K in which:



### Suppose the concentration of “total lead” in one of SIMCAT’s shots is 15 µg/l. Suppose also that the corresponding value for suspended solids is 200 and that Log10(K) is 4 (giving K as 10,000). The calculated concentration of dissolved lead is 12.5 µg/l and the concentration of “solid” lead is 2.5:

[dissolved lead] = [total lead] / ( 1 + ([suspended solids] [ K ] / 1000000))

[solid lead] = [total lead] – [dissolved lead]

### The calculation is repeated for all shots and the results used to calculate summary statistics like means and percentiles of dissolved lead at points in the river. The results are set out in SIMCAT’s output files, including the CSV files picked by spreadsheets and databases.

### An option has been added for a determinand to be split into “dissolved” and “solid” fractions. This is triggered by the addition of an extra item, the partition coefficient. In the following example this is the value of Log10(K) and is “4.48”.

|  |
| --- |
| 1 'Copper ' 'Cu ' 'ug/l ' 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0 **4.48** |

### Where the value is positive, assessments of compliance assume that the standards are set for “total” concentration, the sum of “dissolved” and “solid”.

### If the partition coefficient is entered as a negative value it is used as a code that means that standards are assumed to be for the “dissolved” fraction. The negative sign is ignored in term of the value of the partition coefficient:

|  |
| --- |
| 1 'Copper ' 'Cu ' 'ug/l ' 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0 **-4.48** |

SIMCAT assumes that all inputs from rivers, discharges and diffuse pollution, and the concentrations specified at Monitoring Points, are expressed at “total”. SIMCAT then calculates concentrations and loads in the river as “total”, “dissolved” and “solid”.

Similarly, Gap Filling is done in terms of the “total” quantities.

## Correlation

### The flows of rivers and sewage treatment works are both affected by rainfall. You can introduce this and other correlations between river and discharge flow and quality. This is done through the data on river and discharge flow and quality.

### SIMCAT assumes a default value of the correlation coefficient of 0.6 between river flows and flows of sewage treatment works. Between rivers and tributaries this default coefficient is 1.0. These can be over-written (for example, §83, §99).

### The default correlations within SIMCAT are set out in the following tables. The default values set for determinands within SIMCAT using the short determinand names (§49).

|  |  |
| --- | --- |
| **Default Correlation between Flows** | |
| Correlation | Coefficient |
| River flow on tributary flows | 1.0 |
| River flow on discharge flow from Sewage Treatment Works (Feature 3) | 0.6 |
| River flow on discharge flow from other discharges (Feature 5) | 0.0 |

|  |  |
| --- | --- |
| **Default Correlation between River Flow and River Quality** | |
| Correlation | Coefficient |
| Chloride | -0.3 |
| BOD | 0.0 |
| Ammonia | 0.35 |
| Dissolved Oxygen | 0.3 |
| Total Organic Carbon | 0.3 |
| Phosphate | -0.3 |
| Nitrate | 0.6 |
| Parent Substances | 0.0 |
| Daughter Substances | 0.0 |

|  |  |
| --- | --- |
| **Default Correlation for Discharge Flow on Discharge Quality** | |
| Correlation | Coefficient |
| Chloride | -0.1 |
| BOD | 0.3 |
| Ammonia | 0.4 |
| Dissolved Oxygen | 0.0 |
| Total Organic Carbon | 0.3 |
| Phosphate | -0.1 |
| Nitrate | -0.2 |
| Parent Substances | 0.0 |
| Daughter Substances | 0.0 |

## Determinand Section of a SIMCAT Data file

**======================================================================2**

**======= [2] Determinand ==============================================2**

**======================================================================2**

**======= The code number for each determinand is defined by its order 2**

**======= in the list ... the first is code number 1 etc 2**

**======= There is one line of data for each determinand ... 2**

**======= Each line holds the following items: 2**

**======= (a) defines the type of determinand and the method of 2**

**======= handling River Chemistry and Gap-filling (GF) 2**

**======= The types are: 2**

**======= 1: the determinand is conservative; also, all the 2**

**======= corrections calculated by Gap Filling will be 2**

**======= be applied as a linear function of river length 2**

**======= 2: losses calculated by GF will be applied as an 2**

**======= exponential function of river length; gains will be 2**

**======= linear 2**

**======= 3: Dissolved Oxygen; it is assumed that the second and 2**

**======= third pollutants in the list are BOD and Ammonia 2**

**======= respectively; the Gap Filling corrections 2**

**======= corrections are as for type 2 2**

**======= 4: (or any other number) the determinand will be 2**

**======= excluded from the run 2**

**======= 5: partitioned determinands 2**

**======= (b) the name of the determinand 2**

**======= (c) the short name for the determinand 2**

**======= The names BOD, DO, DOX, AMM, NH4, NH4+ and NH4N are 2**

**======= special and trigger the hard-wired decay rates and 2**

**======= temperature coefficients for BOD, Dissolved Oxygen and 2**

**======= Ammonia 2**

**======= (d) the unit of measurement 2**

**======= (e) the global rate constant (reciprocal days) 2**

**======= (f) the minimum quality achievable by exponential decay with 2**

**======= the rate constants listed above for (e) 2**

**======= (g) the quality of the diffuse inflows added by Gap Filling 2**

**======= Filling when fitting river flows 2**

**======= (h) the minimum quality allowed by extrapolation of the 2**

**======= extra exponential decay introduced by Gap Filling 2**

**======================================================================2**

**======= The following variables (i),(j) and (l) are used as 2**

**======= constraints by Modes 7 - 9. They are mean concentrations 2**

**======================================================================2**

**======= (i) the worst permissible effluent quality (annual mean) 2**

**======= (j) the best feasible effluent quality (annual mean) 2**

**======= (k) a definition of good effluent quality (annual mean) 2**

**======= a negative value excludes the determinand from 2**

**======= calculations 2**

**======================================================================2**

**======= (l) summary statistic used to define river targets: 2**

**======= 1, 2, 3 for mean, 95-percentile and 90-percentile 2**

**======= 4 and 5 for the 5 and 10-percentile 2**

**======= 6 for the 99-percentile 2**

**======= (m) partition coefficient (optional) 2**

**======= A positive value means the standard is total dissolved 2**

**======= plus solid. A negative sign is a code that the standard 2**

**======= applies to dissolved. 2**

**========b===========c======d====e====f=====g====h=====i===j====k==l===m**

**1 'Chloride...' ' Cl' 'mg/l' 0.00 0.0 35.0 20.0 0.0 0.0 0.0 1**

**2 'B.O.D......' ' BOD' 'mg/l' 1.20 1.0 1.0 0.8 500.0 3.0 20.0 3**

**2 'Ammonia....' ' Amm' 'mg/l' 3.00 0.0 0.0 0.0 35.0 2.0 10.0 3**

**3 'Diss.Oxygen' ' DO' 'mg/l' 2.00 0.0 0.0 0.0 0.0 7.0 2.0 5**

**2 'Phosphate..' ' PO4' 'mg/l' 0.05 0.0 0.05 0.0 8.0 0.2 0.0 1**

**\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* indicator of the end of the determinand data \*\*\*\*\*\*\*\*\*2**

# REACH DATA

### You need to define your Reaches and how they are joined together. This Section explains how. The data for the Example Data File are at §**U**. The layout of the example catchment was given in the picture at §15 and at §17.

## Reach Number

### This is a code, an integer, which is used to identify the Reach in later Sections of data.

|  |
| --- |
| **1** 'River Ouse I ' 14.0 0 2 0 10 11 33.0 0.6 |

## Name of Reach

### Next is the Reach Name - 16 characters enclosed in single quotation marks, as in:

|  |
| --- |
| 1 **'River Ouse I '** 14.0 0 2 0 10 11 33.0 0.6 |

## Length of Reach

### This is specified in kilometres.

|  |
| --- |
| 1 'River Ouse I '  **14.0** 0 2 0 10 11 33.0 0.6 |

## Defining the Next Reach

### SIMCAT does the calculations for Reaches in a sequence which you must define. The next three variables define the **next** reach to be processed. The pattern of numbers defines how the next reach will be formed. For example:

|  |
| --- |
| 1 'River Ouse I ' 14.0 **0 2 0**  10 11 33.0 0.6 |

**0 2 0** The first Reach in the Section, Reach Number 1, will be processed first. Reach 1 must be a headwater reach.

In this particular data file, after Reach Number 1 (River Ouse I), the next Reach will be another headwater Reach, number 2 (River Avon). This interpreta­tion is set by the pattern of numbers: 0 2 0. We say that after Reach 1, the next reach will be a Branch to Reach 2:



### Subsequently the Reach to be processed after Reach 2 is directed by the three numbers specified for Reach Number 2. These numbers are 1, 2, 3:

|  |
| --- |
| 2 'River Avon ' 10.0 **1 2 3** 10 11 1.0 1.0 |

**1 2 3** After Reach, Number 2, the next Reach will be Reach Number 3, which will be formed by mixing together Reaches 1 and 2. This interpretation is set by the pattern of the numbers: 1 2 3. Obviously, as in this case, Reaches 1 and 2 must have been processed earlier in the sequence in order to provide data which can be mixed together to form the start of Reach 3:

### After Reach 3, the next Reach is a branch to Reach 4:

|  |
| --- |
| 3 'Middle Ouse ' 2.0 **0 4 0** 10 11 1.0 1.0 |

### Another confluence occurs after Reach 4:

|  |
| --- |
| 4 'Black Brook ' 10.0 **3 4 5** 10 11 1.0 1.0 |

**3 4 5** After the current Reach, Number 4, the next Reach will be Reach Number 5, which will be formed by mixing together Reaches 3 and 4. Obviously Reaches 3 and 4 must have been processed earlier in the sequence.

|  |
| --- |
| 5 'Lower Ouse I ' 14.0 **6 0 0**  10 11 33.0 0.6 |

**6 0 0** After Reach Number 5, the next Reach will be a straight con­tinuation to Reach Number 6. The end of Reach 5 forms the start of Reach Number 6.

|  |
| --- |
| 6 'Lower Ouse II ' 2.0 **0 0 0** 10 11 33.0 0.6 |

**0 0 0** This indicates that Reach 6 will be the last Reach.

## Modelling diffuse inputs

SIMCAT allows the modelling of the addition of diffuse inflows – flow added per kilometre of river length. These inflows are assigned specified sets of data on flows and quality.

### You will probably need to assume that river flow increases in the downstream direction at a rate which is bigger than the result of adding flow from headwaters, discharges and tributaries. This increase might account for flows added directly by groundwater, or by streams and ditches which are too small to be regarded as proper rivers or modelled as Features.

### You can also use this facility to build in diffuse losses of flow along the length of a Reach. The losses are modelled as if they were leaks through the bed of the river, and not as caused by evaporation. This means that river quality is unchanged when flow is lost (though the reduced flow will mean less dilution for downstream discharges).

### You can use this facility to help make SIMCAT's calculations agree with the observed data at river flow gauges.

One such set of inflows and quality is defined can be defined for every one of SIMCAT’s Reaches. In the Reach definition section of the DAT file, each SIMCAT Reach has a single number that identifies a set of data on river flow. These data are interpreted as the flow added per kilometre of the Reach. These are the called “Reach Diffuse Inflows”.

We can also set up such flows and contributions for 11 sectors such as highways, arable agriculture, livestock agriculture and urban run-off. This is done in the Feature section of the DAT file (§177, §32). The types of diffuse pollution based on Features can be stopped and started at any points on a Reach. They can also be expressed as concentrations that are added to a shared addition of river flow.

The diffuse inputs based on Features can also be added to the headwaters of an estuary – the flows defined by Feature Type 10.

## Diffuse Inflow Code (River Flow)

### The amount of the inflow is set by giving a code number which defines a set of data on river flow:

|  |
| --- |
| 2 'River Avon ' 10.0 1 2 3 **10** 11 1.0 1.0 |

### The data on the actual amount of inflow will be specified later in the River Flow Section (§**G**). Each set of river flow data has a code number (§79). For Reach 2, River Avon, the flow will be under code number **10**.

### The flow specified under Code 10 is the amount to be added for each kilometre of Reach 2.

### In the section of data in Features (§**K**), there is an option to use this set of flow data as an extra way of adding diffuse pollution (§141 and §178).

## Diffuse Inflow Code for River Quality

Each Reach has another single number that identifies a set of data on river water quality for the Reach Diffuse Inflows. In the following line of data for a Reach called “River Avon” the sets of data on diffuse river inflow and river quality are numbered **10** and **11** respectively:

### If a Diffuse Inflow Code for River Flow (§69,$32) has been entered the quality of the inflow must be assigned. This is done by another code number:

|  |
| --- |
| 2 'River Avon ' 10.0 1 2 3 10 **11** 1.0 1.0 |

### The data on the actual quality of the inflows will be specified in another part of the data file, the River Quality Section (§**H**), under the code number, 11. A zero code will mean that there is no diffuse inflow to the Reach.

## River Velocity

### In theory, the equations of river chemistry need to know the time taken for a body of water to travel between different points in the catchment. This time will depend on the river flow.

### SIMCAT does not have to know the time-of-travel as a function of river flow be­cause the effect is small compared with other errors in data. But you have the option to use time of travel if you wish.

### A relationship between flow and velocity is used to calculate the time of travel. This has the form:

### 

In this v is the velocity of river flow in kilometres per day and R is the ratio of the river flow to the annual mean flow. The value of *α* is the time-of-travel in kilometres per day when river flow is at its average value. A typical value of *β* is 0.5.

### The items, *α* and *β* are specified for each reach, as in:

|  |
| --- |
| 2 'River Avon ' 10.0 1 2 3 10 11 **30.0 0.5** |

### The first number is *α*, the second is *β*. Values of *α* and *β* can be derived from log-plots of field data from studies of time of travel, though particular values will tend to be characteristic of rivers in a region.

### If you don't want to use this relationship, enter zero values for *α* and*β*. Alternatively, values of 1.0 can be entered. SIMCAT then uses a uniform value of 0.4 metres/sec (33 km/day) to calculate travel time for all the values of river flow.

## Rate constants for individual reaches

### Rate constants can be set for each reach. They will override the Global Rate Constants (§51). These may be useful in calibration.

### These rate constants appear in the reach data as an extra row of numbers, one per determinand, for each and every reach:

|  |
| --- |
| 1 'Reach One' 35.0 0 2 0 10 11 33.0 0.5 |

|  |
| --- |
| 0.0 **0.3** **0.2** 0.0 0.0 0.0 0.0 0.0 0.0 0.0 'Reach rate constants' |

### In this example there are 10 values in the second row. If there are 5 determinands, only the first five numbers will be read and you can have a second row with only the first five numbers. The item 'Reach rate constants' is not essential.

### The second determinand has a Reach Rate Constant for this reach of 0.3; the third determinand has a value of 0.2. These, and any other non-zero value will over-write, for this Reach only, the values specified as Global Rate Constants (§52).

### These Reach Rate Constants, like the Global Rate Constants, will be applied only if the River Chemistry Switch is ON (§33).

### If you want to replace the Global Rate Constant with a value of zero for this reach then enter **-1.0** (minus 1.0) in the appropriate field, as for the third determinand in:

|  |
| --- |
| 0.0 0.3 **-1.0** 0.0 0.0 0.0 0.0 0.0 0.0 0.0 'Reach rate constants' |

## Flow and Quality at the Head of the Reach

### The Reach Section has no mention of the flow and quality at the head of the Reach. For Reaches which are headwaters, the flow and quality at the head of the Reach is specified as a Feature (§169).

### For other Reaches the flow and quality at the head of the Reach are obtained from the values calculated for the downstream limits of upstream reaches.

## Running bits of models

### Some of SIMCAT's data file are very big. You can get SIMCAT to run bits of them by setting to negative, the number of the reach at which you want SIMCAT to start the run and setting to zero the number of the reach at which you want to finish.

### SIMCAT then reads the entire data file but starts its calculations at the reach you've indicated and continues.

## Temperature

### Temperature can be specified as a single set of data that applies to the whole of the modelled river (§29).

### There is also an option to specify annual a distribution of temperature for each reach in the model. Temperature is set up as correlated with river flow.

### This facility is set up by entering an extra line of data for a reach. So, for a reach number 5 called “Lower Ouse I”:

|  |
| --- |
| 5 'Lower Ouse I' 200.0 0 0 0 10 11 etc etc |

We add immediately after this a line that is similar to that described later for entering data on river water quality:

|  |
| --- |
| 'Temperature' **1 11.0 3.0**  -9.9 30 |

### The first four letters of the word “Temperature” are used by SIMCAT to identify that these are data on temperature for the reach. The number “1” is the code for the distribution (Table 0.2) in (§96). In this case it is a normal distribution. Others can be used but the Shift Parameter is not an option (§98). The annual mean temperature is 11.0 and the corresponding standard deviation is 3.0.

The next two items are optional. In this example the correlation coefficient between temperature and river flow is provided by “-9.9”. This triggers the use of SIMCAT’s default value of -0.6. The number “30” is the number of samples.

|  |
| --- |
| 'Temperature' 1 11.0 3.0 **-9.9 30** |

### There is an option to specify monthly temperature distributions for reaches. This is done using distribution Type 8 (§106) as in:

|  |
| --- |
| 'Temperature' 8 'qtemp1.npd' -9.9 30 |

In this option temperature is then set up as correlated with river flow through parallel monthly averages of flow and temperature. At present this option treats as negligible any within month correlation between the daily values of river flow and river temperature.

## Suspended solids

### Similarly, there is an option of distributions for each reach for suspended solids. The first four letters of the phrase “Suspended Solids” is used by SIMCAT to identify that these are data on suspended solids that are to be used specifically for the reach. The process is the same as for temperature.

|  |
| --- |
| 'Suspended Solids' 2 12.0 6.0 0.4 30 |

## Reach-specific standards for determinands

There is an option to set separate standards for each reach. This can be done for all determinands.

|  |
| --- |
| '**Standard**' 1 5 0.02 0.04 -0.12 0.50 9999.9 |

The word “**Standard**” is used by SIMCAT to identify that these are data on special standards for a Reach.

These reach-specific standards replace those from the Targets section in the DAT file (§**J**) and set within the data on Features (§146).

The number “1” is the number of the determinand. This is defined by the order in which the determinands are entered in the DAT file (§46). The next number, “5”, indicates the number of standards that will follow.

A negative value sets the standard to be used as an objective. In the following, 0.12 will be that standard.

|  |
| --- |
| 'Standard' 1 **5** 0.02 0.04 -0.12 0.50 9999.9 |

### The number, 5, might be the number of classes set for, say, a river classification system such as that used for the Water Framework Directive. The next 5 numbers are the standards themselves.

|  |
| --- |
| 'Standard' 1 **5** 0.02 0.04 -0.12 0.50 9999.9 |

### This number of standards might be **1**. In the following, 0.12 will be that standard whether or not it is negative.

|  |
| --- |
| 'Standard' 1 **1** -0.12 |

|  |
| --- |
| 'Standard' 1 **1** -0.12 |

## Reach data section from the example SIMCAT data file

**======================================================================3**

**======= Section [3] Reaches ==========================================3**

**======================================================================3**

**======= For each Reach the following are given: 3**

**======= (a) the code number 3**

**======= (b) the name 3**

**======= (c) length (km) 3**

**======================================================================3**

**======= There are two ways of defining how reaches are connected 3**

**======= In the newer version (no longer preferred): 3**

**======= (d) defines the next downstream reach 3**

**======= (e) and (f) are dummy values 'set as x' and not used by 3**

**======= SIMCAT 3**

**======================================================================3**

**======= The older version is now preferred because of developments 3**

**======= for things like lakes and bifurcations. In this (d), (e) and 3**

**======= (f) define the sequence in which the Reaches will be 3**

**======= processed: 3**

**======= 0,x,0 ... the NEXT Reach will be a branch to Reach 3**

**======= number z 3**

**======= x,0,0 ... the NEXT Reach will be a straight 3**

**======= continuation to Reach number z 3**

**======= z,y,x ... the NEXT Reach, number x, will be formed by 3**

**======= mixing z and y 3**

**======================================================================3**

**======= (g) the flow data-set for any diffuse inflow 3**

**======= (h) the quality data-set for these diffuse inflows 3**

**======= (i) term a for the velocity/discharge relation 3**

**======= (j) term b for the velocity/discharge relation 3**

**======================================================================3**

**======= Then follows an optional line of data on rate constants, for 3**

**======= the reach - one constant for each determinand in the order 3**

**======= the determinands are entered above (2) 3**

**======= If non-zero, these replace any global values set in the 3**

**======= determinand data (at section [C]) 3**

**======= To replace the global value with zero enter '-1.0' 3**

**======================================================================3**

**======= Then follows an optional line of data for Temperature for 3**

**======= the reach. This set replaces any global values set in the 3**

**======= general data (in section [1]). 3**

**======================================================================3**

**======= Then follows an optional line of data for Suspended Solids 3**

**======= for the reach. This set replaces values hard wired within 3**

**======= SIMCAT. 3**

**======================================================================3**

**======= Then follows an optional line of data on river quality 3**

**======= targets and class limits for the reach. These replace values 3**

**======= entered in section [7] which are invoked in the data on 3**

**======= Features in Section [8]. 3**

**=========b==================c===d==e==f====g===h======i===j===========3**

**1 'Upper Ouse' 16.0 0 2 0 10 11 33.0 0.6**

**0.00 0.00 0.00 0.00 0.00**

**2 'River Avon' 12.0 1 2 3 10 11 1.0 1.0**

**0.00 0.00 0.00 0.00 0.00**

**3 'Middle Ouse' 2.0 0 4 0 10 11 1.0 1.0**

**0.00 0.00 0.00 0.00 0.00**

**4 'Black Brook' 10.0 3 4 5 10 11 1.0 1.0**

**0.00 0.00 0.00 0.00 0.00**

**5 'Lower Ouse ' 8.0 0 0 0 10 11 1.0 1.0**

**0.00 0.00 0.00 0.00 0.00**

**\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* indicator of the end of the Reach data \*\*\*\*\*\*\*\*\*\*\*\*\*3**

# RIVER FLOW

### This section shows you how to set up data for river flows. The portion of the Example Data File is shown at §93. Most this is comments. The actual data are in **bold type**.

### To get started you need only the mean river flow and the 5-percentile low flow. You can usually get these from the records for flow gauges. Ask the hydrologist for the Flow Duration Curves and the mean flow for flow gauges within your catchment. These should be readily available.

### The Flow Duration Curve should be constructed from the average daily gauged flows recorded over the period of time which cor­responds to the river quality data you will be using in SIMCAT (say 2 - 4 years). You can read off the 5-percentile low flow from the Flow Duration Curve.

### Alternatively, the flow data for ungauged tributaries and head­waters can be estimated from the data for gauged sites by scaling according to the size of the catchment.

### Each line of data specifies one set of flow data. Each line has a number of items. These are now described in turn.

## River Flow Reference Code

### The first item is a Code Number:

|  |
| --- |
| **1** 2 28.0 4.8 0.0 -9.9 'Head of Upper Ouse ' |

### You have encountered this Code already in §69, above. Similarly, in the other Sections of the data file, all reference to river flows will use a Code Number. Thus, in §69, the Diffuse Inflow for a Reach refers to Code 10:

|  |
| --- |
| **10** 2 1.0 0.07 0.0 -9.9 'Diffuse inflow ... ' |

### Later the river flow associated with headwaters, streams and flow gauges will also refer to a Code Number (for example §153 and §169). The actual flow data as­sociated with all the Codes are specified in this River Flow Sec­tion of the data file.

## River Flow Distribution

### The second item is a code which defines the statistical distribu­tion assumed for this set of river flow data:

|  |
| --- |
| 1 **2**  28.0 4.8 0.0 -9.9 'Head of Upper Ouse ' |

### The above example, which refers to code number 2, will assume that river flow follows a Log-normal Distribution.

### When setting up a new data file, it is good practice to assume that all river flows follow this distribution. More complex assumptions should be introduced later only if the results of SIMCAT are sen­sitive to the assumption that the river flow is Log-normal.

### SIMCAT supports several types of statistical distributions for flow and water quality (Table 0.2) (§80, §96 and §116):

|  |  |
| --- | --- |
| Table 0.2: Types of data on river flow | |
| 0 | Constant |
| 1 | Normal Distribution |
| 2 | Log-normal Distribution |
| 3 | 3 Parameter Log normal Distribution |
| 4 | Non-parametric Distributions |
| 5 | Seasonal (monthly) data |
| 8 | Monthly structure |

## Statistics of River Flow (Types 0 - 3)

### The next few items in the record will depend on the type of dis­tribution that you have selected. In nearly all cases you will want to specify a Log-normal Distribution.

### In most options (Types 0, 1, 2 or 3) the **mean flow** is required, as, for example in the following Log-normal Distribution:

### The Log-normal Distribution also requires the corresponding **5-percentile flow**:

|  |
| --- |
| 1 2 **28.0** 4.8 0.0 -9.9 'Head of Upper Ouse ' |

### The units of flow will those specified in §30. In this case the flow is 28.0 Ml/d.

### The Log-normal Distribution also requires the corresponding **5-percentile flow**:

|  |
| --- |
| 1 2 28.0  **4.8** 0.0 -9.9 'Head of Upper Ouse ' |

### For the Log-normal Distribution the next item is specified **as zero**:

|  |
| --- |
| 1 2 28.0 4.8 **0.0** -9.9 'Head of Upper Ouse ' |

### In the highly unusual case that you required a Normal Distribution (Type 1) for river flow the following line would be used:

|  |
| --- |
| 1 **1 28.0 4.8 0.0**  -9.9 'Head of Upper Ouse ' |

## Shift parameter (Type 3)

### The fifth number in the record is used to specify the Shift for a Three-parameter Log-normal Distribution (Type 3). You will hardly ever need this.

|  |
| --- |
| 1 **3**28.0 4.8  **3.0** -9.9 'Head of Upper Ouse ' |

## Site-specific correlation for river flow

### The sixth item of data in each record for river flow is often set as -9.9. This item is reserved for over-riding the default correlation between the river flow and a master set of river flow data (§62).

### The default correlation coefficient between the flows of rivers and tributaries and the master set is 1.0.

### The value of -9.9, or any other value outside the range from plus 1.0 to minus 1.0, signifies that this option is not to be used and that the default correlation will apply.

### Similarly, the value of 0.0 will be over-written as -9.9 and the default correlation imposed. In the unlikely event that you wanted to impose zero correlation you must specify a near-zero value, say, 0.0001.

### The descriptive text at the end of the record is not used by SIMCAT. You can include such items as your own notes perhaps as a reminder of where you got the data.

|  |
| --- |
| 1 2 28.0 4.8 0.0 -9.9 **'Head of Upper Ouse '** |

## Non-parametric Distributions for River Flow (Type 4)

### Option number 4, a **non-parametric distribution** needs care because the format of the line of data is different:

|  |
| --- |
| 1 **4**  'filnam.npd' -9.9 'Head of Upper Ouse ' |

### Instead of the three numbers giving the mean, the 5-percentile flow and the shift, you specify in single quotes the name of a data file which holds your data for the non-parametric distribution.

### The data file must reside in the same folder as your SIMCAT data file. The stem of the filename, *filnam*, must be 64 characters or less.

### In this case the file is called *filnam.npd*. The data-file for a Non-parametric distribution is a list of up to 100,000 numbers taken equi-spaced from the Flow Duration Curve. An example of 14 numbers is:

**14** 0.0 0.0 12.0 34.0 1.0 2.0 2.0 2.0 2.0 0.0 1.5 5.7 8.1 99.0

### The first value, 14, is the number of values of river flow which follow. The 14 items of data, after ranking, are assumed within SIMCAT as equi-spaced in terms of the Weibull plotting positions, 1/(1+n), for the Cumulative Frequency Distribution. This means that the above 14 points are:

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **From the data-file** | 0. | 0. | 12. | 34. | 1. | 2. | 2. | 2. | 2. | 0. | 1.5 | 5.7 | 8.1 | 99. |
| **After ranking** | 0. | 0. | 0. | 1. | 1.5 | 2. | 2. | 2. | 2. | 5.7 | 8.1 | 12. | 34. | 99. |
| **Rank** | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 |
| **Plotting Position** | .07 | .13 | .20 | .27 | .33 | .40 | .47 | .53 | .60 | .67 | .73 | .80 | .87 | .93 |

### In this case the river flow is zero for about 13% of the time and takes a constant value of 2.0 for about 20% of the time.

## Using monthly data

### SIMCAT retains options to define separate data for each month in the year. Monthly results are also produced.

### These options date from times when certain types of data were available for each month and some users wished them to be part of SIMCAT’s data. Usually such data were loads of pollution from agricultural sources.

### In terms of the overall calculation monthly data are seldom necessary. The full variability is fully and better represented by sets of annual data and the correlations between them.

Problems also occur when some data are assigned monthly structures but others are left with annual descriptions. In such cases SIMCAT attempts to construct a monthly structure for river flows (§88) and for the flows from sewage treatment works (Features 3 (§154 and §121) and 12 (§171)). The imposition of default monthly data changes the correlation coefficients. For example, generally reducing them by 15 to 30% from the values input for annual data.

There are two ways of setting up monthly data for river flow: Type 5 (§86) and Type 8 (§87).

If SIMCAT data contains Type 5 or Type 8 data for river or effluent flow or quality it will check whether the number of shots is a multiple of 365. If it is not the number is changed to a multiple of 365.

## Monthly (Seasonal) Data for River Flow (Type 5)

### SIMCAT retains options to define separate data for each month in the year. The options date from times when certain types of data were available for each month and some users wished them to be part of SIMCAT’s data. Usually such data were loads of pollution from agricultural sources.

### In terms of the overall calculation monthly data are seldom necessary. The full variability is fully and better represented by sets of annual data and the correlations between them.

### Type 5, **monthly data**, is specified in much the same way as a non-parametric distribution (Type 4):

|  |
| --- |
| 1 **5**  'monthly.npd' -9.9 'Head of Upper Ouse ' |

### The data file must reside in the same folder as your SIMCAT data file. The filename, *monthly.npd*, can be 64 characters or less. In this case the data-file itself comprises four rows of numbers:

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 15.0 | 12.0 | 11.0 | 8.0 | 6.0 | 3.0 | 2.0 | 5.0 | 6.0 | 10.0 | 14.0 | 16.0 |
| 3.0 | 2.0 | 1.8 | 1.0 | 0.8 | 0.3 | 0.1 | 0.4 | 0.5 | 1.2 | 2.1 | 3.6 |
| 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| -9.9 | -9.9 | -9.9 | -9.9 | -9.9 | -9.9 | -9.9 | -9.9 | -9.9 | -9.9 | -9.9 | -9.9 |

### Each column is a month in the year from January to December. The following rows give, for each month, the mean flow, the 5-percentile flow, the shift (nearly always zero) and any special correlation coefficient. Each column is a monthly version of the Log-normal data described above (§80, §81).

## Distributions with a monthly structure (Type 8)

### Type 8 is similar to Type 5 except that the monthly structure is fitted within a specified annual structure. Type 8 is also defined in much the same way as a non-parametric distribution (Type 4):

|  |
| --- |
| 1 **8**  'struct.npd' -9.9 'Head of Upper Ouse ' |

### The filename, *struct.npd*, can be 64 characters or less. The file must be placed in the same folder as your SIMCAT data file. The data-file comprises a line of annual data followed by five rows of 12 numbers:

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 2 100.0 10.0 0 .0 -9.9 | | | | | | | | | | | |
| 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 |
| 60.0 | 50.0 | 50.0 | -50.0 | -50.0 | -60.0 | -70.0 | -50.0 | -50.0 | 50.0 | 50.0 | 70.0 |
| 6.0 | 6.0 | 5.0 | -5.0 | -5.0 | -6.0 | -7.0 | -5.0 | -5.0 | 5.0 | 5.0 | 7.0 |
| 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| -9.9 | -9.9 | -9.9 | -9.9 | -9.9 | -9.9 | -9.9 | -9.9 | -9.9 | -9.9 | -9.9 | -9.9 |

The first line in the file gives the annual data. This is similar to that specified above (§81) for an annual distribution. It comprises: the type of distribution (2, for log-normal), the annual mean (100.0), the 5-percentile (10.0), the shift (0.0) and the correlation coefficient for the month (-9.9):

|  |
| --- |
| 2 100.0 10.0 0 .0 -9.9 |

After this there are five rows of 12 numbers. Each row gives values for the months January to December for:

* the type of distribution (Row 1)
* additions to the annual mean flow that will define the mean monthly flow (Row 2) – the 12 values must sum to zero.
* additions in 95-percentile flow that define the monthly 95-percentile flow (Row 3) – these must also sum to zero.
* the changes in shift flow define the monthly shift (Row 4)
* the monthly correlation coefficient (Row 5)

## Imposing a monthly structure on annual data

Problems occur when some data are assigned monthly structures but others are left with annual descriptions. In such cases SIMCAT attempts to construct a monthly structure for river flows.

In this situation SIMCAT the looks at any log-normal distributions of the annual river flow of Types 2 or 3. These are then converted into a monthly structure using the following information that is hard-wired within SIMCAT:

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 |
| 60.0 | 50.0 | 50.0 | -50.0 | -50.0 | -60.0 | -70.0 | -50.0 | -50.0 | 50.0 | 50.0 | 70.0 |
| 6.0 | 6.0 | 5.0 | -5.0 | -5.0 | -6.0 | -7.0 | -5.0 | -5.0 | 5.0 | 5.0 | 7.0 |
| 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| -9.9 | -9.9 | -9.9 | -9.9 | -9.9 | -9.9 | -9.9 | -9.9 | -9.9 | -9.9 | -9.9 | -9.9 |

## Intermittent Discharges

### The procedure described above for Non-parametric Distributions (§84) can also be used to define the flow data for an intermittent discharge.

### This is done by specifying a set of flow data in which the required proportion of items are specified as zero (§84). The discharge itself is then specified as a Feature 2 (a Stream or Tributary) which uses the specified Flow Data-set.

### An intermittent discharge specified in this way will have flows which are correlated with the flow in the receiving river – in the same manner as a Stream or Tributary.

### An intermittent discharge can also be defined by using Feature 3 (§155 – a sewage treatment works) or Feature 5 (§158 – an industrial discharge). These too can be allocated a non-parametric distribution for discharge flow (§120).

### They can also be set up as all or any of the forms of SIMCAT’s “diffuse inputs” (Features 13, 15, 25, 27, 29, 31, 33, 25. 37, 40 and 42).

### For example, a discharge flow can be set up as a non-parametric distribution of flow whose data are defined with, say, 98% of values that are zero. This will produce non-zero flows for 2% of SIMCAT’s Monte Carlo shots. The data on the concentrations associated with these flows can then be set up as the basic “operate all the time” distributions of concentration (Distribution Types 0, 1, 2, 3, 4 etc).

### It may not make sense to specify an intermittent distribution of concentrations to go with your intermittent distribution of flows. In such a case the non-zero flows will have a proportion of zero concentrations according to the percent of time the concentrations are defined to be zero in your data.

## End of Data on River Flows

### Finally, you need to indicate the end of this section of data.

|  |
| --- |
| \*\*\*\*\* indicator of the end of the list of data for river flow \*\*\*\*\*\*\*\* |

## Abstractions

### River flow data-sets are also used to define the data for constant abstractions of flow from rivers.

### More complex abstractions are dealt with by “negative discharges” (Features 18 and 19) or perhaps by exploiting Gap-filling.

### When used in this way all the fields in the river flow data-set are zero except those for the Code Number, the mean flow and the 5-percentile flow. (Non-zero values may be entered but they will be ignored if the Data-set is used for Abstractions).

|  |
| --- |
| **11** 0 20.0 5.0 0.0 0.0 'Abstraction at New Mill ' |

### The number entered for the **mean flow** for data-set number 11 now defines the value of a constant abstraction: 20.0 in this case.

|  |
| --- |
| **11** 0 **20.0** 5.0 0.0 0.0 'Abstraction at New Mill ' |

### The units of flow will those specified in §30. In this case the flow is 20.0 Ml/d.

### The next field defines a limiting flow below which flow may not be removed from the river.

|  |
| --- |
| 9 0 20.0 **5.0** 0.0 0.0 'Abstraction at New Mill ' |

### When SIMCAT encounters an abstraction which uses Flow Data-set Number 9, it will subtract 20.0 from all the river flow shots. Where this would leave less than 5.0 in the river, the abstraction is reduced accordingly so that a level of 5.0 is left in the river.

## Flow Regulation

### River flow data-sets are also used to define the data for River Regulation – a device for adding flow to a river.

### When used in this way all the fields in the data-set are zero except those for the Code Number and the 5-percentile low flow. (Non-zero values may be entered but they will be ignored if the Data-set is used for River Regulation).

|  |
| --- |
| 13 0 **0.0** 5.0 0.0 0.0 'Avon Regulation ' |

### The next field defines a target flow. The units of flow will those specified in §30. In this case the flow is 5.0 Ml/d.

|  |
| --- |
| 13 0 0.0 **5.0** 0.0 0.0 'Avon Regulation ' |

### When SIMCAT encounters Flow Regulation which uses Flow Data-set Number 13, it will add flow to all the river flow shots whose flow is less than 5.0.

## River Flow Section from the Example Data File

**======================================================================4**

**======= Section [4] River Flow =======================================4**

**======================================================================4**

**======= The River Flow Data-Sets follow: 4**

**======= There is one line for each data-set: For each line: 4**

**======= (a) the code number of the data-set that will be referred 4**

**======= in the data on Features (8) and Reaches (3) 4**

**======= (b) the code number of type of distribution: 4**

**======= (for Feature Types 7 and 9 only zero, 1 or 2 can be used 4**

**======= 0 - constant, uniform flow 4**

**======= 1 - flow follows the Normal Distribution 4**

**======= 2 - the Log-Normal Distribution 4**

**======= 3 - a Three-Parameter Log-Normal Distribution 4**

**======= 4 - non-parametric distribution 4**

**======= 5 - monthly data - distribution for each month 4**

**======= 8 - monthly structure 4**

**======================================================================4**

**======= For distribution types 4 and 5 the items (c),(d) and 4**

**======= (e) below do not appear. Instead we show the name 4**

**======= of data file holding the data for these distributions. 4**

**======= For example: 'npar.npd' (Note the need to use this 4**

**======= type of quotation marks) 4**

**======================================================================4**

**======= (c) the mean flow; except when used by: 4**

**======= Feature Type 7 (abstractions): the abstracted flow 4**

**======= Feature Type 9 (river regulation): zero 4**

**======= Distribution Type 3: the mean of transformed data 4**

**======= (d) the 95-percentile low flow: except when used by: 4**

**======= Feature Type 7 (abstractions): the Hands-Off Flow 4**

**======= Feature Type 9 (river regulation): a Maintained Flow 4**

**======= (e) the shift parameter for distribution types 3: 4**

**======= for Distribution Type 0, 1, 2: zero or blank 4**

**======= (f) reserved for a non-standard correlation coefficient 4**

**======= (g) the name of the site. This is used only for help with 4**

**======= preparing the DAT file. It is not needed by SIMCAT. 4**

**===========c=====d======e=======f=============g=======================4**

**1 3 28.0 4.80 -3.0 -9.9 'Head of Upper Ouse'**

**2 2 4.0 1.20 0.0 -9.9 'Head of River Avon'**

**3 3 1.0 0.20 0.1 -9.9 'Head of Black Brook'**

**4 2 30.0 6.00 0.0 -9.9 'Upper Ouse at Pig Farm'**

**5 2 2.0 0.40 0.0 -9.9 'Ouse Stream'**

**6 2 15.0 5.00 0.0 -9.9 'Avon at Valley Bottom'**

**8 2 0.0 0.00 0.0 -9.9 'Middle Ouse Station'**

**9 2 84.0 13.00 0.0 -9.9 'Ouse at New Mill'**

**10 2 1.0 0.07 0.0 -9.9 'Diffuse inflow'**

**11 2 1.0 0.10 0.0 -9.9 'Flow Adjustment'**

**12 2 0.0 3.00 0.0 -9.9 'Avon Regulation'**

**16 2 100.0 15.00 0.0 -9.9 'Ouse Stream'**

**17 2 0.0 40.00 0.0 -9.9 'Regulation'**

**18 2 82.0 0.00 0.0 -9.9 'Abstraction'**

**\*\*\*\*\*\*\*\*\*\*\* indicator of the end of the list of river flow data \*\*\*\*\*\*4**

# RIVER QUALITY

### This section shows you how to set up data for river quality. The portion of the Example Data File is shown at §111. As before, most of §111 is comments. The actual data are in **bold type**.

### To get started you need only the mean river quality, the standard deviation and the number of samples. These should be readily available.

### You may need to estimate data for points that are not monitored directly.

### Each line of data specifies one set of data. Each line has a num­ber of items. These are now described in turn.

|  |
| --- |
| 1 3 2 0.05 0.05 0.0 -9.9 30 'Head of Upper Ouse ' |

## River Quality Reference Code

### The first item is a Code Number:

|  |
| --- |
| **1** 3 2 0.05 0.05 0.0 -9.9 30 'Head of Upper Ouse ' |

### You have met such a Code already in §70 above. Similarly, in the other Sections of the data file, all references to river quality will use a Code Number. Thus, in §70, the quality of the Diffuse Inflow for a Reach refers to Code 11:

|  |
| --- |
| **11** 3 2 0.05 0.05 0.0 -9.9 30 'Diffuse inflow ' |

### Later the river quality associated with headwaters, streams and monitoring points will also refer to a Code Number (For example: §153, §152, §169). The actual data associated with all these Codes are specified in this River Quality Section of the data file.

## Determinand Number

### Next you need to define the Number of the Determinand for which these data refer. The Determinand Number is set according to the order in which the Determinand Data are listed in the Determinand Section (§46). Thus, the following:

|  |
| --- |
| 12 **3** 2 0.05 0.05 0.0 -9.9 30 'Head of Upper Ouse ' |

refers to Determinand Number 3, (or Ammonia in this particular set of data).

## River Quality Distribution

### The third item is a code which defines the statistical distribu­tion assumed for this set of river quality data:

|  |
| --- |
| 12 3 **2** 0.05 0.05 0.0 -9.9 30 'Head of Upper Ouse ' |

### The above example, which refers to code number 2, will assume that this set of river quality data follows a Log-normal Distribution.

### The options are:

|  |  |
| --- | --- |
| Table 0.3: Types of data on river quality | |
| 0 | Constant flow |
| 1 | Normal distribution |
| 2 | Log-normal distribution |
| 3 | 3 parameter log-normal distribution |
| 4 | Non-parametric distributions |
| 5 | Monthly (seasonal) data |
| 6 | As 1 but the data are loads and not concentrations (see §97) |
| 7 | As 2 but the data are as loads and not concentrations (see §97) |
| 8 | Monthly structure |
| 9 | Non-parametric distribution of loads |
| 10 | Power curve distribution for concentrations (see §109) |
| 11 | Power curve distribution for loads (see §108) |

### When setting up a new data file, it is good practice to assume that BOD and Ammonia follow a Log-normal distribution and that Dis­solved Oxygen is Normal. More complex assumptions can be intro­duced later if the results of SIMCAT turn out to be sensitive to the simpler choices. Such elaborations are nearly always less important say, than the statistical errors introduced by the number of samples taken of rivers and discharges.

## Specifying river quality data as loads

### Types 6 and 7 are similar to types 1 and 2 except that they will specify loads, not concentrations. Type 9 is like type 4 but for loads, not concentrations.

### The units of load are assumed to be those corresponding to the product of flow and concentration. This would be “kg/day” if flow were “megalitres per day” and if concentration were “mg/litre”.

### The distributions are assumed to be normal for type 6 and log-normal for type 7. For type 9, non-parametric, the data are placed a file whose structure is the same as for Type 4, except that the values are loads.

## Statistics of River Quality (Types 0 - 4)

### Some of the next few items in the record will depend on the type of distribution which has been selected. As a rule, however you will need to specify the **mean**:

|  |
| --- |
| 12 3 2  **0.05**  0.05 0.0 -9.9 30 'Head of Upper Ouse ' |

This is followed by the corresponding **standard deviation**:

|  |
| --- |
| 12 3 2 0.05  **0.05**  0.0 -9.9 30 'Head of Upper Ouse ' |

and the number of samples:

|  |
| --- |
| 12 3 2 0.05 0.05 0.0 -9.9  **30** 'Head of Upper Ouse ' |

### The units will be those specified for the determinand (§51).

### The sixth number in the record is used to specify the Shift for a Three-parameter Log-normal Distribution (Type 3). You will hardly ever need this.

|  |
| --- |
| 12 3  **3** 0.05 0.05 **0.01** -9.9 30 'Head of Upper Ouse ' |

## Site Specific Correlation for River Quality

### The seventh item of data in each record for river quality data is nearly always given the value -9.9. This item is reserved for in­troducing special correlation between the river quality and river flow at the same site (§62).

|  |
| --- |
| 12 3 2 0.05 0.05 0.0 **-9.9**  30 'Head of Upper Ouse ' |

### The value of -9.9, or any other value outside the range from plus 1.0 to minus 1.0, signifies that this option is not to be used and that the default option will apply. This imposes zero correlation between this river quality and river flow at this site.

### Similarly, the value of 0.0 will be over-written as -9.9 and the default correlation imposed. If you want to impose zero correlation you must specify a near-zero value, say, 0.0001.

## Number of Samples for River Quality

### The eighth item of data in each record for river quality data is number of samples used to calculate the annual mean and standard deviation. The number is used to calculate confidence limits and the confidence that standards are failed.

### The numbers of samples are critical in the assessment of the confidence that the correct actions are calculated to protect water quality. The errors stemming from limited sampling are usually the biggest uncertainty in the calculations.

|  |
| --- |
| 12 3 2 0.05 0.05 0.0 -9.9 **30** 'Head of Upper Ouse ' |

The number of samples is also used to calculate compliance with standards and targets in terms of the confidence of failure. This helps confirm the need to act and to decide places where action is most necessary.

## Descriptive Text

### The descriptive text at the end of the record is not used by SIMCAT. You can include such items as your own notes perhaps as a reminder about some problem with the data.

|  |
| --- |
| 12 3 2 0.05 0.05 0.0 -9.9 30 **'Head of Upper Ouse '** |

## Non-parametric Distribution for River Quality (Type 4)

### Option number 4, a non-parametric distribution, needs special care because the format of the line of data is different:

|  |
| --- |
| 17 3 **4** 'qual.npd' -9.9 30 'Head of Upper Ouse ' |

### Instead of the three numbers giving the mean, the standard devia­tion and the shift, you will need to specify in single quotes the name of a data file which holds your data for the non-parametric distribution. The format of this data file is exactly the same as that described for river flow (§84).

|  |
| --- |
| 17 3 4 **'qual.npd'** -9.9 30 'Head of Upper Ouse ' |

### The value of -9.9 is as discussed above (§99), and the value, 30, is the same item as before – the number of samples that SIMCAT will use to estimate confidence limits. Even if this is the same as the number of items in the file ‘qual.npd’ it needs to be specified here too.

### The file must be in the same folder as your main SIMCAT data-file. The stem of the filename, *qual*, can be 64 characters or less.

## Monthly (Seasonal) Data for River Quality (Type 5)

### Type 5, **seasonal data** is specified in much the same way as a non-parametric distribution (Type 4):

|  |
| --- |
| 18 3 **5 'mon.npd'** -9.9 10 'Head of Upper Ouse ' |

### The stem of the filename, *mon.npd*, must be 64 characters or less. The data file is placed in the same folder as your SIMCAT data file. The data-file comprises four rows of numbers:

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 15.0 | 12.0 | 11.0 | 8.0 | 6.0 | 3.0 | 2.0 | 5.0 | 6.0 | 10.0 | 14.0 | 16.0 |
| 3.0 | 2.0 | 1.8 | 1.0 | 0.8 | 0.3 | 0.1 | 0.4 | 0.5 | 1.2 | 2.1 | 3.6 |
| 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| -9.9 | -9.9 | -9.9 | -9.9 | -9.9 | -9.9 | -9.9 | -9.9 | -9.9 | -9.9 | -9.9 | -9.9 |

### Each column is a month in the year. The rows give, for each month, the mean, the standard deviation, the shift (nearly always zero) and any special correlation coefficient. These are all monthly versions of the Log-normal data described above (§98).

### One reason for setting up such methods (Type 5 and Type 8 (§106)) has been that some data on diffuse pollution were available as monthly discharges of load - expressed as a distinct mean and standard deviation for each month. SIMCAT was then used to try and answer questions like – what is the January contribution to the annual mean concentration or to the annual 95-percentile?

### This last point is important because water quality standards are, and need to be as a minimum requirement, expressed as annual summary statistics such as the annual mean or an annual percentile[[5]](#footnote-5).

## Normal Distribution for Loads (Type 6)

This type of data (Type 6) is the same as Type 1 but the numbers refer to loads and not concentrations,

## Log-normal Distribution for Loads (Type 7)

This type of data (Type 7) is the same as Types 2 and 3 but the numbers refer to loads and not concentrations,

## Distributions with a monthly structure (Type 8)

### Type 8 is similar to Type 5 except that the monthly structure is fitted within a specified annual structure. Again, **monthly structure** is specified in much the same way as a non-parametric distribution:

|  |
| --- |
| 19 3 **8**  'struct.npd' -9.9 26 'Head of Upper Avon ' |

### The filename, *struct.npd*, can be 64 characters or less. The data file must reside in the same folder as your SIMCAT data file. The data-file comprises the line of annual data followed by five rows of numbers:

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 2 1.0 0.4 0 .0 -9.9 | | | | | | | | | | | |
| 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 |
| 0.6 | 0.4 | 0.4 | -0.5 | -0.5 | -0.5 | -0.5 | -0.5 | -0.5 | 0.5 | 0.5 | 0.9 |
| 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| -9.9 | -9.9 | -9.9 | -9.9 | -9.9 | -9.9 | -9.9 | -9.9 | -9.9 | -9.9 | -9.9 | -9.9 |

The first line in the file is the annual data. This is similar to that specified above (§98) for an annual distribution. The first line comprises: the type of distribution (2), the annual mean (1.0), the standard deviation (0.4), the shift (0.0) and the correlation coefficient (-9.9).

|  |
| --- |
| 2 100.0 10.0 0 .0 -9.9 |

After this come rows of 12 numbers. Each row gives values for the months January to December:

* the types of distribution (Row 1)
* the additions to the annual mean that define the monthly mean (Row 2). The 12 items must sum to zero.
* the change in standard deviation that define the monthly standard deviation (Row 3). These must sum to zero.
* the changes in annual shift define the monthly shift (Row 4)
* the monthly correlation coefficient (Row 5)

## Non-parametric Distribution of Loads (Type 9)

This type of data is the same as Type 4 but the numbers refer to loads and not to concentrations.

## Power Curves for Loads (Type 11)

Type 11 has proved useful in dealing with data on diffuse pollution. This type is a log-normal distribution of loads.

In the following example of a set of data of Type 11, the first, second and third items are the same as in other types of data such as Types 2 or 7. They define the number of this set of data (28), the number of the determinand (3) and the type of data (11). Similarly, the values of 1.0 and 36 are the correlation coefficient and number of samples just as for other Types of data.

|  |
| --- |
| **28 3** **11** 1.52 0.81 0.76 1.0 5.0 **1.0 36** ''diffuse load” |

The definitions of the middle five numbers are set out below:

|  |
| --- |
| 28 3 11 **1.52 0.81 0.76 1.0 5.0** 1.0 36 ''diffuse load” |

* The mean load, m (1.52 in this case)
* The standard deviation, (0.81)
* The power index, p (0.76)
* The base load, b, (is specified as a percentage of the mean) (1.0)
* The cut off percentile; values below this are set to zero), c (5.0)

SIMCAT then calculates the 5000 values of load by assuming a log-normal distribution and the using same processes as for Type 7.

For Type 11 the calculations are taken further. The power index is used to modify the initial values of the 5000 values. Each initial value of *load* is raised to the power of the power index, p (0.76 in this case):

Values of for percentiles that are less than the specified cut-off-percentile are set to zero. In the current example, the cut-off is the 5-percentile, 5% of the values of will be zero.

SIMCAT then calculated the average value of the 5000 results:

Then when setting up the values of *(shot)* that are to be used by SIMCAT in the calculation of river quality, every value of is multiplied by the input mean, m, and divided by the value calculated for

The full calculation brings in the value entered for the base load (b):

## Power Curves for Concentrations (Type 10)

In Type 10, the first, second and third items are the same as in other types of data such as Types 2 or 7. They define the number of this set of data (29), the number of the determinand (3) and the type of data (10). Similarly, the values of 1.0 and 36 are the correlation coefficient and number of samples just as for other Types of data.

|  |
| --- |
| **29 3** **10** 1.52 0.81 0.76 1.0 5.0 **1.0 36** ''diffuse concentration” |

The definitions of the middle five numbers are set out below:

|  |
| --- |
| 29 3 10 **1.52 0.81 0.76 1.0 5.0** 1.0 36 ''diffuse concentration” |

* The mean concentration, m (1.52 in this case)
* The standard deviation (0.81)
* The power index, p (0.76)
* The base concentration, b, (is specified as a percentage of the mean) (1.0)
* The cut off percentile; values below this are set to zero), c (5.0)

SIMCAT calculates the standard deviation by multiplying the mean by the coefficient of variation. SIMCAT then calculates the 5000 values of load by assuming a log-normal distribution and the using same processes as for Type 7.

For Type 11 the calculations are taken further. The power index is used to modify the initial values of the 5000 values. Each initial value of *concentration* is raised to the power of the power index, p (0.76 in this case):

Values of for percentiles that are less than the specified cut-off-percentile are set to zero. In the current example, the cut-off is the 5-percentile, 5% of the values of will be zero.

SIMCAT then calculated the average value of the 5000 results:

Then when setting up the values of *(shot)* that are to be used by SIMCAT in the calculation of river quality, every value of is multiplied by the input mean, m, and divided by the value calculated for

The full calculation brings in the value entered for the base load (b):

## End of Data on River Quality

### Finally, you need to indicate the end of the section of data on river quality.

|  |
| --- |
| \*\*\*\*\* indicator of end of the list data for river quality \*\*\*\*\*\*\*\* |

## River Quality Section from the Example Data File

**======================================================================5**

**======= Section [5] River Quality ====================================5**

**======================================================================5**

**======= The River Quality Data-Sets follow. For each Data-Set 5**

**======= there is a line of data for each determinand. 5**

**======================================================================5**

**======= For each line the following items are required: 5**

**======= (a) the code number of the data-set that will be referred 5**

**======= in the data on Features (8) and Reaches (3) 5**

**======= (b) the code number for the determinand. 5**

**======= (This is defined by its order in the above list of 5**

**======= determinands (2) ... the first is code number 1 etc) 5**

**======= (c) the code number of type of distribution: 5**

**======= (for Feature types 7 and 9: this is zero, 1 or 2) 5**

**======= 0 - constant, uniform concentration 5**

**======= 1 - concentration follows the Normal Distribution 5**

**======= 2 - the Log-Normal Distribution 5**

**======= 3 - a Three-Parameter Log-Normal Distribution 5**

**======= 4 - non-parametric distribution 5**

**======= 5 - monthly data - a distribution for each month 5**

**======================================================================5**

**======= For distribution types 4,5,8 and 9 the items (d),(e) and 5**

**======= (f) below do not appear. Instead is shown the name of 5**

**======= the data file holding the data for the distribution. 5**

**======= For example: 'npar.npd' (Note the need for this type of 5**

**======= quotation marks) 5**

**======================================================================5**

**======= 8 - monthly structure 5**

**======= 6 - as 1 but the data (d) and (e) refer to loads 5**

**======= 7 - as 2 but the data (d) and (e) refer to loads 5**

**======= 9 - non-parametric distribution of loads 5**

**======= 10 - a power-curve distribution for concentrations 5**

**======= 11 - a power-curve distribution for loads 5**

**======================================================================5**

**======= (d) the mean concentration 5**

**======= (e) the standard deviation 5**

**======= (f) the shift parameter for distribution types 3 5**

**======= for Distribution Type 0, 1 or 2: zero or blank 5**

**======= (g) reserved for a non-standard correlation coefficient 5**

**======= (h) number of samples used to compute the mean 5**

**======= (i) the name of the site (this is used for identification. 5**

**======= It is not needed by SIMCAT. 5**

**======================================================================5**

**======= For the power curves (10) and (11) items (f), (g) and (h) 5**

**======= become: 5**

**======= (f) the power index 5**

**======= (g) the base concentration (specified as a percentage of the 5**

**======= mean 5**

**======= (h) the cut off percentile (values below this are set to 5**

**======= zero) 5**

**======= (g) reserved for a non-standard correlation coefficient 5**

**======= (h) number of samples used to compute the mean 5**

**======= (i) the name of the site (this is used for 5**

**======= identification. It is not needed by SIMCAT) 5**

**=====b==c======d======e====f=======g===h=======i======================5**

**1 1 1 35.00 4.60 0.0 -9.9 30 'Head of Upper Ouse'**

**1 2 3 1.90 0.90 -0.5 -9.9 30 ''**

**1 3 2 0.05 0.05 0.0 -9.9 30 ''**

**1 4 1 9.00 1.50 0.0 -9.9 30 ''**

**1 5 2 0.07 0.07 0.0 -9.9 30 ''**

**2 1 2 35.00 4.60 0.0 -9.9 30 'Head of River Avon'**

**2 2 2 1.80 0.90 -0.5 -9.9 30 ''**

**2 3 2 0.07 0.10 0.0 -9.9 30 ''**

**2 4 1 9.00 1.50 0.0 -9.9 30 ''**

**2 5 2 0.09 0.09 0.0 -9.9 30 ''**

**3 1 2 35.00 4.60 0.0 -9.9 30 'Head of Black Brook'**

**3 2 3 1.90 1.00 0.5 -9.9 30 ''**

**3 3 2 0.04 0.04 0.0 -9.9 30 ''**

**3 4 3 9.00 1.00 0.0 -9.9 30 ''**

**3 5 2 0.05 0.05 0.0 -9.9 30 ''**

**4 1 1 33.60 4.60 0.0 -9.9 12 'Upper Ouse at Pig Farm'**

**4 2 2 2.00 0.80 0.0 -9.9 12 ''**

**4 3 2 0.00 0.00 0.0 -9.9 12 ''**

**4 4 1 8.80 1.20 0.0 -9.9 12 ''**

**4 5 2 0.10 0.10 0.0 -9.9 12 ''**

**5 1 2 36.00 4.20 0.0 -9.9 30 'Ouse Stream'**

**5 2 2 1.20 3.50 0.0 -9.9 26 ''**

**5 3 2 0.70 0.60 0.0 -9.9 30 ''**

**5 4 1 5.20 2.00 0.0 -9.9 26 ''**

**5 5 2 0.10 0.50 0.0 -9.9 30 ''**

**6 1 2 42.90 7.10 0.0 -9.9 30 'Black Brook'**

**6 2 2 2.00 1.00 0.0 -9.9 30 ''**

**6 3 2 0.04 0.04 0.0 -9.9 30 ''**

**6 4 1 8.80 1.00 0.0 -9.9 30 ''**

**6 5 2 0.05 0.06 0.0 -9.9 30 ''**

**7 1 2 50.00 5.70 0.0 -9.9 0 'Temply Station'**

**7 2 2 3.90 2.10 0.0 -9.9 0 ''**

**7 3 2 0.10 0.10 0.0 -9.9 0 ''**

**7 4 1 7.20 2.10 0.0 -9.9 0 ''**

**7 5 2 0.25 0.20 0.0 -9.9 26 ''**

**8 1 2 50.00 5.70 0.0 -9.9 26 'Middle Ouse Station'**

**8 2 2 3.90 2.10 0.0 -9.9 26 ''**

**8 3 2 0.30 0.30 0.0 -9.9 26 ''**

**8 4 1 7.20 2.10 0.0 -9.9 26 ''**

**8 5 2 0.11 0.80 0.0 -9.9 26 ''**

**9 1 2 53.00 5.30 0.0 -9.9 26 'Ouse at New Mill'**

**9 2 2 4.10 2.40 0.0 -9.9 26 ''**

**9 3 2 0.30 0.20 0.0 -9.9 30 ''**

**9 4 1 8.10 2.40 0.0 -9.9 26 ''**

**9 5 2 0.25 0.20 0.0 -9.9 26 ''**

**10 1 2 46.00 4.90 0.0 -9.9 12 'Avon at Valley Bottom'**

**10 2 2 3.90 2.20 0.0 -9.9 12 ''**

**10 3 2 0.50 0.50 0.0 -9.9 12 ''**

**10 4 1 5.90 2.20 0.0 -9.9 12 ''**

**10 5 2 1.15 0.80 0.0 -9.9 12 ''**

**11 1 1 10.00 2.00 0.0 -9.9 36 'Diffuse inflows'**

**11 2 2 0.50 0.20 0.0 -9.9 36 ''**

**11 3 2 0.00 0.00 0.0 -9.9 36 ''**

**11 4 1 8.80 0.00 0.0 -9.9 36 ''**

**11 5 2 0.05 0.05 0.0 -9.9 36 ''**

**14 1 2 90.00 6.00 0.0 -9.9 36 'Diffuse inflows'**

**14 2 2 60.00 40.00 0.0 -9.9 36 ''**

**14 3 2 40.00 5.00 0.0 -9.9 36 ''**

**14 4 1 0.00 0.00 0.0 -9.9 36 ''**

**14 5 1 4.00 4.00 0.0 -9.9 36 ''**

**\*\*\*\*\*\*\*\*\* indicator of end of the list of river quality data \*\*\*\*\*\*\*\*\*5**

# DISCHARGE FLOW AND QUALITY

## Introduction

### The discharge flow and quality data are entered together. The layout of the data is the same as that used for river quality ex­cept that discharge flow is entered with the data for discharge quality.

### The portion of the Example Data File is shown at §126. As before, most is comments.

### To get started you need the mean and standard deviation of dis­charge flow and the mean discharge quality, the standard deviation of discharge quality and the number of samples.

### You must use the same units as for rivers (§30). Each line of data specifies one set of data:

|  |
| --- |
| 21 3 2 12.0 9.0 0.0 -9.9 55 'Wellington STW ' |

### Each line has a num­ber of items. These are now described in turn.

## New Discharge

### You may need to make special provision for discharges that do not exist now but which are planned for the future. You will see later in §**K** on Features and Gap-filling that you should include the data for these discharges but give them zero flow when doing calculations for conditions before they come into operation.

## Discharge Flow and Quality Reference Code

### The first item is a Code Number:

|  |
| --- |
| **21** 2 12.0 9.0 0.0 -9.9 55 'Wellington STW ' |

### In other Sections of the data file, all references to the flow and quality of the discharge will use a Code Number. The code numbers should be defined sequentially.

## Determinand Number

### Next you need to define the Number of the Determinand to which these data refer. The Determinand Number is set according to the order in which the Determinand Data are listed in the Determinand Section (see above at §**E**). Thus, the following refers to Determinand Number 3, or Ammonia.

|  |
| --- |
| 21 **3** 2 12.0 9.0 0.0 -9.9 55 'Wellington STW ' |

### A Determinand Number of zero is used for discharge flow as in:

|  |
| --- |
| 22 **0** 2 2.5 0.5 0.0 -9.9 365 'Brickton STW - flow ' |

## Distributions of Discharge Flow and Discharge Quality

### The third item is a code which defines the statistical distribu­tion assumed for this set of data on discharge quality (or flow):

|  |
| --- |
| 21 3 **2** 12.0 9.0 0.0 -9.9 55 'Wellington STW ' |

### The protocol is the same used for river quality and river flow.

### The above example, which refers to code number 2, will assume that discharge quality follows a Log-normal Distribution (for determinand number 3, Ammonia).

### The options are listed below. Types 6, 7 and 9 apply only to discharge quality and not to discharge flow:

|  |  |
| --- | --- |
| Table 0.4: Types of data on discharge flow and quality | |
| 0 | Constant |
| 1 | Normal Distribution |
| 2 | Log-normal Distribution |
| 3 | 3 parameter Log-normal Distribution |
| 4 | Non-parametric Distributions |
| 5 | Seasonal (monthly) data |
| 6 | As 2 but the data are taken as loads and not as concentrations (§117) |
| 7 | As 5 but the data are taken as loads and not as concentrations (§117) |
| 8 | Monthly structure |
| 9 | Non-parametric distribution of loads |

### When setting up a new data file, it is good practice to assume that flow and quality are Log-normal (Type 2). More complex distributions can be introduced later if the results of SIMCAT prove sensitive to these assumptions and similar in scale to the impacts of the numbers of samples.

## Specifying discharge data as loads

### Types 6 and 7 are similar to types 1 and 2 except that they specify loads, not concentrations. Type 9 is like type 4 but for loads, not concentrations.

### The units of load are assumed to be those corresponding to the product of flow and concentration. This would be “kg/day” if flow were “megalitres per day” and if concentration were “mg/litre”.

### The distributions are assumed to be normal for type 6 and log-normal for type 7. For type 9, non-parametric, the data are placed a file whose structure is the same as for Type 4, except that the values are loads.

## Statistics of Discharge Flow and Quality (Types 0 - 4)

### Some of the next few items in the record will depend on the type of distribution which has been selected. As a rule, however you will need to specify the **mean**:

|  |
| --- |
| 21 3 2 **12.0** 6.0 0.0 -9.9 55 'Wellington STW ' |

This is followed by the corresponding **standard deviation**:

|  |
| --- |
| 21 3 2 12.0 **6.0**  0.0 -9.9 55 'Wellington STW ' |

### The sixth number in the record is the value for the Shift for a Three-parameter Log-normal Distribution. You will seldom need a value that is not zero.

|  |
| --- |
| 21 3 **2** 12.0 6.0 **0.0**  -9.9 55 'Wellington STW ' |

After this there are the correlation coefficient (§119) and the number of samples.

|  |
| --- |
| 21 3 2 12.0 6.0 0.0 **-9.9** **55** 'Wellington STW ' |

### For the discharge flow the second number is always zero.

|  |
| --- |
| 21 **0** 2 13.0 9.0 0.0 -9.9 55 'Wellington STW - flow ' |

### The units for discharge flow will be the same as those for river flow and as defined earlier (§30; §81). The units for discharge quality will be the same used for river qu2ality as defined above (§51; §96).

### The number of samples, "55", cited in the example for discharge flow given above and below, can be a surrogate for uncertainty in the estimates of the summary statistics, or it may be that the estimates of the summary statistics (the mean and standard deviation of 12.0 and 9.0, respectively) are based on a particular number of sample results. Use a high value for the number of samples if you are confident you have precise estimates.

|  |
| --- |
| 21 **0**  2 13.0 9.0 0.0 -9.9 **75** 'Wellington STW - flow ' |

### You might be dealing with discharges that do not operate now, but which may do so in future. It can be important to include these throughout the study, but to enter zero for the mean and standard deviation when the discharge is not operating. This discipline can be important if you want to use Gap Filling.

### Later, when calculating the effect of the new discharges you would replace these zeroes with the expected flows.

## Site Specific Correlation for Discharge Flow and Quality

### The seventh item of data in each record for the discharge data is nearly always given the value -9.9. This item is reserved for in­troducing special correlation. For discharge flow, the correlation defines that between the discharge flow and the master set of river flow data. For discharge quality, the correlation defines that between the discharge flow and discharge quality (§62).

|  |
| --- |
| 21 3 2 12.0 9.0 0.0 **-9.9** 55 'Wellington STW ' |

### The value of -9.9, or any other value outside the range from plus 1.0 to minus 1.0, signifies that this option is not to be used and that the default option will apply. This imposes a default correlation coefficient of 0.6 between river flow and the flow from sewage treatment works. Or, if the record applies to discharge quality, zero correlation between this discharge quality and discharge flow at this site.

### Similarly, the value of 0.0 will be over-written as -9.9 and the default correlation imposed. If you wanted to impose zero correlation you must specify a near-zero value, say, 0.0001.

## Non-parametric Distributions (Type 4)

### Option number 4, non-parametric distributions need special care because in this case the format of the line of data is different.

### Instead of the three numbers giving the mean, the standard devia­tion and the shift, you will need to specify in single quotes the name of a data file which holds your data for the non-parametric distribution. The format of this data file is the same as described for river flow in §84.

|  |
| --- |
| 21 3 4 ‘Wflow.npd ' -9.9 55 'Wellington STW ' |

### The value of -9.9 is as discussed above (§119), and the value, 55, is the same item as before – the number of samples that SIMCAT will use to estimate confidence limits. Even if this is the same as the number of items in ‘Wflow.npd’ it needs to be specified here too.

### The file must be in the same folder as your main SIMCAT data-file. The stem of the filename, *Wflow*, must be 64 characters or less.

### As before, the number of samples, "55", cited in the example for discharge flow given above and below, can be a surrogate for uncertainty in the estimates of the summary statistics. You can use a high value for the number of samples if you are confident you have precise estimates.

### The following structure, with no entry for the number of samples, is also read as correct by SIMCAT for non-parametric distributions of discharge flow and discharge quality. In this case the number of samples will be set within SIMCAT to a default value of 24.

|  |
| --- |
| 1 0 4 ‘Wflow.npd’ -9.9 'Wellington STW ' |

|  |
| --- |
| 1 3 4 ‘Wflow.npd’ -9.9 'Wellington STW ' |

## Monthly Data for Discharge Flow and Quality (Type 5)

### Type 5, **monthly data** are specified in much the same way as a non-parametric distribution:

|  |
| --- |
| 1 3 **5 'mon.npd'** -9.9 'Wellington STW ' |

### The data file must reside in the same folder as your SIMCAT data file. The stem of the filename, *seas*, must be 64 characters or less.

### In this case the file is called *mon.npd*. The data-file comprises four rows of numbers:

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 15.0 | 12.0 | 11.0 | 8.0 | 6.0 | 3.0 | 2.0 | 5.0 | 6.0 | 10.0 | 14.0 | 16.0 |
| 3.0 | 2.0 | 1.8 | 1.0 | 0.8 | 0.3 | 0.1 | 0.4 | 0.5 | 1.2 | 2.1 | 3.6 |
| 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| -9.9 | -9.9 | -9.9 | -9.9 | -9.9 | -9.9 | -9.9 | -9.9 | -9.9 | -9.9 | -9.9 | -9.9 |

### Each column is a month in the year. The rows give, for each month, the mean, the standard deviation, the shift (nearly always zero) and any special correlation coefficient. These are all monthly versions of the Log-normal data described above (§118)

## Distributions with a monthly structure (Type 8)

### Type 8 is similar Type 5 except that the monthly structure is fitted within a specified annual structure. Type 8, **monthly structure** is specified in much the same way as a non-parametric distribution:

|  |
| --- |
| 1 3 **8**  'struct.npd' -9.9 33 'Head of Upper Ouse ' |

### The filename, *struct.npd*, can be 64 characters or less. The data file must reside in the same folder as your SIMCAT data file. The data-file comprises the line of annual data followed by five rows of numbers:

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 2 1.0 0.4 0 .0 -9.9 | | | | | | | | | | | |
| 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 |
| 0.6 | 0.4 | 0.4 | -0.5 | -0.5 | -0.5 | -0.5 | -0.5 | -0.5 | 0.5 | 0.5 | 0.9 |
| 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| -9.9 | -9.9 | -9.9 | -9.9 | -9.9 | -9.9 | -9.9 | -9.9 | -9.9 | -9.9 | -9.9 | -9.9 |

The first line in the file is the annual data. This is similar to that specified above (§98) for an annual distribution. The first line comprises: the type of distribution (2), the annual mean (1.0), the standard deviation (0.4), the shift (0.0) and the correlation coefficient (-9.9).

|  |
| --- |
| 2 100.0 10.0 0 .0 -9.9 |

After this come rows of 12 numbers. Each row gives values for the months January to December:

* the types of distribution (Row 1)
* the additions to the annual mean that define the monthly mean (Row 2). The 12 items must sum to zero.
* the changes in standard deviation that define the monthly standard deviation (Row 3). These must sum to zero.
* the changes in shift that define the monthly shift (Row 4)
* the monthly correlation coefficient (Row 5)

### One reason for setting up this method is that some forms of diffuse pollution were best described as monthly discharges of load. This type of pollution might be specified as a distinct mean and standard deviation for each month. This means answering questions like – what is the contribution of the load in January to the annual mean concentration or to the annual 95-percentile?

## Intermittent Discharges

### The procedure described above (§120) for Non-parametric Distributions can also be used to define the flow data for an intermittent discharge (§M).

### This is done by specifying a set of flow data in which the required proportion of items are specified as zero. The discharge is then specified as a Feature 3 (Sewage Treatment Works - §155) or Feature 5 (Industrial Discharge - §158) which uses the specified Discharge Flow and Quality Data-set.

### An intermittent discharge specified in this way will have flows which are correlated with the flow in the receiving river if Feature 3 is used. The default correlation coefficient, 0.6, will be the same as that between river flow and the flow from a Sewage Treatment Works. The default is zero correlation for an Industrial Discharge.

### As noted above (§84), an intermittent discharge can also be defined by using Feature 2 (§153) with a Non-parametric Distribution for River Flow.

## End of Discharge Flow and Quality

### Finally, you need to use the usual device to indicate the end of this section of data.

|  |
| --- |
| \*\*\*\*\* indicator of end of data for discharges \*\*\*\*\*\*\*\* |

## Discharge Flow and Quality from the Example Data File

**======================================================================6**

**======= Section [F] Effluent Flow & Quality ==========================6**

**======================================================================6**

**======= Effluent Flow and Quality Data-Sets follow. For each Data-Set 6**

**======= there is a line for the flow and a line for each determinand 6**

**======= each determinand in turn: 6**

**======= For each line the following are entered: 6**

**======= (a) the code number of the data-set (this will be referred 6**

**======= to in the data on Feature (8) 6**

**======= (b) the code number for the determinand (zero for flow) 6**

**======= (c) the code number of type of distribution: 6**

**======= 0 - constant, uniform values 6**

**======= 1 - a Normal Distribution 6**

**======= 2 - the Log-Normal Distribution 6**

**======= 3 - a Three-Parameter Log-Normal Distribution 6**

**======= 4 - non-parametric distribution 6**

**======= 5 - monthly data - distribution for each month 6**

**======= For distribution types 4,5 and 9 the items (d),(e) and 6**

**======= (f) below do not appear. Instead is shown the name of 6**

**======= the data file holding the data for the distribution. 6**

**======= For example: 'npar.npd' (Note the need for this type of 6**

**======= quotation marks) 6**

**======= 6 - as 2 but the data (d) and (e) refer to loads 6**

**======= 7 - as 5 but the data in the data file refer to loads 6**

**======= 8 - monthly structure 6**

**======= 9 - non-parametric distribution of loads 6**

**======= (d) the mean value 6**

**======= (e) the standard deviation 6**

**======= (f) the shift parameter for distribution types 3: for 6**

**======= Distribution Type 0, 1 or 2: zero or blank 6**

**======= (g) reserved for non-standard correlation coefficient 6**

**======= (h) number of samples used to compute the mean 6**

**======= (i) the name of the discharge. This is used for 6**

**======= identification. It is not needed by SIMCAT 6**

**======================================================================6**

**======= The following types of Feature use effluent data: 6**

**======================================================================6**

**======= 3 - sewage works or sewage discharge 6**

**======= 5 - industrial effluent discharge 6**

**======= 12 - intermittent discharge 6**

**======= 15 - start point for diffuse pollution 6**

**======= (effluent type) 6**

**======= 40 - start point for aggregated CSOs 6**

**======= 42 - start point for aggregated sewage works 6**

**======= 60 - other point sources 6**

**======= 61 - private wastewaters 6**

**======b=c=========d========e=====f========g===h=====i=================6**

**1 0 2 4.00 1.80 1.00 -9.9 365 'Wellington STW'**

**1 1 2 91.50 8.20 0.00 -9.9 30 ''**

**1 2 2 35.00 30.00 20.00 -9.9 56 ''**

**1 3 2 15.00 9.00 0.00 -9.9 55 ''**

**1 4 2 0.50 0.20 0.00 -9.9 56 ''**

**1 5 2 4.50 2.20 0.00 -9.9 56 ''**

**2 0 2 2.50 0.80 0.00 -9.9 365 'Brickton STW'**

**2 1 2 95.00 4.60 0.00 -9.9 30 ''**

**2 2 2 35.00 30.00 0.00 -9.9 56 ''**

**2 3 2 15.00 9.00 0.00 -9.9 55 ''**

**2 4 2 1.00 0.50 0.00 -9.9 56 ''**

**2 5 2 4.50 2.20 0.00 -9.9 56 ''**

**3 0 2 2.00 0.70 0.00 -9.9 365 'Appleford STW'**

**3 1 2 95.00 4.60 0.00 -9.9 30 ''**

**3 2 3 17.00 9.00 4.00 -9.9 56 ''**

**3 3 2 15.00 9.00 0.00 -9.9 55 ''**

**3 4 3 2.00 1.20 0.00 -9.9 56 ''**

**3 5 2 1.50 2.20 0.00 -9.9 56 ''**

**4 0 2 0.10 0.10 0.00 -9.9 365 'Allied Industries'**

**4 1 1 380.00 22.00 0.00 -9.9 10 ''**

**4 2 2 80.00 50.00 0.00 -9.9 10 ''**

**4 3 2 0.00 0.00 0.00 -9.9 10 ''**

**4 4 2 0.00 0.00 0.00 -9.9 10 ''**

**4 5 2 4.50 2.20 0.00 -9.9 56 ''**

**6 0 4 'inter.npd' -9.9 365 'New Mill Storm Overflows'**

**6 1 2 60.00 4.60 0.00 -9.9 30 ''**

**6 2 3 163.00 30.00 4.00 -9.9 26 ''**

**6 3 2 20.00 6.00 0.00 -9.9 27 ''**

**6 4 3 0.00 0.00 0.00 -9.9 28 ''**

**6 5 2 2.50 2.20 0.00 -9.9 56 ''**

**8 0 2 1.00 0.40 0.00 -9.9 365 'Diffuse Source'**

**8 1 2 91.00 12.60 0.00 -9.9 30 ''**

**8 2 2 61.00 30.00 0.00 -9.9 56 ''**

**8 3 2 15.00 9.00 0.00 -9.9 55 ''**

**8 4 2 1.00 0.50 0.00 -9.9 56 ''**

**8 5 2 4.50 2.20 0.00 -9.9 56 ''**

**\*\*\*\*\*\*\*\*\*\*\*\* indicator of end of effluent flow and quality data \*\*\*\*\*\*6**

# RIVER QUALITY TARGETS

## Introduction

### River water quality targets are used in SIMCAT’s assessment of compliance. Also, when run with Automatic Permit-setting (Run Types 7, 8 or 9), SIMCAT seeks to calculate automatically the discharge standards needed to achieve the river targets at the point of mixing. This is called a backward calculation within the system called RQP (River Quality Planning) used for single discharges.

### The portion of the Example Data File dealing with targets is shown at §131. Again, most of this is made up of comments. The actual data are in **bold type**.

### If you do not plan to use River Quality Targets and you will have no entries to make to this section of SIMCAT's data. Even if no data are entered, an End of Data indicator is still required.

### Each line of data specifies one set of data. Each line has a num­ber of items. These items are now described in turn.

|  |
| --- |
| 1 0.0 2.0 1.5 0.0 |

## Code Number for a Set of River Targets

### The first item is a Code Number for a set of Targets – the Target Data Set:

|  |
| --- |
| **1**  0.0 5.0 1.5 0.0 |

### The Code Number will be used further down the data file in the data for Features (§146, §147). It will refer, for example, to a set of targets downstream of a discharge.

### After the Code Number, the next few items are the river quality targets for the individual determinands. A zero means that no tar­get applies.

### The targets apply to the determinands according to the order of the Determinand Codes (§46). In this data file Determinand Number 1 is Chloride and no target is specified:

|  |
| --- |
| 1  **0.0**  5.0 1.5 8.0 |

### In this set of targets, the target for the second determinand, BOD, is 5.0 mg/l:

|  |
| --- |
| 1 0.0 **5.0** 1.5 8.0 |

### The third target is for Ammonia:

|  |
| --- |
| 1 0.0 5.0 **1.5** 8.0 |

### The fourth target is for Dissolved Oxygen but SIMCAT cannot calculate automatically (by Run Types 7, 8 or 9 (§7)), the discharge standards needed to achieve targets in the river for Dissolved Oxygen.

|  |
| --- |
| 1 0.0 5.0 1.5 **8.0** |

### You can of course work out by trial-and-error the measures needed to achieve any targets.

## Standards for a System of Classification

### This section of data can also be used to enter a system of classification. This is done by entering data with a negative number for the code number. In the following example the standards are taken to apply to Class 1.

|  |
| --- |
| **-1**  0.0 5.0 1.5 0.0 |

### Subsequent entries, each with a negative Code number, define, for example, the standards for classes 2, 3 and 4.

### The system of classification is applied throughout the entire modelled catchment. It is overruled by any extra information on classification that is defined for particular Reaches (§77) or Features (§146).

## End of Data on River Quality Targets

### Finally, you need to indicate the end of this section of data.

|  |
| --- |
| \*\*\*\*\* indicator of end of data for river quality targets \*\*\*\*\*\*\*\* |

### You will need this indicator even if your data file contains no data on River Targets.

## Compliance with river quality targets

### The code that is used to define the summary statistics for river quality targets is set as part of the determinand data (§60).

### SIMCAT can handle the case where in the same run a single determinand has several standards provided all the targets for the determinand have the same summary statistic. (A mix of targets with different summary statistics can be looked at by setting up a data file in which a determinand is duplicated).

## River Quality Targets

**======================================================================7**

**======= Section [6] River Quality Targets ============================7**

**======================================================================7**

**======= The data sets for River Quality Targets follow. There is one 7**

**======= line for each set. It contains: 7**

**======= (a) a code number to be cited in the Feature data below (8) 7**

**======================================================================7**

**======= The targets follow. These are defined as the statistics 7**

**======= entered above (as item (l)) within data on Determinands (1) 7**

**======================================================================7**

**======= If the Determinand data contain no such definition, these 7**

**======= standards are defined as the statistic set up above (Set 0) 7**

**======= as the definition of Mean Mode 7**

**======================================================================7**

**======= (b-k) the targets for up to 10 determinands. Zero indicates 7**

**======= that no target is to be applied. 7**

**======================================================================7**

**======= These targets will be over-written by any targets that have 7**

**======= been specified above with the data for individual Reaches (3) 7**

**======================================================================7**

**======= Negative values specified for (a) are taken as defining a 7**

**======= system of classification. (The positive value of (a) is still 7**

**======= used as a target within the data on Features). 7**

**======= This classification is over-written by any classification 7**

**======= entered for particular reaches with the Reach Data (3) 7**

**======a======b======c======d======e======f======g======h======i=======7**

**1 0.00 5.00 1.50 0.00 0.10**

**2 0.00 8.00 3.00 0.00 0.10**

**3 250.00 5.00 1.50 0.00 0.10**

**\*\*\*\*\*\*\*\*\* indicator of the end of data on river quality targets \*\*\*\*\*\*7**

# DATA ON FEATURES

### This section shows you how to set up data for Features. This por­tion of the Example Data File is shown at §184. Most of §184 is comments. The actual data are in **bold type**.

### There are 49 types of Feature (§132). Each has a unique Code Number. The different types of Features are outlined in the next sections of text. First, we go through setting up of the data which are common to all Features. Then we deal with and the rest of the data for the most common Features (Numbers 1-5, 7, and 10). Special aspects of the less common Features (Numbers 6, 8, 9, 11-16) are detailed from §162.

## Table: Types of Feature

|  |  |
| --- | --- |
| Code Number | Description of Feature |
| 1 | River Quality Monitoring Point |
| 2 | Stream or Tributary |
| 3 | Sewage Treatment Works |
| 4 | River Flow Gauging Station |
| 5 | Industrial Discharge |
| 6 | Plotting Point |
| 7 | Abstraction |
| 8 | Weir |
| 9 | Point of River Flow Regulation |
| 10 | Upstream Boundary |
| 11 | Bifurcation |
| 13 | Start of Diffuse Pollution (River Type) |
| 14 | End of Diffuse Pollution (River Type) |
| 15 | Start of Diffuse Pollution (Discharge Type) |
| 16 | End of Diffuse Pollution (Discharge Type) |
| 17 | Discharge with zero flow |
| 18 | Abstraction (the Negative Discharge) |
| 19 | Abstraction (the Negative Discharge) |
| 20 | Bifurcation Start (abstraction of river flow distribution) |
| 21 | Bifurcation End (re-entry of river flow distribution) |
| 22 | Bifurcation Start (abstraction of discharge flow distribution) |
| 23 | Bifurcation End (re-entry of discharge flow distribution) |
| 24 | Sub-catchment boundary |
| 25 | Switch on Diffuse Pollution - agriculture (livestock) |
| 26 | Switch off Diffuse Pollution - agriculture (livestock) |
| 27 | Switch on Diffuse Pollution - agriculture (arable) |
| 28 | Switch off Diffuse Pollution - agriculture (arable) |
| 29 | Switch on Diffuse Pollution - highways |
| 30 | Switch off Diffuse Pollution - highways |
| 31 | Switch on Diffuse Pollution - urban |
| 32 | Switch off Diffuse Pollution - urban |
| 33 | Switch on Diffuse Pollution - atmospheric deposition |
| 34 | Switch off Diffuse Pollution - atmospheric deposition |
| 35 | Switch on Diffuse Pollution - background |
| 36 | Switch off Diffuse Pollution - background |
| 37 | Switch on Diffuse Pollution - septic tanks |
| 38 | Switch off Diffuse Pollution - septic tanks |
| 39 | Mine waters |
| 40 | Switch on Aggregated CSOs |
| 41 | Switch off Aggregated CSOs |
| 42 | Switch on Aggregated sewage works |
| 43 | Switch off Aggregated sewage works |
| 44 | Flow into lake |
| 45 | Flow from lake |
| 46 | Switch on Diffuse Pollution - mines |
| 47 | Switch off Diffuse Pollution - mines |
| 48 | Switch on Diffuse Pollution - birds, boats and angling |
| 49 | Switch off Diffuse Pollution - birds, boats and angling |
| 50 | Switch on User-defined Diffuse Pollution |
| 51 | Switch off User-defined Diffuse Pollution |
| 52 | Switch on User-defined Diffuse Pollution |
| 53 | Switch off User-defined Diffuse Pollution |
| 54 | Switch on User-defined Diffuse Pollution |
| 55 | Switch off User-defined Diffuse Pollution |
| 56 | Switch on User-defined Diffuse Pollution |
| 57 | Switch off User-defined Diffuse Pollution |
| 58 | Switch on User-defined Diffuse Pollution |
| 59 | Switch off User-defined Diffuse Pollution |
| 60 | Discharges from Landfill |
| 61 | Private Wastewater Discharges |

## Data Common to All Features

### Each line of data specifies the data for one Feature. Each line has a number of items. These are now described in turn. First, we deal with four items which are common to all types of Feature. These are the first four items in each line.

|  |
| --- |
| 'Pig Farm Gauging Station ' 4 1 4.0 4 0 4 0 0 |

## Name of the Feature

### First is the Feature Name - up to 40 characters enclosed in single quotation marks, as in:

|  |
| --- |
| 'Pig Farm Gauging Station ' 4 1 4.0 4 0 4 0 0 |

## Feature Code

### Next come the Code Number, defined in Table §132, which tells SIM­CAT whether this Feature is a sewage treatment works, a monitoring station or whatever:

|  |
| --- |
| 'Pig Farm Gauging Station '  **4**  1 4.0 4 0 4 0 0 |

## Negative Value of the Feature Code for a Discharge

### If the Code Number is present as a negative number it tells SIM­CAT that in Run Types 7, 8 or 9 this Feature will not be subject to calculations of a discharge quality needed to meet a river quality target (§3).

|  |
| --- |
| 'Wellington STW ' **-3** 1 8.0 0 1 0 0 7 |

## Reach Code

### The next item defines the Reach on which the Feature is located. The Reach Codes will have been set up in §64. In following example, Pig Farm Gauging Station is on Reach Number 1:

|  |
| --- |
| 'Pig Farm Gauging Station ' 4  **1** 4.0 4 0 4 0 0 |

## Distance from Head of Reach

### The next item defines the location of the Feature in terms of the distance, in kilometres, from the head of the reach. Pig Farm Gauging Station is 4.0 km from the head of Reach Number 1:

|  |
| --- |
| 'Pig Farm Gauging Station ' 4 1  **4.0** 4 0 4 0 0 |

### For Bifurcations, Feature 11, the value entered in this field takes a different meaning (§170).

## Code Numbers for Flow and Quality

### This concludes the description of the first four fields. The entries for the remaining fields vary according to the type of Feature and are discussed from §143 onwards. The fifth and sixth fields are used, as necessary, to define the Code Numbers for sets of data in flow and quality. The seventh and eighth fields define the same types of codes but these are used for Gap-filling. The ninth code is used to refer to the Code Number for a set of River Quality Targets (§127).

### The requirements for each type of Feature are listed in a table (§140). In this table, a tick, √, indicates that a non-zero entry is required. A zero, 0, means that the item is not required and that a zero should be entered. The letter, “U”, indicates that a non-zero value can be entered if you want it. This last case applies only to the fields used for Gap-filling - all Features can be used as a point of Gap-filling.

## Table showing fields used for features

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | Type of Feature (1) | | | Field  (see below for the key) | | | | | | | | |
| 2 | 3 | 4 | 5 | 6 | 7 | | 8 | 9 |
| 1 | River Quality Monitoring Point | | | √ | √ | √ | 0 | √ | U | | U | U |
| 2 | Stream or Tributary | | | √ | √ | √ | √ | √ | U | | U | U |
| 3 | Discharge from Sewage Treatment Works | | | √ | √ | √ | 0 | √ | U | | U | U |
| 4 | River Flow Gauging Station | | | √ | √ | √ | √ | 0 | U | | U | U |
| 5 | Industrial Discharge | | | √ | √ | √ | 0 | √ | U | | U | U |
| 6 | Plotting Point | | | √ | √ | √ | 0 | 0 | U | | U | U |
| 7 | Abstraction | | | √ | √ | √ | √ | √ | U | | U | U |
| 8 | Weir | | | √ | √ | √ | 0 | 0 | U | | U | U |
| 9 | Point of River Flow Regulation | | | √ | √ | √ | √ | √ | U | | U | U |
| 10 | Upstream Boundary | | | √ | √ | 0 | √ | √ | U | | U | U |
| 11 | Bifurcation | | | √ | √ | 0 | √ | √ | U | | U | U |
| - | Start any form of Diffuse Pollution (River Type) | | | √ | √ | √ | √ | √ | U | | U | U |
| - | End Diffuse Pollution (River Type) | | | √ | √ | √ | 0 | 0 | U | | U | U |
| - | Start form of Diffuse Pollution (Discharge Type) | | | √ | √ | √ | 0 | √ | U | | U | U |
| - | End Diffuse Pollution (Discharge Type) | | | √ | √ | √ | 0 | 0 | U | | U | U |
| 17 | Discharge with zero flow | | | √ | √ | √ | 0 | 0 | U | | U | U |
| 18 | Abstraction (the Negative Discharge) | | | √ | √ | √ | √ | 0 | U | | U | U |
| 19 | Abstraction (the Negative Discharge) | | | √ | √ | √ | √ | 0 | U | | U | U |
| 20 | Bifurcation Start (removal of river flow) | | | √ | √ | 0 | √ | √ | U | | U | U |
| 21 | Bifurcation End (re-entry of river flow) | | | √ | √ | 0 | √ | √ | U | | U | U |
| 22 | Bifurcation Start (removal of discharge type distribution) | | | √ | √ | 0 | √ | √ | U | | U | U |
| 23 | Bifurcation Start (re-entry of discharge flow) | | | √ | √ | 0 | √ | √ | U | | U | U |
|  | Key for the columns | | | | | | |  | | | |
| 1 | Name of Feature | | | | | | |
| 2 | Code for Type of Feature | | | | | | |
| 3 | Number of Reach | | | | | | |
| 4 | Distance from Head of Reach | | | | | | |
| 5 | Code Number for a River Flow Dataset | | | | | | |
| 6 | Code Number for a Quality Dataset | | | | | | |
| 7 | Code Number for a River Flow Dataset | | | | | | |
| 8 | Code Number for a Quality Dataset | | | | | | |
| 9 | Code Number for any River Quality Target | | | | | | |
| 10 | Code Number for any reference to GIS data | | | | | | |

## Code of -1 for a River Flow Dataset for a Diffuse Input Feature

### For the types of Features that are used to define diffuse pollution there is an option to declare a value of -1 for the River Flow Dataset.

### This is used for types of diffuse pollution that will share a single set of flow data. The set of flow data to be shared is the Diffuse Reach Inflow that has been defined for the Reach (§69) on which the Feature is declared as located. In the following data for a Reach this will be flow data defined for as number **14**:

**6** 'River Avon ' 10.0 1 2 3 **14** 11 1.0 1.0

### If the Code Number for the river flow dataset for a Feature located on this Reach is replaced by **-1** it tells SIM­CAT that the Feature is one of what may be several Features that will share a common dataset for river flow:

'Livestock (25) ' 25 **6** 0.0 **-1** 2 0 0 0 ' '

'Arable (27) ' 27 **6** 0.0 **-1** 3 0 0 0 ' '

'Arable (29) ' 29 **6** 0.0 **-1** 4 0 0 0 ' '

'Urban (31) ' 31 **6** 0.0 **-1** 5 0 0 0 ' '

The shared dataset of river flow will be the particular set of flow data specified as the Diffuse Reach Inflow for Reach Number **6** (§69) – number **14** in the above example.

No extra flow will be added to the river by the four features listed above with **-1** as their definition of their river flow datasets. Instead the quality (concentrations) specified for each of these four will be added to whatever concentrations have been assigned to the set of river flow defined for Reach Number 6 – the Diffuse Inflow Code for River Quality (§70). For example, river quality set number **11** for Reach **6**:

**6** 'River Avon ' 10.0 1 2 3 14 **11** 1.0 1.0

The process continues down the Reach until the type of Diffuse Pollution is switched off (§132) or until the end of the Reach Number 6.

Further details are at paragraph (§178) – specifying diffuse pollution as an added concentration. I

If the sets of data for quality are include determinands whose levels are expressed as loads rather than concentrations (Type 7, for example, rather than number 2 used for a log-normal distribution), the load added to the river is calculated from the values derived from the data-set multiplied by the length of river since the last addition of the particular type of diffuse pollution – that is, since the previous upstream Feature (or if there are none – since the head of the Reach).

This applies to data-sets numbered **2, 3** etc in the following, for any determinands defined as added using loads rather than concentrations.

'Livestock (25) ' 25 **6** 0.0 **-1** **2** 0 0 0 ' '

'Arable (27)' 27 **6** 0.0 **-1** **3** 0 0 0 ' '

‘Highway (29)' 29 **6** 0.0 **-1** **4** 0 0 0 ' '

'Urban (31)' 31 **6** 0.0 **-1** **5** 0 0 0 ' '

## Negative Feature Code for a Reach Headwaters (add diffuse pollution)

Feature Code 10 sets up the flow and quality at head of a new Reach – a reach not formed by the mixing together of any of the other Reaches.

A negative sign in front of this Feature Code (10) tells SIMCAT to add diffuse pollution (§176 and §177) to the flow specified for Feature Type 10 for the starting headwaters of the Reach – a Reach Boundary (§169).

This is done by changing the Feature Type from 10 to **-10** as in:

'Head of River Avon ' **-10** 2 0.0 **22** **2** 0 0 0

The diffuse pollution will be added to the flows defined by set number **22** – an addition the concentrations define by the set of river quality data – **2**.

The types of diffuse pollution that can be added in this way are those defined as Features:

* agricultural livestock (Features 25 and 26)
* agricultural arable (Features 27 and 28)
* highway runoff (Features 29 and 30)
* urban runoff (Features 31 and 32)
* atmospheric deposition (Features 33 and 34)
* natural background (Features 35 and 36)
* septic tanks (Features 37 and 38)
* aggregated CSOs (Features 40 and 41)
* aggregated sewage works (Features 42 and 43) (discharge)
* diffuse mines (Features 46 and 47)
* birds, boats and angling (Features 48 and 49)
* named by user (Features 50 and 51)
* named by user (Features 52 and 53)
* named by user (Features 54 and 55)
* named by user (Features 56 and 57)
* named by user (Features 58 and 59)

Diffuse Types (13) and (15) cannot be added to the flows of the Reach Headwaters.

The types of diffuse pollution in the above list that will be added to the Reach Headwaters are those Features which in the data file have been assigned negative Feature Type number for their own value. They have also been given a distance of zero (from the head of the Reach) and a negative code number for their own set of flow data (§141).

In the cases listed below for Livestock (**25**), Arable (**27**) and Urban (31), the Feature Code is set as negative. In these cases (but not for Highway (**29**)), the quality specified by the sets of quality data numbered 2, 3 and 5 will be added to the flows (set number **22**) defined as added by Feature Type 10:

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| ‘Livestock (25) ' | **-25** | 6 | 0.0 | **-1** | **2** | 0 | 0 | 0 | ‘ ‘ |
| 'Arable (27) ' | -**27** | 6 | 0.0 | **-1** | **3** | 0 | 0 | 0 | ‘ ‘ |
| 'Highway (29) ' | **29** | 6 | 0.0 | **-1** | **4** | 0 | 0 | 0 | ‘ ‘ |
| 'Urban (31) ' | **-31** | 6 | 0.0 | **-1** | **5** | 0 | 0 | 0 | ‘ ‘ |

For the sets of river quality data numbered 2, 3, 6, 7, 5 and 8 diffuse additions will be made to the headwaters (for data are defined as concentrations or loads). Data types 4 (non-parametric of concentrations), 9 (non-parametric loads), 10 (power-curve for concentrations) and 11 (power-curve for loads) are not yet included.

## Other Fields

### We now go through the different types of Feature and describe the remaining fields. We start with fields 7 and 8. These deal with Gap-filling.

## River Flow Data-set for Gap-filling

### This item is often zero but can be specified for any type of Fea­ture. A non-zero entry defines the Feature as a **Flow Gap Filling Point.** This need not be a Flow Gauge, it can be any Feature where you have measured or estimated flow and where you might want to make SIMCAT's calculations produce the same flows.

### This item defines the Code Number of a River Flow Data-set in §79 which SIMCAT will use in Gap-filling (Run Type 1, 3, 5 or 6). SIMCAT will invent the sources and sinks of river flow which are needed to obtain a perfect fit to the mean and 5-percentile river flow defined in the Data-set (§**G**).

### So, for Pig Farm Gauging Station, SIMCAT will fit to the flow data defined for Data-set number 4:

|  |
| --- |
| 'Pig Farm Gauging Station ' 4 1 4.0 4 0  **4** 0 0 |

### For a Flow Gauging Station, this Data-set will usually be the same as that specified earlier, as in:

|  |
| --- |
| 'Pig Farm Gauging Station ' 4 1 4.0  **4**  0  **4** 0 0 |

### But this is not essential.

### Often you will have estimated flow data for a point on a river just upstream of a discharge of discharge. You can then make a Sewage Treatment Works into a Flow Gap Filling Point, as in:

|  |
| --- |
| 'Wellington STW ' 3 1 2.0 0 1 **16**  0 3 |

### Left to itself, SIMCAT, will extrapolate in the downstream direc­tion any adjustment to river flow needed to secure a fit. If you prefix the Data-set Code with a minus sign you will suppress this:

|  |
| --- |
| 'Pig Farm Gauging Station ' 4 1 4.0 4 0 **-4** 0 0 |

### Left to itself, SIMCAT, will interpolate in the upstream direction and average out over the upstream length of river any adjustments to river flow needed to secure a fit. The upstream boundary for this interpolation will be set by the boundary of the Reach or the last Flow Gap Filling Point, whichever is closest. If you start a new Reach at the Feature for which you calculated the adjustment you will suppress this upstream interpolation.

### Using these two devices you can use SIMCAT to transform the Flow Duration Curve at any point in the river system. This is useful in simulating the effects of abstractions which take water intermit­tently and in a way which may not be governed by a simple rule based on the prevailing flow in the river (§164).

## River Quality Data-set for Gap-filling

### This item is often zero but can be specified for any type of Fea­ture. A non-zero entry defines the Feature as a **River Quality Gap Filling Point**. This need not be a **River Quality Monitoring Station**, it can be any Feature where you have measured or es­timated river quality data and where you want to make SIMCAT's calculations reproduce the same river quality.

### This item defines the Code Number of a River Quality Data-set in §94 which SIMCAT will use in Gap-filling (Run Type 3, 5 or 6). SIMCAT will invent the sources and sinks of pollution which are needed to obtain a perfect fit to the mean and 95-percentile river quality defined in the Data-set.

### So for New Mill Monitoring Station, 1.0 km from the top of Reach Number 5, SIMCAT will fit to the river quality data defined for Data-set number 9:

|  |
| --- |
| 'New Mill Monitoring Station ' 1 5 1.0 0 9 0  **9**  0 |

### For a River Quality Monitoring Station, this Data-set will often be the same as that specified earlier, as in:

|  |  |
| --- | --- |
| |  | | --- | | 'New Mill Monitoring Station ' 1 5 1.0 0 **9** 0  **9**  0 | |

But this is not essential. You can also make any Feature into a River Quality Gap Filling Point, as in:

|  |
| --- |
| 'Wellington STW ' 3 1 2.0 0 1 0 **16**  3 |

### Left to itself, SIMCAT, will extrapolate in the downstream direc­tion any adjustment to river quality needed to secure a fit. If you prefix the Data-set Code with a minus sign you will suppress this:

|  |
| --- |
| 'New Mill Monitoring Station ' 1 5 1.0 0 9 0 **-9** 0 |

### Left to itself, SIMCAT, will interpolate in the upstream direction and average out over the upstream length of river any adjustments to river quality needed to secure a fit. The upstream boundary for this interpolation will be set by the boundary of the Reach or the last River Quality Gap Filling Point, whichever is closest. If you start a new Reach at the Feature you will suppress this.

### Using these two devices you can use SIMCAT to transform the River Quality Distribution at any point in the river system. This is useful in investigating cases where the data appear to indicate an unknown source of pollution.

### For Feature 8, **Weirs** (§168), this item is used to specify the code number for the river quality Data-Set defining quality downstream of the Weir. In other words, SIMCAT treats Weirs as a special River Quality Gap Filling Point which operates only on Dissolved Oxygen.

## River Quality Target

### The next field provides the option to include a River Quality Target by entering a code number for the required target (§127). For Features that are not discharges (Features that are not Types 3 and 5) this field can be used indicate a point on the reach where the Target changes. This will be reflected in the plotting of the targets on graphs.

|  |
| --- |
| 'New Mill Monitoring Station ' 1 5 1.0 0 9 0 9 **3** |

### 

### The target will use be used in Modes 7, 8 and 9 in SIMCAT’s efforts to calculate the discharge quality needed to meet targets of river quality.

Any targets specified for Features will be over-written by targets that are set out for Reaches as part of the set of data on Reaches.

## Zero River Quality Target Specified for Features

When the effluent has a zero value of the target set with the Feature Data (and there are no reach standards) the backward calculation is not done. A forward calculation (the effect of the current discharge) is done when the backward calculation is not required.

|  |
| --- |
| 'Wellington STW ' 3 1 2.0 01 0 0 **0** |

## River Quality Target Specified as 999 for Discharge

When the effluent has a value of 999 for the target set with the Feature Data, the backward calculation is not done for this effluent even if there are Reach standards.

|  |
| --- |
| 'Wellington STW ' 3 1 2.0 01 0 0 **999** |

## River Quality Target Specified as negative for Discharge

When the effluent has a value that is negative the target specified here will be used instead of any specified set for the Reach:

|  |
| --- |
| 'Wellington STW ' 3 1 2.0 01 0 0 **-3** |

## Reference to data held on a Geographical Information System

### The final field provides the option to include a reference. It can be used in data-files created by GIS as a means of transferring SIMCAT’s results back to the GIS for plotting on maps and diagrams.

### The field is up to 40 characters. SIMCAT still runs if it missing. An example follows as ‘568500337502’. This particular code is a map reference

|  |
| --- |
| 'Heacham Flow Gauge' 1 5 1.0 0 9 0 9 3 '568500337502' |

## Other Data for Features

### We now go through each type of feature in turn and set out the data required for each.

## River Quality Monitoring Station (Feature 1)

### This will usually be a point at which river quality is measured routinely. After the first four, common, items we need the following.

River Flow Data-set

### In other types of Feature, the next item refers usually to a set of data on river flow. This is not needed for a River Quality Monitoring Station. Zero is entered, as in:

|  |
| --- |
| 'Valley Bottom Monitoring Station ' 1 2 9.0  **0** 10 0 10 0 |

Quality Data-set

### The next item refers either to a set of data on river quality.

### For a River Quality Monitoring Station, you may want to specify the river quality measured at the site. You do this by specifying one of the Code Numbers for the sets of River Quality Data which you have listed in §94.

### If you choose to do this, details of these measurements of river quality will appear as information in the output from SIMCAT. For Valley Bottom Monitoring Station, a Feature of Type 1 located 9.0 km from the head of Reach Number 2, this is River Quality Data-set Number 10:

|  |
| --- |
| 'Valley Bottom Monitoring Station ‘ 1 2 9.0 0 **10** 0 10 0 |

### After these items, the next two fields will cover options discussed above (§144 and §145) for Gap-filling.

### The last field is the code number for the River Quality Target.

River Quality Target

### The final field provides the option to include a River Quality Target by entering a code number for the required target (§127). This will be reflected in the plotting of the targets on graphs.

|  |
| --- |
| 'New Mill Monitoring Station ' 1 5 1.0 0 9 0 9 **3** |

## Stream or Tributary (Feature 2)

### This Feature is used for a river which is too small to be defined as a Reach. Usually this will be a tributary which contains no discharges of importance, nor any other attributes considered important enough to be defined as Features. The stream is treated as a dis­charge of river water into the Reach.

### After the first four items of data, you will want to specify river flow and quality for the Feature.

River Flow Data-set

### The next item refers usually to a set of data on river flow. This is done by specifying one of the Code Numbers specified in §94. In this case, number 5.

|  |
| --- |
| 'Ouse Stream ' 2 1 6.0 **5**  1 0 0 0 |

Quality Data-set

### The next item refers to a set of data on river quality.

### ForStreams or Tributaries, you will specify the quality of the flow added to the Reach. In this case, number 1.

|  |
| --- |
| 'Ouse Stream ' 2 1 6.0 5  **1** 0 0 0 |

### After these items, the next two fields will cover options discussed above (§144 and §145) for Gap-filling.

### The last field is the code number for the River Quality Target.

River Quality Target

### The final field provides the option to include a River Quality Target by entering a code number for the required target (§127). This will be reflected in the plotting of the targets on graphs.

|  |
| --- |
| 'Ouse Stream ' 2 1 6.0 5 1 0 0 **2** |

## Flow Gauge (Feature 4)

### This will usually be a point at which river flow is measured routinely though it can be any point for which you have estimates of river flow.

### After the first four, common, items (§133) we need the following.

River Flow Data-set

### After the first four items, the next item refers usually to a set of data on river flow. This is done by specifying one of the Code Numbers set up in §79.

### For Flow Gauging Stations, you can specify the river flow measured or es­timated at this site. If you do this, details of these measure­ments will appear as information in the output from SIMCAT. For Pig Farm Gauging Station this is River Flow Data-set Number 4:

|  |
| --- |
| 'Pig Farm Gauging Station ' 4 1 4.0 **4** 0 4 0 0 |

Quality Data-set

### The next item refers usually to a set of data on river or discharge quality. This is not needed for a Flow Gauging Station. Zero is entered.

|  |
| --- |
| 'Pig Farm Gauging Station ' 4 1 4.0 4  **0** 4 0 0 |

### After these items, the next two fields will cover options discussed above (§144 and §145) for Gap-filling.

### The final field provides the option to include a River Quality Target.

River Quality Target

### The final field provides the option to include a River Quality Target by entering a code number for the required target (§127). This will be reflected in the plotting of the targets on graphs.

|  |
| --- |
| 'Pig Farm Gauging Station ' 4 1 4.0 4 0 4 0 **1** |

## Sewage Treatment Works (Feature 3)

### This is any continuous discharge of discharge. You will want to specify the flow and quality of the discharge and will eventually need to specify the river quality targets to be achieved downstream of the discharge.

### You need to make special provision for discharges that do not exist now but which are planned for the future. You should include these discharges as Features but give them zero flow when doing calculations for conditions before they come into operation.

### Flows from discharges from sewage treatment works are assumed correlated with river flow unless this is over-written (§119). The correlation coefficient is 0.6.

### After the first four, common, items we need the following.

River Flow Data-set

### Some types of feature, like Sewage Treatment Works (Type 3) or **In­dustrial Discharges** (Type 5) need no data on river flow. For these, a zero is entered:

|  |
| --- |
| 'Wellington STW '  **3**  1 2.0  **0** 1 0 0 3 |

Quality Data-set

### For the Feature called **Sewage Treatment Works**, you will want to specify the flow and quality of the discharge. In this case this item of data will refer not to a set of data on river quality but to one of the Data-sets for the flow and quality of discharges, as in:

|  |
| --- |
| 'Wellington STW ' 31 2.0 0 **1**  0 0 3 |

in which Wellington STW is characterised by Data-set Number 1.

### After these items, the next two fields will cover options discussed above (§144 and §145) for Gap-filling.

River Quality Target

### The final field provides the option to include a River Quality Target.

|  |
| --- |
| 'Wellington STW '  **3** 1 2.0 0 1 0 0  **3** |

### This item defines the Code Number of a River Quality Target Data-set in §127 which SIMCAT will use in Automatic Permit-setting Run Types (7, 8 or 9) – a backward calculation. SIMCAT will calculate and impose the discharge quality needed to meet this target.

## Negative, Zero or 999 River Quality Target Specified for Discharges

When the effluent has a zero value for the target set with the Feature Data (and there are no reach standards) the backward calculation is not done. A forward calculation is done.

|  |
| --- |
| 'Wellington STW ' 3 1 2.0 01 0 0 **0** |

If there are Reach Standards, this target is replaced by any target specified for the Reach within the Reach Data (§**F**). A default target of Good is implemented if none of the class limits is assigned negative value – the method by which a target is assigned to a Reach.

When the effluent has a value of 999 for the target set for the Feature, the backward calculation is not done even if there are Reach Standards:

|  |
| --- |
| 'Wellington STW ' 3 1 2.0 01 0 0 **999** |

## River Quality Target Specified as negative for Discharge

When the effluent has a value that is negative the target specified here will be used instead of any specified set for the Reach:

|  |
| --- |
| 'Wellington STW ' 3 1 2.0 01 0 0 **-3** |

## Industrial Discharge (Feature 5)

### This is the same as for the Sewage Treatment Works (Feature 3 - §155 and §156) except that the discharge will be assumed uncorrelated with river flow unless this is over-written (§119).

### After the first four, common, items we need the following.

### You will want to specify the flow and quality of the discharge and may need to specify the river quality targets to be achieved downstream of the discharge (§127).

River Flow Data-set

### In­dustrial Discharges need no data on river flow. Zero is entered:

|  |
| --- |
| 'Allied Industry '  **5**  4 1.0  **0** 1 0 0 3 |

Quality Data-set

### For the Feature called Industrial Discharge, you will want to specify the flow and quality of the discharge. In this case this item of data will refer not to a set of data on river quality but to one of the Data-sets for the flow and quality of discharges, as in:

|  |
| --- |
| 'Allied Industry '  **5** 4 1.0 0 **1**  0 0 3 |

in which Allied Industry is characterised by Data-set Number 1.

### After these items, the next two fields will cover options discussed above (§144 and §145) for Gap-filling.

### The final field provides the option to include a River Quality Target.

|  |
| --- |
| 'Allied Industry '  **5** 4 1.0 0 1 0 0 **3** |

### This item defines the Code Number of a River Quality Target Data-set (§**J**, page77) which SIMCAT will use in Automatic Permit-setting Run Types (7, 8 or 9). SIMCAT will calculate and impose the discharge quality needed to meet this target.

## Discharge from “Other Discharges” (Feature 60)

### This too is the same as for the Industrial Discharge (Feature 5). The discharge flow is also assumed uncorrelated with river flow unless this is over-written (§119).

## Discharge from Private Wastewater Works (Feature 61)

### This too is the same as for the Industrial Discharge (Feature 5). The discharge flow is also assumed uncorrelated with river flow unless this is over-written (§119).

## Discharge with Zero Flow (Feature 17)

### This is the same as for the Sewage Treatment Works (Feature 3) (§155) except that the discharge will be assumed to have zero flow. You can achieve the same effect with Feature 3 or 5 by specifying zero mean flow in the Discharge Dataset.

### You might use this in cases where a new discharge was expected at some future date. It is helpful because Gap-filling cannot work if you introduce a new feature into a calibrated model.

### You get round this by using this feature in modelling and calibrating for present conditions. You then activate the new discharge and calculate its impact by changing the Feature from 17 to 3 or 5.

## Plotting Point (Feature 6)

### Although SIMCAT knows the flow and quality of the river at all points in the catchment, it produces output only at Features and the beginning and end of a Reach. This is because SIMCAT needs to be told where to convert the Shots into estimates of Summary Statistics like means and percentiles.

### A Plotting Point is used only if you want to tell SIMCAT to produce output for a particular place which is not the location of any other Feature. You can put in several Plotting Points to describe, in detail, the longitudinal profile of flow and quality.

### As an alternative to the direct insertion of Plotting Points, the Interpolation Option, see the General data (§34), operates by automatically inserting hidden Plotting Points into your data).

### After the first four, common, items we consider the following.

River Flow Data-set

### This Feature needs no data on river flow. A zero is entered:

|  |
| --- |
| 'Plotting Point '  **6**  1 4.0 **0** 0 0 0 0 |

Quality Data-set

### The next item refers usually to a set of data on river quality. This is not needed for this type of Feature. Zero is entered.

|  |
| --- |
| 'Plotting Point ' 6 1 4.0 0  **0** 0 0 0 |

### After these items, the next two fields will cover options discussed above (§144 and §145) for Gap-filling.

River Quality Target

### The final field provides the option to include a River Quality Target by entering a code number for the required target (§127). This will be reflected in the plotting of the targets on graphs.

|  |
| --- |
| 'Plotting Point ' 6 1 4.0 0 0 0 0 **1** |

## Sub-catchment boundary (Feature 24)

### A Feature (Feature 24) is used to mark a point in the modelled river that denotes the downstream limit of a section of river. This might be the boundary of a sub-catchment such as a water body defined for the Water Framework Directive.

### The feature is used to mark out sections of rivers upstream of the boundary as far as the headwaters of rivers or the locations of upstream boundaries.

### SIMCAT’s output then includes the loads emanating from each sub-catchment. This is in *filename*.ALC

### After the first four, common, items we consider the following.

River Flow Data-set

### This Feature needs no data on river flow. A zero is entered:

|  |
| --- |
| ‘Water body one '  **24**  1 4.0 **0** 0 0 0 0 |

Quality Data-set

### The next item refers usually to a set of data on river quality. This is not needed for this type of Feature. Zero is entered.

### After these items, the next two fields will cover options discussed above (§144 and §145) for Gap-filling.

River Quality Target

### The final field provides the option to include a River Quality Target by entering a code number for the required target (§127). This will be reflected in the plotting of the targets on graphs.

|  |
| --- |
| ‘’Water body boundary '  **24**  1 4.0 0 0 0 0 **1** |

## Abstraction (Feature 7)

### This allows you to abstract (subtract) a set amount of flow from the river. You can also specify a minimum flow such that the abstraction will take place only to the extent that the specified flow is left in the river.

### Intermittent abstractions and others developments which have an irregular effect on the Flow Duration Curve can be simulated by Gap-filling (§144).

### There are two other types of Feature for dealing with abstractions. In earlier versions of SIMCAT abstractions could be modelled only as a fixed constant removal of flow, subject to enough flow in the river, and subject to leaving any specified residual flow in the river.

### You can now use Feature 18 to specify that a distribution of river flow is to be abstracted. This feature acts as a kind of negative discharge. The distribution of flow to be abstracted is specified as a river flow dataset. In this, for example, you specify the mean and 95-percentile low flow for the distribution of the abstracted flow. You can also specify how the abstraction is correlated with flow in the river.

### Intermittent or seasonal abstractions can be modelled by using non-parametric distributions for the abstracted flow.

### The second type of extra Feature, Feature 19, is the same as number 18 except that the value entered in the space for the 95-percentile low river flow is interpreted as a standard deviation.

### After the first four, common, items we need the following.

River Flow Data-set

### The next item refers usually to a set of data on river flow.

### For an Abstraction Point the number entered here will also be a code number for one of the sets of data on river flow. However, the actual data entered for this Code Number will define the amount of water abstracted and the residual flow which must be left in the river (§91).

### This is done by specifying one of the Code Numbers specified in §79. In this case, number 9.

|  |
| --- |
| 'New Mill Intake '  **7**  1 4.0 **9** 0 0 0 0 |

Quality Data-set

### After these items, the next two fields will cover options discussed above (§144 and §145) for Gap-filling.

River Quality Target

### The final field provides the option to include a River Quality Target by entering a code number for the required target (§127). This will be reflected in the plotting of the targets on graphs.

|  |
| --- |
| 'New Mill Intake ' 7 1 4.0 9 0 0 0 **2** |

## Abstraction (the Negative Discharge - Type 18)

### This allows you to abstract (subtract) a distribution of river flow from the river. You can also specify a minimum flow such that the abstraction will take place only to the extent that the specified flow is left in the river.

### Intermittent abstractions and others developments which have an irregular effect on the Flow Duration Curve can be simulated by Gap-filling (§144).

### After the first four, common, items we need the following.

River Flow Data-set

### The next item refers usually to a set of data on river flow.

### The number entered here will also be a code number for one of the sets of data on river flow. The data entered for this Code Number will define the distribution of flows abstracted (§**G**).

|  |
| --- |
| 'Abstraction I ' 18 1 4.0 **7** 0 0 0 0 |

Quality Data-set

### The next item refers usually to a set of data on river quality. This is not needed for this type of Feature. Zero is entered.

### After these items, the next two fields will cover options discussed above (§144 and §145) for Gap-filling.

### The final field provides the option to include a River Quality Target.

River Quality Target

### The final field provides the option to include a River Quality Target by entering a code number for the required target (§127). This will be reflected in the plotting of the targets on graphs.

## Abstraction (the Negative Discharge – Type 19)

### This is the same as Feature 18 (§165) except that except that the 95-percentile low river flow in the specified dataset for river flow is interpreted as a standard deviation and not as a 5-percentile flow.

|  |
| --- |
| 'Abstraction II ' 19 1 4.0 **8** 0 0 0 0 |

## Flow Regulation (Feature 9)

### In certain catchments, the flow in a river may be artificially augmented up to some specified level, called the Maintained Flow. This might be done by the addition of flow from a reservoir, another river, or from groundwater. Feature 9 enables SIMCAT to represent this operation.

### For Feature 9, you will need to specify the value of the Maintained Flow. When SIMCAT comes across a Flow Regulation Point, it looks at each Monte Carlo Shot and checks whether the river flow is less than the Maintained Flow and where it is less it adds flow to make up the shortfall.

### After the first four, common, items we need the following.

River Flow Data-set

### In the following record, river flow will be augmented at a point 1.0 kilometre from the head of Reach Number 2. The Maintained Flow is given in the data specified for river flow, in this case, River Flow Data-set Number 12.

|  |
| --- |
| 'Avon Regulation ' 9 2 1.0 **12** 11 0 0 0 |

### In the sets of data for River Flow, Data-set Number 12 might be:

|  |
| --- |
| 12 0 0.0  **3.0** 0.0 0.0 'Avon Regulation ' |

### This shows that the Maintained Flow is 3.0. The value is entered in the space occupied in most Data-sets by the 95-percentile low flow.

Quality Data-set

### The next item refers to a set of data on river quality. The quality of any water added to make up flow is given by the River Quality Data-set, as in:

|  |
| --- |
| 'Avon Regulation ' 9 2 1.012 **11** 0 0 0 |

### After these items, the next two fields will cover options discussed above (§144 and §145) for Gap-filling.

### The final field provides the option to include a River Quality Target.

River Quality Target

### The final field provides the option to include a River Quality Target by entering a code number for the required target (§127). This will be reflected in the plotting of the targets on graphs.

## Weir (Feature 8)

### Weirs can increase the level of oxygen in a river. They are treated as a type of Gap-filling.

### After the first four, common, items we need the following.

River Flow Data-set

### This Feature needs no data on river flow. A zero is entered:

|  |
| --- |
| 'Weir ' 8 10 0.0  **0** 0 0 12 0 |

Quality Data-set

### The next item refers usually to a set of data on river quality. This is not needed for this type of Feature. Zero is entered.

|  |
| --- |
| 'Weir ' 8 10 0.0 0 **0** 0 12 0 |

### After these items, the next two fields will cover options discussed above (§144 and §145) for Gap-filling.

### The first gives you the option to calibrate for river flow.

|  |
| --- |
| 'Weir ' 8 10 0.0 0 0 **0** 12 0 |

### For all other types of Feature, the second field gives you the option to calibrate for river quality.

### For Weirs, Gap-filling for river quality is restricted to Dissolved Oxygen. For the following data-set, SIMCAT will look up the data on the distribution of Dissolved Oxygen for Quality Data-set Number 12. It will then adjust the shots for Dissolved Oxygen to reproduce these.

|  |
| --- |
| 'Weir ' 8 10 0.0 0 0 0 **12** 0 |

### The final field provides the option to include a River Quality Target.

## Upstream Boundary (Feature 10)

### This is how SIMCAT gets flow and quality data for the start of a calculation. The first feature in any Reach whose upstream limit is a model boundary (§14) must be a Feature of this Type (an Upstream Boundary). You will need to specify the river flow and quality for this Feature.

### After the first four, common, items we need the following.

River Flow Data-set

The next item refers usually to a set of data on river flow. This is done by specifying one of the Code Numbers specified in §79. In this case, number **2**.

|  |
| --- |
| 'Head of River Avon ' 10 2 0.0 **2** 2 0 0 0 |

Quality Data-set

### The next item refers to a set of data on river quality.

### You will want to specify the quality of the flow at the head of the Reach. In this case, number 2.

|  |
| --- |
| 'Head of River Avon ' 10 2 0.0 2  **2** 0 0 0 |

### After these items, the next two fields will cover options discussed above (§144 and §145) for Gap-filling.

### The final field provides the option to include a River Quality Target.

River Quality Target

### The final field provides the option to include a River Quality Target by entering a code number for the required target (§127). This will be used in the plotting of the targets on graphs.

Added Diffuse Pollution

Types of diffuse pollution that are defined as Features, and which have a distance of zero and a negative code number for the set of flow data can also be added to the flows added by Feature Type 10 (§169). This is done by changing the Feature Type 10 to **-10** (§142).

|  |
| --- |
| 'Head of River Avon ' **-10** 2 0.0 **22** 2 0 0 0 |

The types of diffuse pollution that can be added in this way are those defined as Features:

* agricultural livestock (Features 25 and 26)
* agricultural arable (Features 27 and 28)
* highway runoff (Features 29 and 30)
* urban runoff (Features 31 and 32)
* atmospheric deposition (Features 33 and 34)
* natural background (Features 35 and 36)
* septic tanks (Features 37 and 38)
* aggregated CSOs (Features 40 and 41)
* aggregated sewage works (Features 42 and 43) (discharge)
* diffuse mines (Features 46 and 47)
* birds, boats and angling (Features 48 and 49)
* named by user (Features 50 and 51)
* named by user (Features 52 and 53)
* named by user (Features 54 and 55)
* named by user (Features 56 and 57)
* named by user (Features 58 and 59)

Types (13) and (15) cannot be added to the flows of the Reach Headwaters.

The types of diffuse pollution that will be added to the Reach Headwaters are those Features which have a negative Feature Type, a distance of zero and a negative code number for the set of flow data (§141).

In the cases listed below for Livestock (**25**), Arable (**27**) and Urban (31), the Feature Code is set a negative. In these cases (but not for Highway (**29**)), the quality specified by the sets of quality data numbered 2, 3 and 5 will be added to the flows (set number **22**) defined as added by Feature Type 10:

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| ‘Livestock (25) ' | **-25** | 6 | 0.0 | **-1** | 2 | 0 | 0 | 0 | ‘ ‘ |
| 'Arable (27) ' | -**27** | 6 | 0.0 | **-1** | 3 | 0 | 0 | 0 | ‘ ‘ |
| 'Highway (29) ' | **29** | 6 | 0.0 | **-1** | 4 | 0 | 0 | 0 | ‘ ‘ |
| 'Urban (31) ' | **-31** | 6 | 0.0 | **-1** | 5 | 0 | 0 | 0 | ‘ ‘ |

For the above the above four types of diffuse pollution the amount of added pollution is the same as would have been added if there is a flow of 1.0 kilometre upstream of the start of Reach 6. This scaling can be altered by inserting a negative value of distance. The following data set 5.0 kilometres for the first two and 2.0 for the last. The value of -1.0 set for the third row actually produces the same outcome as 0.0.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| ‘Livestock (25) ' | **-25** | 6 | **-5.0** | **-1** | 2 | 0 | 0 | 0 | ‘ ‘ |
| 'Arable (27) ' | -**27** | 6 | **-5.0** | **-1** | 3 | 0 | 0 | 0 | ‘ ‘ |
| 'Highway (29) ' | **29** | 6 | **-1.0** | **-1** | 4 | 0 | 0 | 0 | ‘ ‘ |
| 'Urban (31) ' | **-31** | 6 | **-2.0** | **-1** | 5 | 0 | 0 | 0 | ‘ ‘ |

## Bifurcation (Feature 11)

### This Feature deals with the case where a river splits into two or more branches. These may re-join further downstream.

### Consider the case where a river divides into two branches. SIMCAT demands that you treat the point at which the branch occurs as the end of the Reach. Each branch is then treated as the start of a new Reach.

### Suppose the upstream Reach is number 6 and the bifurcation forms the two new Reaches, numbers 7 and 9. Suppose these recombine later to form Reach 15.

### You need make no special changes to the data for Reach 6.

### Reaches 7 and 9 are specified in the Reach Data (Section 2.9) as if they were branches to a new Reach. (That is, as if they had no upstream Reaches, and their headwaters defined a boundary of the catchment).

### The data on the Features in Reach 7 will then start not with an Upstream Boundary (Feature 10) but with a Bifurcation (Feature 11). This will look like the following. The Feature and Reach Number are indicated:

|  |
| --- |
| 'Bifurcation Start ' **11 7** 0.4 6 0 0 0 0 |

### For most Features, the fourth item of data, 0.4 in this example, will be the distance from the head of the Reach. For a Bifurcation, this distance is, by definition, zero, and the actual value entered in this field takes on a different meaning.

### The value in the length field defines the proportion of the river flow which passes down this branch of the bifurcation. In this case this proportion is 0.4, or 40%.

|  |
| --- |
| 'Bifurcation Start ' 11 7 **0.4** 6 0 0 0 0 |

### The next field, 6 in this example, also takes on a different meaning for a Bifurcation. It defines the number of the Reach which will contribute to the head of the bifurcation.

### So, for this example, 40% of the flow at the end of Reach 6 will form the flow at the head of Reach 7.

### Similarly, for the other arm of this bifurcation, 60% of the flow at the end of Reach 6 will form the flow at the head of Reach 9.

|  |
| --- |
| 'Bifurcation Start ' 11  **9** **0.6**  **6** 0 0 0 0 |

### In both cases the quality at the head of Reaches 7 and 9 will be that calculated for the end of Reach 6.

### Reaches 7 and 9 may re-join, say, to form Reach 15. This is done in the Reach Data (§**F**, page 43) using the normal procedure for mixing Reaches.

### After these items, the next two fields will cover options discussed above (§144 and §145) for Gap-filling.

## Additional methods for Bifurcations (Types 20, 21, 22 and 23)

### A bifurcation is the name given to the situation in which the river splits into two portions. These usually re-join downstream. In the old form of bifurcation (Feature 11) a fixed proportion of the flow is sent down one arm of the bifurcation and the rest of the flow is passed down the second arm.

### We have added extra Features to improve the representation of a bifurcation. We have kept the old one (Feature Type 11). The new Features abstract a distribution of river flow. The abstracted distribution of flow is sent down one arm of the bifurcation; the flow left behind goes down the second arm.

### The “abstracted” flow can be made to be subject to a minimum (hands-off) flow that must be left in the second arm. This can represent a bifurcation that operates only when a weir is overtopped.

### The features can also be used to represent a flow split through a fish farm that is subsequently returned to the river. Previously we had to represent this as two features – an abstraction followed by a discharge.

### The new bifurcations operate in pairs: 20 and 21 – abstraction of a river flow type of distribution; 22 and 23 – abstraction of a discharge data type of flow distribution.

### 20 Bifurcation – second arm – this will contain the remaining river flow after the diversion of the flow specified for this feature

### 21 Bifurcation – first arm – this will contain the diverted river flow distribution

### 22 Bifurcation – second arm – this will contain the residual discharge flow after diversion of the flow specified for this feature

### 23 Bifurcation – first arm – this will contain the diverted discharge flow distribution

### Suppose the upstream Reach is number 6 and the bifurcation forms the two new Reaches, numbers 7 and 9. Suppose these recombine later to form Reach 15. You need make no special changes to the data for Reach 6.

### Reaches 7 and 9 are specified in the Reach Data (§**F**) as if they were branches to a new Reach. (That is, as if they had no upstream Reaches, and their headwaters defined a boundary of the catchment).

### The data on the Features in Reach 7 will then start not with an Upstream Boundary (Feature 10) but with a Bifurcation (Feature 20 or 22). This will look like the following. The Feature and Reach Number are indicated as “20” and “7”, respectively:

|  |
| --- |
| 'Bifurcation Start (1) ' **20 7** 0.0 **6** 2 0 0 0 |

### The fourth item of data, 0.0 in this example, is the distance from the head of the Reach. For any Bifurcation, this distance is, by definition, zero.

### The next field, **6**, in this example defines the code number of the reach whose flow at the end of the reach is to be split between the two arms of the bifurcation.

### The next field, **2**, defines the code number of the flow data set that gives the distribution of flows that will be abstracted.

### Similarly, for the other arm of this bifurcation:

|  |
| --- |
| 'Bifurcation Start (2) ' 21  **8** **0.0**  **6** **2** 0 0 0 |

### In both cases the quality at the head of Reaches 7 and 8 will be that calculated for the end of Reach 6.

### Reaches 7 and 8 may re-join, say, to form Reach 15. This is done in the Reach Data (§**F** and §67) using the normal procedure for mixing Reaches.

### After these items, the next two fields will cover options discussed above (§144 and §145) for Gap-filling.

## Intermittent Discharge (Feature 12)

### SIMCAT's method of dealing with Intermittent Discharges is based on the use of river quality standards expressed as 99-percentiles. River quality should be satisfactory if, for example, the required pairs of 90 and 99-percentiles standards are met:

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Class | Limits on BOD | | Limits on Ammonia | |
| 90-percentile | 99-percentile | 90-percentile | 99-percentile |
| High | 2.5 | 5 | 0.25 | 0.6 |
| Good | 4 | 9 | 0.6 | 1.5 |
| Moderate | 6 | 14 | 1.3 | 3.0 |
| Poor | 8 | 19 | 2.5 | 6.0 |

### Most intermittent discharges will operate with a frequency which is low enough not to threaten a 95 or 90-percentile standard in the long run. (In other words, they operate for less than 5 or 10% of the time). If an intermittent discharge did operate so often as to breach a 95-percentile standard then we shall need to set conditions which will meet both standards.

### SIMCAT has three ways in which you can model an Intermittent Discharge (§**M**). These involve specifying a Non-parametric Distribution either for river flow (§84) or for discharge flow (§120) in which most of the flows are zero.

### The river flow option is used with Feature 2 (Stream or Tributary). The discharge flow option is used for Feature 3 (Sewage Treatment Works) or Feature 5 (Industrial Discharge).

### You call also use Feature 12, as in:

|  |
| --- |
| 'New Mill Storm Overflow ' **12** 5 3.0 0 6 00 0 |

Feature 12 is used as a category of intermittent discharges though such discharges are treated as continuous discharges (such as Features 3 and 5) except that they are expected to be characterized by non-parametric flows.

## Diffuse Pollution

### SIMCAT has several ways by which you can add diffuse pollution. This section explains how to do it by Features.

### At §32 we discussed the use of the Diffuse Inflow Switch to add flow and quality. This particular device is intended mainly to add extra flow so that calculated river flows agree with the measured flows for Flow Gauges (§154).

### You could also use this procedure to add diffuse pollution to an entire Reach or to the whole catchment. To this you would need to define the diffuse inflow to the Reach with a River Quality Data-set which defined its quality (§94).

### We also looked at the use of Gap-filling to add diffuse inputs and losses to river flow and quality.

### The Features described here give you extra ways of adding diffuse pollution. These additions will be superimposed on top of any others you introduce via Reaches with the Diffuse Inflow Switch, or via Gap-filling.

### In the next sections (§174 and §175) we describe procedures (more than 10 pairs of types of Features) allow you to add diffuse pollution to all or part of a Reach. The first of these (Type 13/14) adds pollution which is defined by the statistics of river flow. The second method (Type 15/16) adds pollution which is characterised by the statistics of discharge flow and quality.

### The two types may be superimposed or overlap.

## River Type (Features 13 and 14)

### The method uses two Features to designate the start and end of a source of dif­fuse pollution to a Reach.

### The first Feature, Type 13, marks the point where diffuse pollution will start.

|  |
| --- |
| 'Diffuse Pollution ‑ Start ' **13** 9 1.0 10 14 0 0 0 |

### In this example diffuse pollution to Reach Number 9 will start 1.0 kilometre from the head of the Reach.

### The inflow is defined by the summary statistics entered for River Flow Data-set Number 10 (§79) and will be added at this rate for each kilometre. The quality of the inflow is defined by the summary statistics entered for the River Quality Data-set (§94).

### Correlation is applied as between rivers and tributaries (§99).

### The diffuse inflow will be added until a Feature of Type 14 is encountered, or until the end of a reach is encountered:

|  |
| --- |
| 'Diffuse Pollution ‑ End ' **14** 9 8.0 0 0 0 0 0 |

### In the above example, the inflow will cease at a point that is 8.0 kilometres from the head of Reach Number 9.

### Once diffuse pollution has been switched on using Feature 13, you cannot switch in a second input of this type further down the Reach until the first has been switched off using Feature 14. In other words, only one Type 13/14 Feature can be switched in over the same length of river. You can, however, superimpose a Type 13 and any or all of Types 15, 27, 29, 31, etc (§175 and §176).

## Discharge Type (Features 15 and 16)

### The method also uses two Features to designate the start and end of a source of dif­fuse pollution to a Reach.

### As before the first Feature, type 15, marks the point where diffuse pollution will start.

|  |
| --- |
| 'Diffuse Pollution ‑ Start ' **15** 10 2.0 0 8 0 0 0 |

### In this example diffuse pollution to Reach Number 10 will start 2.0 kilometres from the head of the Reach.

### The inflow is defined by the summary statistics for flow and quality entered for Discharge Data-set Number 8 (§114). It will be added at this rate for each kilometre.

### Correlation is applied as between rivers and discharges (§119).

### The diffuse inflow will be added until a Feature of Type 16 is encountered (or the end of the reach encountered):

|  |
| --- |
| 'Diffuse Pollution ‑ End ' **16** 10 7.0 0 0 0 0 0 |

### In the above example, the inflow will cease at a point 7.0 kilometres from the head of Reach Number 10.

### Once diffuse pollution has been switched in using Feature 15 you cannot switch in a second input of this type further down the Reach until the first has been switched off using Feature 16. In other words, only one Type 15/16 Feature can be switched in over the same length of river. You can, however, superimpose any or all of Types 13, 27, 29, 31, etc. (§174 and 175).

## Diffuse Pollution (Features 25 and 26, 27 and 28, etc)

### SIMCAT has 11 more types of diffuse pollution. These are the same as Features 13/14. They can overlap. They are labelled:

* agricultural livestock (Features 25 and 26)
* agricultural arable (Features 27 and 28)
* highway runoff (Features 29 and 30)
* urban runoff (Features 31 and 32)
* atmospheric deposition (Features 33 and 34)
* natural background (Features 35 and 36)
* septic tanks (Features 37 and 38)
* aggregated CSOs (Features 40 and 41)
* aggregated sewage works (Features 42 and 43) (discharge)
* diffuse mines (Features 46 and 47)
* birds, boats and angling (Features 48 and 49)
* named by user (Features 50 and 51)
* named by user (Features 52 and 53)
* named by user (Features 54 and 55)
* named by user (Features 56 and 57)
* named by user (Features 58 and 59)

### Any, some or all of these sectors can be set up in the set of data on SIMCAT Features in the DAT file. Inputs from things like highways can be switched on and off at any points in the SIMCAT Reach that contains the Feature. Each of these types of Features is defined with a set of data on flow and quality. For example, the sets of data are numbered **2** and **3** in the line of data shown below for a Feature called Urban Runoff:

|  |
| --- |
| 'Urban Runoff ' 31 1 0.0 **2** **3** 0 0 0 |

### In this case SIMCAT assumes that set 2 provides the flow per kilometre that is added to the downstream Reach for the feature called “Urban Runoff”. Set 3 provides data on quality that will be assigned to these inflows and mixed into the river.

### This diffuse inflow cuts in 0.0 kilometres from the head of Reach Number 1 – that is, at the very start of the Reach:

|  |
| --- |
| 'Urban Runoff ' 31 1 **0.0** 2 3 0 0 0 |

## Use-named Sources of Diffuse Pollution (Features 50 and 51 etc)

### The last section (§176) mentions five Features that can be used to set and track up extra types of diffuse pollution. The even numbers: 50, 52, etc are used to define the starting point of the pollution in a Reach. The odd numbers: 51, 53, etc, shut down the contribution.

SIMCAT uses the name of the Feature as if it were a description of the type of pollution. In the following example, type 52 will be called “Pine Forests”:

|  |
| --- |
| Pine Forests ' 52 1 0.0 2 3 0 0 0 |

### All sections of type 52 inputs defined in a set of data will be accumulated throughout the modelled rivers, even if the Feature Name is changed from Reach to Reach.

## Modelling diffuse inputs as added concentrations with no extra flow

### SIMCAT has another way of adding diffuse inflows of pollution. It can be used for any or all of the 16 types of diffuse inflow described above.

### In this, the diffuse inputs are treated as additions of concentration (§141) to a set of flow data defined for the Reach itself and not for the Feature. No extra flow is added by the Feature.

### This method is activated if we replace with **-1**, the number that is used to define the set of data on river flow for the Features for the above 16 types of diffuse pollution. The following feature of Type 31 is set up to start at 0.0 km from the head of Reach

|  |
| --- |
| ‘Urban runoff from Clifton ' 31 2 0.0 **-1** **3** 0 0 0 |

### When this **-1** is present, no extra flow will be added to the Reach by this section of Feature Type 31.

### The concentrations defined by set number **3** define an addition to the concentration of the Reach Diffuse Inflow set up in the data for the Reach 2 itself (§69). The example for the Reach number 2 (called River Avon), has been assigned a set of river flows that define the diffuse input as set number **10**:

|  |
| --- |
| 2 'River Avon ' 10.0 1 2 3 **10** 11 1.0 1.0 |

### Any or all of the other types of diffuse pollution in the above list of 16 can also be set up in this way with a flow dataset defined as -1 and a set number the defines concentrations. In the following example, the set number for concentration is **7**:

|  |
| --- |
| 'Highway runoff from Clifton' 29 2 0.0 -1 **7** 0 0 0 |

### The actual concentration that enters the river is the total defined for all of these types of diffuse pollution. And SIMCAT keeps track of the contributions from each type of diffuse pollution as they proceed downstream

## Mine waters (Feature 39)

### A point source discharge has been added as a Feature to cover mine waters. This will allow SIMCAT to express the contribution of mine waters, individually and collectively, to failures to meet water quality standards.

### The new Feature has the code number 39. It has the same properties as an industrial discharge (Feature 5).

## Lakes (Feature 44 and 45)

### SIMCAT assumes that a lake will be modelled outside SIMCAT’s model of the catchment and its rivers. SIMCAT supplies the Lake Model with full data on the flow and quality of inflows to the lake from any number of rivers and streams. This can include flows that run directly into the lake as rivers or streams, or flows that enter the lake as diffuse run-off from the land that drains directly into the lake. It can also include volumes pumped in from, say, rivers or groundwater.

## Inflow to a lake (Feature 44)

### The data on flow and quality that are passed to the Lake Model are set up for a type of Feature, number 44. There can be any number of these Features in SIMCAT’s model of the catchment and its rivers.

|  |
| --- |
| 'Inflow to Lake' ' 44 7 0.0 0 0 0 0 0 ' ' |

### The data for each Feature are provided as part of the CSV files that SIMCAT creates for use by databases, and Geographical Information Systems such as SAGIS.

### The data in the CSV file are based on monthly and annual mean summary statistics such as means, standard deviations and percentiles of flows, concentrations and loads.

### (It may be better to pass to the Lake Model the actual Monte-Carlo shots of flow and concentration used by SIMCAT to calculate the summary statistics. These would give a more precise expression of the seasonal variations in the inputs to the lake, and the more detailed aspects of correlation between flow and quality.)

### Along with the data on flow and quality at these points of inflow to the lake, the SIMCAT CSV files provide a breakdown of the contributions to water quality from all types of inputs and losses – tributaries, natural decay, effluent discharges, and all 14 types of diffuse pollution. This breakdown also includes the inputs from all of the different sources of pollution from individual discharges that enter all the upstream rivers.

### The Lake Model is then expected to use these inputs to help calculate the quality of the lake.

## Outflow from a lake (Feature 45)

### The Lake Model then passes back to SIMCAT, data on the flow and quality of any rivers that are fed from the lake. Another type of Feature has been set up in SIMCAT to receive this information. This is Feature Type 45. When encountering such a Feature, SIMCAT checks whether a file of data has been provided by the Lake Model.

### SIMCAT can also receive from the Lake Model, details of the relative contributions to water quality from all types of inputs – rivers, effluent discharges and all the various types of diffuse pollution, no matter how they entered the lake.

### The modelling process for a lake requires an initial run of SIMCAT setting up the data for Feature Types 44. These are picked up by the Lake Model and used to calculate data for SIMCAT’s Feature Types 45. SIMCAT then picks up this information and calculates the impacts on rivers downstream of the lake.

### Features 44 and 45 are designed to interact with a lake model that is part of SAGIS. Feature 44 passes data to the lake model.

### Feature 45 is provided with data from the lake model that is used as the headwaters of a Reach within the river system modelled by SIMCAT.

## Outflow from a lake (Feature 45)

### Feature 45 sets up flows from the lake into the headwaters of a SIMCAT River Reach. The present version of SIMCAT expects Feature (45) to be placed in the Feature section of the DAT file just as for the headwaters of a new River Reach, Feature 10, as in:

|  |
| --- |
| 'Outflow from Lake' ' 45 7 0.0 11 15 0 0 0 ' ' |

### In this row of data, the code number of the Feature is “45”, and the new River Reach that will receive the flow from the lake is number 7. The value “0.0” is the position in the Reach that receives the inflow. In any Reach headed by Feature 45 this is always assigned zero for the length for its distance from the head of the Reach.

### The value “11” refers in the normal way to a set of SIMCAT data on river flow. This will be used to input the flows from the lake into the river. The value “15” refers to the set of data on river quality. This will define the quality of the flows from the lake to the river.

### All the existing options for types of data on flow and quality are available for these two items. These include all the various statistical distributions, non-parametric distributions, distributions of load, and data expressed as a monthly structure in the form of 12 separate distributions.

### For the flow from the lake, SIMCAT used the correlation coefficient specified within the river flow data. This correlates the inflow from the lake with the river flows used elsewhere in SIMCAT.

### For each chemical discharged from the lake within these flows, SIMCAT uses the correlation coefficients set up in the river quality data with respect to the calculated daily shots of the river flows from the lake.

### Again, all the various ways of specifying data on water quality can be used: statistical distributions summarising a year, separate distributions for each month, non-parametric distributions (including intermittent discharges), and the specification of quality as loads or concentrations with flows.

### (For chemicals defined as “partitioned” in the DAT file, SIMCAT requires parallel data on the second partition, or information and assumptions that allow SIMCAT to calculate these values. Again, this can be done in the same way as for current River Reaches. Parallel information on sediments and temperature can be provided in terms of data for the new zero-length Reach.)

### SIMCAT also requires for each chemical, and probably for each month, data or assumptions on the mean and standard deviation for the concentrations and loads contributed by the lake for each of SIMCAT’s 16 different types of sector or source of pollution, and how these daily values (the Monte Carlo shots) are correlated with the flow of water from the lake. By default, these are set to zero.

### The only difference is that the contributions of diffuse pollution are specified and added as if they were net effect of point sources at the point the lake water enters the river. SIMCAT interprets the data for these “diffuse” sources as if they were a point source.

### At the end of the zero-length reach. All “diffuse” inputs are automatically switched off by the current version SIMCAT, just as they are for all other Reaches.

### If there are several point discharges into the lake itself, these can be defined as separate inputs to the zero-length Reach. SIMCAT can then keep track their distinct impacts throughout all the downstream stretches of river. This can also be done for discharges to rivers that then flow INTO the lake, and pass through the lake and into downstream Reaches.

### The zero-length Reach then forms a “straight continuation” into a new and normal SIMCAT reach. All the new and distinct levels of diffuse pollution can be specified for this new reach.

## Features

**======================================================================8**

**======= Section [I] Features =========================================8**

**======================================================================8**

**======= The Data-Sets for Features follow. There is one line for 8**

**======= each feature. Each line holds: 8**

**======= (a) the name of the Feature 8**

**======= (b) the code for the type of Feature, these are: 8**

**======= 1 - monitoring station 8**

**======= 2 - stream or tributary 8**

**======= 3 - sewage works or sewage discharge 8**

**======= 4 - river flow gauge 8**

**======= 5 - industrial effluent discharge 8**

**======= 6 - plotting point 8**

**======= 7 - abstraction (of flow) 8**

**======= 8 - weir 8**

**======= (must be at head of Reach) 8**

**======= 9 - river flow regulation point 8**

**======= (switched on only in Modes 3-8) 8**

**======= 10 - upstream river boundary 8**

**======= 11 - bifurcation 8**

**======= (must be at head of Reach) 8**

**======= 12 - intermittent discharge 8**

**======= 13 - start point for diffuse pollution 8**

**======= (river type) 8**

**======= 14 - end point for diffuse pollution 8**

**======= 15 - start point for diffuse pollution 8**

**======= (effluent type) 8**

**======= 16 - end point for diffuse pollution 8**

**======= 17 - a feature that has no flow, eg. a future 8**

**======= effluent discharge in a current model 8**

**======= Allow "what-if" runs based on gap-filled 8**

**======= model 8**

**======= 18 - an abstraction which removes a set 8**

**======= distribution of flow feature. A sort 8**

**======= of negative discharge. The 8**

**======= distribution to be abstracted is 8**

**======= entered with the river flow data sets 8**

**======= 19 - as 18 but the distribution to be 8**

**======= abstracted is entered with the effluent 8**

**======= data sets 8**

**======= 20 - bifurcation (first arm) 8**

**======= distribution to be abstracted to second 8**

**======= arm is entered as a river flow data set 8**

**======= (Feature must be at head of the Reach) 8**

**======= 21 - bifurcation (second arm) 8**

**======= distribution to be diverted to this 8**

**======= arm is entered as a river flow data set 8**

**======= (Feature must be at head of the Reach) 8**

**======= 22 - bifurcation (first arm) 8**

**======= the distribution to be abstracted 8**

**======= to second arm (23) is entered with 8**

**======= the effluent data sets 8**

**======= (Feature must be at head of the Reach) 8**

**======= 23 - bifurcation (second arm) 8**

**======= the distribution to be diverted to this 8**

**======= arm (23) is entered with the effluent 8**

**======= data sets (the feature must be at the 8**

**======= head of a Reach) 8**

**======= 24 - boundary of a sub-catchment 8**

**======= 25 - start point for agricultural livestock 8**

**======= 26 - end point for agricultural livestock 8**

**======= 27 - start point for agricultural arable 8**

**======= 28 - end point for agricultural arable 8**

**======= 29 - start point for highway runoff 8**

**======= 30 - end point for highway runoff 8**

**======= 31 - start point for urban runoff 8**

**======= 32 - end point for urban runoff 8**

**======= 33 - start point for atmospheric deposition 8**

**======= 34 - end point for atmospheric deposition 8**

**======= 35 - start point for natural background 8**

**======= 36 - end point for natural background 8**

**======= 37 - start point for septic tanks 8**

**======= 38 - end point for septic tanks 8**

**======= 39 - point discharge from mine water 8**

**======= 40 - start point for aggregated CSOs 8**

**======= 41 - end point for aggregated CSOs 8**

**======= 42 - start point for aggregated sewage works 8**

**======= 43 - end point for aggregated sewage works 8**

**======= 44 - flow into a lake 8**

**======= 45 - flow from a lake 8**

**======= 46 - start point for - diffuse mines 8**

**======= 47 - end point for - diffuse mines 8**

**======= 48 - start for - birds, boats and angling 8**

**======= 49 - end point - birds, boats and angling 8**

**======= 50 - start for - "user defined type" 8**

**======= 51 - end point - "user defined type" 8**

**======= 52 - start for - "user defined type" 8**

**======= 53 - end point - "user defined type" 8**

**======= 54 - start for - "user defined type" 8**

**======= 55 - end point - "user defined type" 8**

**======= 56 - start for - "user defined type" 8**

**======= 56 - end point - "user defined type" 8**

**======= 58 - start for - "user defined type" 8**

**======= 59 - end point - "user defined type" 8**

**======= 60 - other point sources 8**

**======= 61 - private wastewaters 8**

**======================================================================8**

**======= (c) the code number of the Reach on which the 8**

**======= Feature is located (Set 2) 8**

**======= (d) distance from the head of the reach (km) 8**

**======= (except for Feature Type 11 where it defines 8**

**======= the fraction of flow passing down the 8**

**======= bifurcation) 8**

**======= (e) the code number of the river flow Data-Set 8**

**======= (discharged from Feature Types 2 & 13) 8**

**======= (recorded at Feature Type 4) 8**

**======= (abstracted at Feature Type 7 or 18) 8**

**======= (for feature types 20 and 21 where this 8**

**======= is the Reach number that provides flow data 8**

**======= at the end of the Reach for the bifurcation) 8**

**======= (f) the code number for the river quality 8**

**======= Data-Set(4) or the effluent flow/quality 8**

**======= Data-Set(5) (non-zero for Feature Types 2,3,5, 8**

**======= 13 and 15, 19) 8**

**======= (data-set for quality produced by Weir(8) 8**

**======= (for feature types 20 and 21 where this 8**

**======= the river flow data set giving flow for the 8**

**======= bifurcation) 8**

**======= (for feature types 22 and 22 where this 8**

**======= the discharge data set giving flow for the 8**

**======= bifurcation) 8**

**======= (g) the code number of any river flow Data-Set to 8**

**======= be fitted by Gap-filling. Prefixing a minus 8**

**======= sign will suppress downstream extrapolation 8**

**======================================================================8**

**======= (h) the code number of any river quality Data-Set 8**

**======= to be fitted by SIMCAT Gap-filling. 8**

**======= Prefixing a minus sign will suppress downstream 8**

**======= extrapolation. 8**

**======= For Feature Type 8 the code number for this 8**

**======= river quality Data-Set defines quality 8**

**======= downstream of the Weir. 8**

**======================================================================8**

**======= Defining the Feature to be at the Head of a 8**

**======= Reach will suppress upstream interpolation. 8**

**======================================================================8**

**======= (i) the code number for any Data-set of river 8**

**======= quality targets specified above in Set 7. 8**

**======= If a Reach Target is in Set 3 this target will 8**

**======= be replaced by that Reach Target. 8**

**======= If value is 999 for a discharge, its quality 8**

**======= will not be tuned to achieve any target 8**

**======= If value is -ve the target will be retained 8**

**======= despite the presence of Reach Targets (Set 3) 8**

**======================================================================8**

**======= (j) user notes such as grid reference for GIS (not 8**

**======= required by SIMCAT but often helpful to users) 8**

**===========a=======================b==c=====d===e===f==g==h=i====j====8**

**'Head of Upper Ouse' 10 1 0.0 1 1 0 0 0**

**'Pig Farm Gauging Station' 4 1 4.0 4 0 4 0 0**

**'Ouse Stream' 2 1 6.0 5 1 0 0 0**

**'Wellington STW' 3 1 8.0 0 1 0 0 3**

**'Middle Ouse Monitoring Station' 1 1 14.0 0 8 0 8 0**

**'Head of River Avon' 10 2 0.0 2 2 0 0 0**

**'Avon Regulation' 9 2 1.0 12 11 0 0 0**

**'Brickton STW' 3 2 3.0 0 2 0 0 1**

**'Valley Bottom Monitoring Station' 1 2 9.0 0 10 0 10 0**

**'Valley Bottom Gauging Station' 4 2 9.0 6 0 6 0 0**

**'Allied Industries' 5 3 1.0 0 4 0 0 3**

**'Head of Black Brook' 10 4 0.0 3 3 0 0 0**

**'Black Brook Monitoring Station' 1 4 2.0 0 6 0 6 0**

**'Appleford STW' 3 4 3.0 0 3 0 0 2**

**'Intermittent' 12 4 6.1 0 4 0 0 3**

**'Avon Stream' 2 5 1.0 16 1 0 0 0**

**'NM Monitoring Station' 1 5 1.5 0 9 0 9 0**

**'NM Flow Gauging Station' 4 5 2.0 9 0 9 0 0**

**'Storm Overflow' 12 5 4.0 0 6 0 0 0**

**'Abstraction' 7 5 7.0 18 0 0 0 0**

**\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* indicator of end of all data \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\***

# OUTPUT

## Output for Mapping Systems (GIS)

### A file is created by SIMCAT for import into data-bases and Geographical Information Systems. The following information, also set out at the head of the SIMCAT output file, is provided for each point of interest in the river. This includes all the Features, points up and downstream of discharges and tributaries, and points at the start and end of all the reaches.

|  |
| --- |
| The following items occur for each row of information ... |
| 1: the code number of the reach |
| 2: the GIS code for the location |
| 3: the name of the reach |
| 4: the name of the feature or a mark for the end of reach |
| 5: indication of downstream or upstream of feature |
| 6: the code number for the type of feature - or 99 for the end of reach |
| 7: the distance from the head of the reach |
| 8: the type of data |
| 9: the units for the data |
| Subsequent items in the record depend on the type of data |
| For records for river flow ... 8 items |
| 10: the mean river flow |
| 11: the 90-percentile of river flow |
| 12: the 95-percentile of river flow |
| 13: the 99-percentile of river flow |
| And for some features such as flow gauges ... |
| 14: the observed mean river flow |
| 15: 90-percentile of observed river flow |
| 16: 95-percentile of observed river flow |
| 17: 99-percentile of observed river flow |
| For river quality ... 42 items |
| 10: the name of the determinand |
| 11: the units of concentration |
| 12: the calculated value of the mean concentration |
| 13: the lower confidence limit on the estimate of the mean |
| 14: the upper confidence limit on the estimate of the mean |
| 15: calculated value of the 90-percentile concentration |
| 16: lower confidence limit on this percentile |
| 17: upper confidence limit on this percentile |
| 18: calculated value of the 95-percentile concentration |
| 19: lower confidence limit on this percentile |
| 20: upper confidence limit on this percentile |
| 21: calculated value of the 99-percentile concentration |
| 22: lower confidence limit on this percentile |
| 23: upper confidence limit on this percentile |
| 24: the calculated value of the mean load |
| 25: lower confidence limit on the estimate of the mean load |
| 26: upper confidence limit on the estimate of the mean load |
| 27: calculated value of the 90-percentile load |
| 28: lower confidence limit on the 90-percentile load |
| 29: upper confidence limit on the 90-percentile load |
| 30: calculated value of the 95-percentile load |
| 31: lower confidence limit on the 95-percentile load |
| 32: upper confidence limit on the 95-percentile load |
| 33: calculated value of the 99-percentile load |
| 34: lower confidence limit on this 99-percentile load |
| 35: upper confidence limit on this 99-percentile load |
| 36: river water target |
| 37: per cent confidence of compliance with the target |
| 38: per cent of load from discharge discharges |
| 39: (redundant field: a value of zero) |
| And, relevant for features such as monitoring stations ... |
| 40: any observed value of the mean concentration |
| 41: the observed value of the 90-percentile concentration |
| 42: the observed value of the 95-percentile concentration |
| 43: the observed value of the 99-percentile concentration |
| 44: the confidence that the class is High |
| 45: the confidence that the class is Good |
| 46: the confidence that the class is Moderate |
| 47: the confidence that the class is Poor |
| 48: the confidence that the class is Bad |
| 49: a label for the next three items ... |
| 50: the length of upstream river complying with 50% confidence |
| 51: length of river failing with 50% confidence |
| 52: length of river failing with 95% cent confidence |
| Items 1 - 52 are then repeated in records for 9 more determinands |
| For overall confidence of class across all determinands ... 55 items |
| 11: the confidence that the overall class is High |
| 12: the confidence that the overall class is Good |
| 13: the confidence that the overall class is Moderate |
| 14: the confidence that the overall class is Poor |
| 15: the confidence that the overall class is Bad |
| 16: the confidence that the class is High |
| 17: the confidence that the class is Good |
| 18: the confidence that the class is Moderate |
| 19: the confidence that the class is Poor |
| 20: the confidence that the class is Bad |
| Items 16 - 20 are then repeated in this record for 9 more determinands |
| 56: the face value class across all determinands |
| 57: the face value class for determinand 1 |
| Item 58 is then repeated for the other 9 determinands |
| 67: the model number in a batch run |

For some determinands, usually metals, the “total” concentration of load is partitioned (§61) into two fractions, “dissolved” and “solid”. In these cases, the results for the “total” appear first in the records for the determinand. Immediately after this record there is a second that deals with the “dissolved” fraction, and a third that deals with the “solid” fraction.

Results for compliance will assume that the standard is for “total” unless the “partition coefficient” is entered as a negative number within the determinand data (§61). This negative is taken as a sign that the standard is for “dissolved” fraction, and the partition coefficient is converted into the positive number for subsequent use by SIMCAT.

## Monthly output

### The output file *filename*.ALC includes lists of the loads and concentrations in each month and the contributions in each month to the annual load and to annual summary statistics like the annual mean concentration or the annual 95-percentile concentration.

### Separate files are produced for each determinand. They are labelled *filename*D1.ALC, *filename*D2.ALC etc.

### These results show, for example, the contribution of each month to failure to meet a water quality standard that is expressed as a summary statistic such as the annual 95-percentile.

### The results also show the total monthly contribution from all the upstream pollution within categories that include:

* agricultural livestock (Feature 25)
* agricultural arable (Feature 27)
* highway runoff (Feature 29)
* urban runoff (Feature 31)
* atmospheric deposition (Feature 33)
* natural background (Feature 35)
* septic tanks (Feature 37)
* aggregated combined sewer overflows (Features 40)
* aggregated small sewage works (Features 42)
* sewage treatment works (Feature 3)
* industrial discharges (Feature 5)
* intermittent discharges of sewage (Feature 12)
* mine waters (Feature 39)

### The output also shows the % of time in each month that exceeds a concentration threshold such as the concentration specified as an annual mean or annual 95-percentile standard.

## Monthly output for export to Geographical Information Systems

### The information in the *filename* .ALC file is also produced in a file of comma-separated-variables, a CSV file. This can be imported into a database or spreadsheet, and into systems for producing maps (GIS).

### Separate files are produced for each determinand. They are labelled *filename*D1.CSV, *filename*D2.CSV etc.

### These files also show the relative contribution to water quality of all upstream discharges.

## Types of point sources

### There are 4 distinct Input Types of pollution from point sources:

* sewage treatment works (Feature 3)
* industrial discharges (Feature 5)
* intermittent discharges of sewage (Feature 12)
* streams and tributaries (Feature 12)

### All these inputs can be expressed as annual or monthly distributions of load, or of flow and quality. The output from SIMCAT expresses discharge loads, for example, as total loads, as well as loads broken down between sewage treatment works (Feature 3), industrial discharges (Feature 5), and intermittent discharges (Feature 12).

## Apportionment

### A key requirement for water quality planning is the calculation of the proportions of pollution from different sources. For the SIMCAT data called, say, EG.DAT, the output files now include EG.ALD. This lists the proportion of the total river load supplied by discharges and the proportion of the total discharge load provided by each upstream discharge.

### This gives you, for example, the proportion of a discharge in Birmingham that reaches the River Trent at Nottingham, or which enters the estuary at the tidal limit of the River Trent.

### In doing this calculation SIMCAT takes account of losses of discharge load, in the river, through abstractions and through the processes you have specified for natural purification. Similarly, SIMCAT adjusts for losses applied through gap-filling.

# INTERMITTENT DISCHARGES

## Modelling intermittent discharges as flow and concentration

### Intermittent discharges can be modelled by defining them as “streams or tributaries” (Feature 2) with a non-parametric distribution of flows. These can be set up with the required proportion of zero flows.

### Similarly, intermittent discharges may be defined as “discharge discharges” (Features 3 and 5). They can also be set up as all or any of the forms of SIMCAT’s “diffuse inputs” (Features 13, 15, 25, 27, 29, 31, 33, 25. 37, 40 and 42).

### For example, a discharge flow can be set up as a non-parametric distribution of flow whose data are defined with, say, 98% of values that are zero. This will produce non-zero flows for 2% of SIMCAT’s Monte Carlo shots. The data on the concentrations associated with these flows can then be set up as the basic “operate all the time” distributions of concentration (Distribution Types 0, 1, 2, 3, 4 etc).

### It may not make sense to specify an intermittent distribution of concentrations to go with your intermittent distribution of flows. In such a case the non-zero flows will have a proportion of zero concentrations according to the percent of time that the concentration is defined to be zero in your data.

## Correlation within the data for intermittent discharges

### The correlation coefficient between the added flows and the flows in the receiving water will be SIMCAT’s default value of 1.0 for “streams and tributaries” (Feature 2). It will be 0.6 for “sewage works” (Feature 3) and 0.0 for “industrial discharges” (Feature 5) (§62).

### As noted above these defaults can be over-written by you in any set of flow data you use by Features.

### In your data for discharge quality, the correlation coefficient you enter defines the correlation between the added flow and the added quality. The values of the correlation coefficients used by SIMCAT as defaults are set out for certain determinands in §62 for Features 2, 3 and 5. For other determinands the defaults are zero.

### You can over-write these defaults in any of the individuals set of quality data you assemble.

### The load added to the river depends on this correlation you set up in the data for the added flow and its added quality, by default or otherwise, between:

1. the added flows and the flows in the receiving river (as set for your data for the added flow)
2. the added flows and the concentration in the added flow (as set in your data for the added concentrations

### (The items (a) and (b) define the linear regressions you would do to calculate actual correlation coefficients.)

### For Feature 12 (Intermittent Discharges of Sewage Effluent), a default correlation coefficient of 1.0 is hard-wired into SIMCAT for item (a). This means that the correlation coefficient for the added concentrations is the same between both the added flows and the flows in the receiving river. Again, such a correlation coefficient can be calculated by linear regression using the concentrations with either type of flow. But this is a special case.

### We to look now at how SIMCAT selects a concentration to go with a selected non-zero flow discharged to the river.

### Suppose you have set up the added flows to be non-zero for 2% of the time. The correlation of these added flows with the flows in the receiving river is set in the data you define for the distribution of the added flows. This will dictate whether, for example, the added flows tend to occur when flows in the receiving river are high or low.

### Now look at the correlation coefficient between the added flows and the concentration of a substance in those flows. If this coefficient is close to 1.0, the old versions of SIMCAT will select a concentration from the top end of the specified distribution of the added concentration. In such a case the average value of the selected concentrations across all the non-zero flows will exceed the mean value you specified in the data for the concentrations. This may not be what you wanted. We are talking here of the difference between, say, a mean for the whole year (to which non-zero flows are contribute a zero concentration) and the mean of the concentrations in the non-zero flows.

### This difference can be made to vanish if you set the correlation coefficient to zero in the data for the distribution for the added concentrations. In this case, the concentrations in the added flow will vary randomly according to the mean and standard deviation (or non-parametric distribution) you have specified for the added concentration.

### Another option is to set the standard deviation for the added concentrations to zero. In this case all the added flows will have the same concentration – the one you specified as the mean.

## Correlation between added flow and the added concentrations

### Complication arise if you do not want to use the simplifications discussed above and actually want the concentrations in the added flows to have a non-zero correlation with the non-zero values of the added flows. In such a case you will have calculated the correlation coefficient in a linear regression between the non-zero flows and the concentrations in those particular flows.

### SIMCAT assumes that whenever the added flows are defined to be non-parametric, the associated data on concentrations applies only to the non-zero flows. This works as follows. Suppose the discharge operates for 2% of the time. This is set up as an intermittent discharge of flow; SIMCAT assumes, say, that the mean and standard deviation of a log-normal distribution specify the concentrations in the non-zero flows.

### In terms of generating random numbers to calculate the shots, a non-zero shot for the added flows occurs whenever the random number exceeds 0.9800. (Though you may have set up these “random” numbers as correlated with say, the flows in the receiving river).

### To generate a “random number” that applies to the non-zero component of the discharged flows the calculations in SIMCAT subtract 0.9800 from the random number used to generate the non-zero discharge flows. The set of results that are bigger than zero, defines the structure of the set of random numbers used to generate only the distribution of the non-zero flows. Such a set of numbers can be used to link to a distribution of concentrations (or loads) that is specified to cover only the non-zero flows. Correlation is then imposed that models the required link between the added flow and its quality.

## Non-parametric distributions of intermittent load

### It may be better to express the additions in terms of zero flow all the time coupled with an intermittent distribution of load. This has been set up in SIMCAT as a facility to add non-parametric distributions of load.

### A form of input, called a type 9 distribution, allows a type 4 distribution to specify loads rather than concentrations (Table 0.1) (§80, §96 and §116):

|  |  |
| --- | --- |
| Table 0.1: Types of data | |
| Code number | Type |
| 0 | Constant |
| 1 | Normal Distribution |
| 2 | Log-normal Distribution |
| 3 | 3 Parameter Log normal Distribution |
| 4 | Non-parametric Distributions |
| 5 | Seasonal (monthly) data |
| 6 | As 1 but the data are taken as loads and not concentrations |
| 7 | As 2 but the data are loads and not concentrations |
| 9 | As 4 but the data are loads and not concentrations |

### Type 9 is used is the same way as type 4 except that the code number is 9 rather than 4:

|  |
| --- |
| 1 **9**  'npload.npd' -9.9 'Diffuse pollution ' |

### Similarly, the data file must reside in the same folder as your SIMCAT data file (§2). In this case the file is called *npload.npd*. The stem of the filename, *npload*, must be 64 characters or less.

### The data-file for the Non-parametric distribution is a list of up to 100,000 numbers taken equi-spaced from the cumulative distribution of loads. For example, the contents of the data-file for 14 numbers might be:

14 0.0 0.0 12.0 34.0 1.0 2.0 2.0 2.0 2.0 0.0 1.5 5.7 8.1 99.0

### The first value, 14, is the number of values which follow. These 14 items are the values of the load. They are expressed in the units set by the units of flow and concentration used for the run of SIMCAT and specified in other data.

### After ranking, as in the case of type 4, the values are assumed equi-spaced in terms of the Weibull plotting positions, 1/(1+n), for the Cumulative Frequency Distribution. This means that the above 14 points are:

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| From the data-file | 0. | 0. | 12. | 34. | 1. | 2. | 2. | 2. | 2. | 0. | 1.5 | 5.7 | 8.1 | 99. |
| After ranking | 0. | 0. | 0. | 1. | 1.5 | 2. | 2. | 2. | 2. | 5.7 | 8.1 | 12. | 34. | 99. |
| Rank | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 |
| Plotting Position | .07 | .13 | .20 | .27 | .33 | .40 | .47 | .53 | .60 | .67 | .73 | .80 | .87 | .93 |

### In this case the load is zero for about 13% of the time and takes a constant value of 2.0 for about 20% of the time (four of the 14 values are equal to 2.0).

### When used by SIMCAT the loads are used in the same way as loads specified under distribution types 6 and 7 (Table 0.1). For a particular discharge to a river there will be data on flow and quality. For a determinand expressed as load, any non-zero flow specified for the discharge will still be added to the river. The calculations are such as would apply if buckets of solid were tipped into the river, followed up with the added flows at zero concentration.

### For a particular discharge, there may be several determinands for water quality. Some can be expressed as concentration and others as loads.

### If all the determinands for a particular discharge are expressed as load any discharge flow you have defined for the discharge will still be added to the river. To add a discharge that has no actual flow you need to actually specify in the data that the added flow is always zero.

## Non-sequenced non-parametric distributions

### A capacity has been added to suppress the ranking of the data set up for non-parametric distributions. This option is helpful in the modelling of inputs of intermittent flows whose quality varies in a complex way with the flow. Recent data on the effects of the run-off from highways appears to be like this.

### This option allows you to correlate concentrations described in non-parametric distribution in any way.

### To use the example set up in the last section, this option is switched in happens if the number of items is set to be negative. The data are then used in the order specified.

-14 0 0 12 34 1 2 2 2 2 0 3 6 8 99

### In this case the ranking is suppressed and the numbers are used in the order in which they are entered:

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| From the data-file | 0 | 0 | 12 | 34 | 1 | 2 | 2 | 2 | 2 | 0 | 3 | 6 | 8 | 99 |
| Rank | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 |

## Site Specific Correlation for Discharge Load

### The item of data in the above example of a line of data has a default value -9.9.

|  |
| --- |
| 1 9 load.npd' **-9.9** 'Diffuse pollution ' |

### This means that SIMCAT will use its default settings for correlation between the discharge flow and the discharge concentration (and in the case of type 9, the discharge load). This is usually zero.

### In type 9, and especially for intermittent discharges, it is unlikely that the default value will be suitable.

# MODELLING DIFFUSE POLLUTION

## Adding Diffuse Pollution as Loads

### Information provided for agriculture may lead to data by which diffuse pollution entering rivers is expressed as something like the total load over a year that is added to the rivers in a catchment. The data are not provided as combinations of concentrations and flows.

### Pollution expressed as loads must be expressed as pairings of loads and flow so that sensible concentrations are calculated for river quality. We must avoid the incorrect and unreal concentrations that might result if a load is added to a river at a place where river flow is sometimes negligible.

### Loads can be represented as the mean and standard deviation of a distribution, with a specified correlation with the flows that convey the loads into the river (§104,105). They can also be represented as non-parametric distribution (§107) or as a power curves (§108).

### We have also set up SIMCAT so that lots of different inputs of diffuse loads can be linked to a single addition of river flow (§141).

### We will wish to calibrate our models so that the effects of the diffuse inflows can (where data are complete and reasonably correct) match the mean and 95-percentile concentrations observed in receiving rivers.

### To do this we must look at how the added loads vary with the flows that “bring” them into the river and avoids cases where a load is “added” to and with low flows and so produce ridiculous over-estimates concentration in some of the Monte Carlo shots.

## Adding Diffuse Pollution as Concentrations

### More recently we have introduced methods based on adding concentrations to river flows without, at the same time, adding more flow (§141). Such additions can also be added to the flows defined as reach headwaters by Feature Type 10 (§142).

# The Monthly Structure Switch

### A complication occurs with using an option for monthly data like Type 8 (§87) if such monthly data are used alongside other data that are specified only as annual distributions.

### For example, suppose that some of the data on diffuse pollution are specified as a set of 12 distinct monthly distributions, but other data on river or discharge flows and quality are set up as annual distributions. How do we ensure that the monthly data is “discharged” into the river flows for the right month?

### (When all the data are annual summaries this problem is managed in a simple way by calculating and using the correlation coefficients between the paired sets of daily values that make up the annual summaries. As discussed later, it is arguable that this process is superior to the use of type 8 distributions.)

### One remedy is to set up all flow and quality data for rivers and discharges as type 8. (Another would be to use a more complex model than the current version of SIMCAT – modelling all the data for the sequence of individual days over the years.)

### On the other hand, there are hundreds of SIMCAT data files, covering the whole of England and Wales, which are based on annual data. It would save time and effort if we could insert a monthly structure for some of the data, whilst retaining annual data elsewhere.

### A key point in all this is that such annual summaries of data for water quality are the logical match to current and historic frequencies of sampling in terms of statistical errors from sampling. There are few daily or weekly records for water quality.

### To allow type 8 data to be used alongside annual data a special switch has been placed in SIMCAT. On detecting any data of type 8, all the annual data are broken into a Standard Monthly Structure. This switch is called the Monthly Structure Switch.

### The Monthly Structure Switch is turned off if the number of Monte Carlo shots you specify in the main data file is not a multiple of 365 (§28). It is also switched off if there are no data that are expressed as type 8.

## The Standard Monthly Structures

### At present these standard monthly structures are hard-wired into SIMCAT. We are looking at ways of allowing them to be specified by users. The values for river flow and the flows from sewage works are:

|  |  |  |
| --- | --- | --- |
| Month | Scaling factor to calculate monthly mean from annual mean | |
| River flow | Flows from sewage works |
| January | 1.9 | 1.3 |
| February | 1.6 | 1.2 |
| March | 1.4 | 1.0 |
| April | 1.2 | 1.0 |
| May | 0.6 | 0.8 |
| June | 0.5 | 0.8 |
| July | 0.3 | 0.8 |
| August | 0.4 | 0.8 |
| September | 0.4 | 0.8 |
| October | 0.8 | 1.0 |
| November | 1.2 | 1.2 |
| December | 1.7 | 1.3 |

## The monthly structure data files

### We now look at the way in which type 8 data are set up for flow or quality.

### If you look at the section in this manual on data on river flow (§80), you will see that this form of data is entered in the same way as those with code numbers 4 and 5. In these a separate data file is specified by name. In the following example the name of this separate file is MONTH3.NPD. Such a set of river flow data is specified in the main SIMCAT data file within the list of all the data on river flows. In this set an individual row would be such as:

### 1 **8** 'month3.npd' -9.9 'Head of Upper Ouse'

### The items in this row of data take the same form as types 4 and 5. This means that the value “1” is a code number of the set of river flow data. The value “8” identifies that the method used is for “monthly structured data”.

### The procedure is similar for data on river quality and for data on discharge flow and quality. For example, for river water quality (§96 and §116) we would have:

### 7 1 **8** 'qmonth.npd' -9.9 30 'Ouse Stream'

### In this, as in methods 4 and 5, the number “7” is the code number of the data set, and “1” signifies that the data are for the first determinand. As usual, the field occupied by value of “-9.9” is for a special, non-default, value of the correlation coefficient. The value, “30”, is the number of samples.

### The form of the file QMONTH.NPD is as follows. You will need to create such a file for each set of data of type 8. Such files must sit as separate files in the same folder as your main SIMCAT data file.

2 100.0 10.0 0.0 -9.9

2 2 2 2 2 2 2 2 2 2 2 2

60.0 50.0 50.0 -50.0 -50.0 -60.0 -70.0 -50.0 -50.0 50.0 50.0 70.0

6.0 5.0 5.0 -5.0 -5.0 -6.0 -7.0 -5.0 -5.0 5.0 5.0 7.0

0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0

-9.9 -9.9 -9.9 -9.9 -9.9 -9.9 -9.9 -9.9 -9.9 -9.9 -9.9 -9.9

### The first line sets out the annual data. The first number, the value of 2, defines the type of distribution, in this case, as throughout SIMCAT, the number “2” defines a log-normal distribution.

2 100.0 10.0 0.0 -9.9

The annual mean is 100.0 and the annual 95-percentile is 10.0. The annual shift-parameter is 0.0 (this is used only for the shifted log-normal distribution). The space for a special correlation coefficient is, as is common, occupied by a value of -9.9.

### The subsequent lines in MONTH3.NPD list, in columns, the values that allow the calculation of these variables for each of the months in the year, from January to December. For example, in the column for February, highlighted below in yellow, these values can be seen to be 2, 50.0, 5.0 0.0 and -9.9. The value “50.0” is the mean river flow for February expressed as an addition to the expressed annual mean of 100.0. This gives the monthly mean for February of 150.0. Similarly the value given for June is -60.0, giving a monthly mean as 40.0.

2 2 2 2 2 2 2 2 2 2 2 2

60.0 50.0 50.0 -50.0 -50.0 -60.0 -70.0 -50.0 -50.0 50.0 50.0 70.0

6.0 5.0 5.0 -5.0 -5.0 -6.0 -7.0 -5.0 -5.0 5.0 5.0 7.0

0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0

-9.9 -9.9 -9.9 -9.9 -9.9 -9.9 -9.9 -9.9 -9.9 -9.9 -9.9 -9.9

### An important (and logical) constraint is that the total of these monthly differences must sum to zero. This is checked by SIMCAT as the data are read or used. SIMCAT also checks that the resulting monthly means are not less than zero.

### If for some reason the data used to calculate the monthly means are all zero, or if any of the monthly adjustments lead to negative values of the average flow, SIMCAT will ignore the month-by-month adjustments and use only the data you have specified in the first row as annual data.

### The development of the type 8 option is at an early stage. Its flexibility will be enhanced in subsequent upgrades to SIMCAT. At present, for example, all the months must have the same type of distribution. It is not possible, for example, to specify that some months have a log-normal distribution whilst others have normal or non-parametric distributions.

### In using this form of monthly data, biased results can occur if the number of Monte Carlo shots you have specified in the main data file is not a multiple of 365. In any run, SIMCAT will check whether you have specified any data as type 8. If type 8 is found, SIMCAT checks whether the requested number of Monte Carlo shots is a multiple of 365. SIMCAT then produces a message that it has reset the number of shots to a multiple of 365. SIMCAT also switches on the Monthly Structure Switch in order to impose a default monthly structure on the data you have expressed only as annual summaries.

### After the row of monthly averages, the next row of data for river flows gives similar information for the monthly 95-percentiles of low flow. These numbers must also sum to zero:

2 2 2 2 2 2 2 2 2 2 2 2

60.0 50.0 50.0 -50.0 -50.0 -60.0 -70.0 -50.0 -50.0 50.0 50.0 70.0

6.0 5.0 5.0 -5.0 -5.0 -6.0 -7.0 -5.0 -5.0 5.0 5.0 7.0

0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0

-9.9 -9.9 -9.9 -9.9 -9.9 -9.9 -9.9 -9.9 -9.9 -9.9 -9.9 -9.9

### The final rows give, respectively, the shifts for a three-parameter log-normal distribution, and the entry in the space for a special correlation coefficient (-9.9). At the time of writing these notes, the scope to deploy variations in these particular rows of numbers has not been developed.

### Data expressed as type 8 are processed as follows. The Monte-Carlo shots are generated so as to reproduce both the summary statistics for the annual data and the summary statistics for the individual months.

### As part of this process of assembling the shots the data given for months are assumed to apply to the number of days in the month. They are corrected by SIMCAT for the fact that months have different numbers of days. Leap years are ignored.

### SIMCAT has a procedure for ensuring that the defined annual and monthly data are compatible. This uses an iterative scheme to adjust the shapes of the monthly distributions to ensure this happens. This involves checks that the monthly data that you entered are compatible with the annual data.

### The outcome is a set of shots that can covers many years but also covers the twelve individual months within these years.

### For data on river water quality, or on the flow and quality of discharges, the file for distributions of type 8 are the same as discussed above for river flow, but the 95-percentile low flows are replaced with values of the standard deviation. As in:

1 11.0 4.0 0.0 -9.9

1 1 1 1 1 1 1 1 1 1 1 1

-5.0 -5.0 -2.0 0.0 2.0 5.0 5.0 4.0 2.0 0.0 -2.0 -4.0

0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0

0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0

-9.9 -9.9 -9.9 -9.9 -9.9 -9.9 -9.9 -9.9 -9.9 -9.9 -9.9 -9.9

### Here the first row gives the annual data:

1 11.0 4.0 0.0 -9.9

### This line specifies the type of distribution (in this case type 1, a normal distribution), the annual mean (11.0), the annual standard deviation (4.0), the shift parameter for a three-parameter log-normal distribution (0.0) and the special correlation coefficient (-9.9).

### The subsequent rows spell out the month-by-month variations. As with river flow, the second line gives the addition to the previously given annual mean. The mean for March is therefore equal to 9.0, 2.0 units less than 11.0.

1 1 1 1 1 1 1 1 1 1 1 1

-5.0 -5.0 -2.0 0.0 2.0 5.0 5.0 4.0 2.0 0.0 -2.0 -4.0

0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0

0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0

-9.9 -9.9 -9.9 -9.9 -9.9 -9.9 -9.9 -9.9 -9.9 -9.9 -9.9 -9.9

### As before the sum of the monthly adjustments must equal zero.

### The next row, corresponding to standard deviations, contains a dummy set of zeros. For data on river water quality (or on discharge flow and quality) the calculations start with a standard deviation set initially using the coefficient of variation for the annual data and adjusting this, as necessary, to generate a compatible set of annual and monthly data.

### In creating shots that can be regarded as monthly data it is important to preserve the relation within the structure of the annual data – to be able to calculate annual summary statistics like the annual mean or annual percentiles. This dictates the form of procedure that has been set up in SIMCAT.

### The reason for this discipline is that, as noted above, water quality standards, the basis for taking big decisions to protect water quality, are defined as annual summary statistics and not as monthly or seasonal summary statistics. This fact is unlikely to change – it ensures that we have standards that model the type of impact and the risk of impact.

## Correlation within and between months

### Nearly all the uses of SIMCAT have been based on annual data. This includes as those of types 0 to 4 in Table 0.1. The statistical correlations between flow and quality in rivers, tributaries and discharges are modelled by specifying correlation coefficients. This means, for example, that the tendency for ammonia concentrations in sewage effluents to peak in winter, is modelled by working out the correlation coefficient between paired daily values of river flow and discharge quality.

### Then when the sets of 500 or so shots are generated from say, the annual means and standard deviations, the values of the individual shots are related for, say, river flow and discharge quality, as directed by the correlation coefficient. This ensures that flows from sewage works, and ammonia concentrations in sewage effluents, can tend to be biggest when river flows are high.

### It is arguable that this process is superior to the use of type 8 distributions. One reason for this lies in the complications with correlation. We have yet to sort out the mathematics by which the following correlations are inter-related. Those correlations between, say:

* the daily flow and quality within the years of the simulation
* the monthly averages of flow and quality
* the daily flow and quality within each of the separate months.

### In replacing annual data with 12 sets of monthly data we need to specify the 12 values of the correlation coefficients for the daily flows and quality within each month. It is unhelpful (and wrong) to leave these as zero.

### SIMCAT attempts to ensure that the month to month correlation (for example, the correlation between mean monthly concentrations and mean monthly flows), and the within-month correlation (for example, the correlation in a month between the daily concentration and the daily flow) are compatible with correlations specified for annual data (the correlations between the daily concentration and the daily flow over the whole year). If the within-month correlation is specified as -9.9 they are over-written by SIMCAT with values that mirror the values specified for the correlation coefficient between daily values throughout the year, and the correlation implied by the specified monthly means.

### As noted above, there is an issue if we use monthly data for some inputs and annual data for others. This difficulty and the associated danger of producing misleading results, coupled with the fact that standards are defined on an annual basis, are strong reasons for dealing with monthly and seasonal data by calculating the correct correlation coefficients within a regime based entirely on annual data.

### Another reason is the large statistical errors produced in monthly data by dividing samples into 12 groups. If there are 36 samples of water quality over three years then each month will have only three samples. The confidence limits for estimates monthly summary based only on three samples renders them useless.

### Our decision to base water quality planning on taking, say, 12 samples a year, makes sense in terms of errors and statistical confidence in taking decisions, mainly if we deal with annual summaries of data. The data are not up to a more detailed breakdown into monthly and daily values.

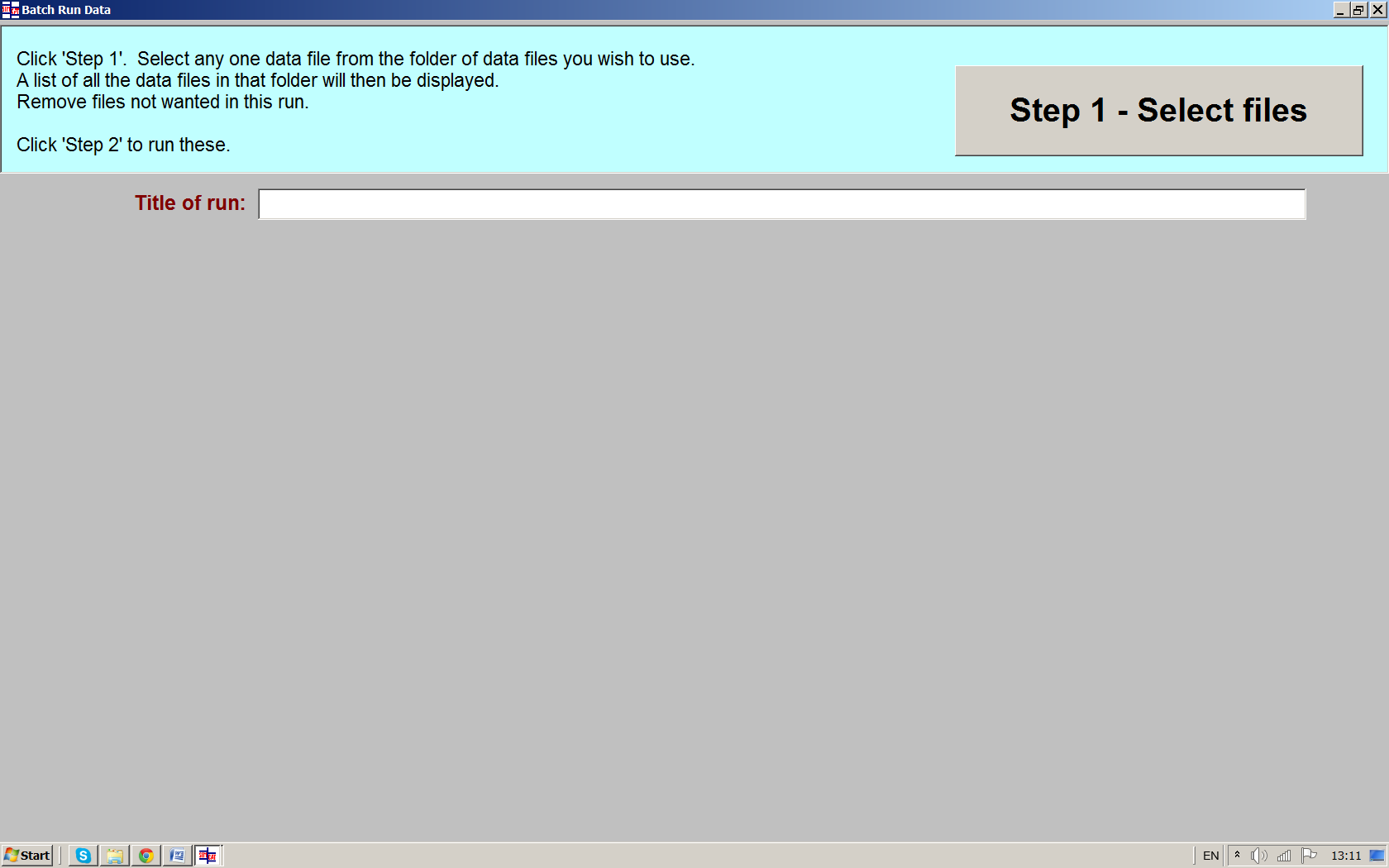
## Time series

### A future stage in the development of the type 8 way of describing data might be to add the option to set up and model time-series of data that preserve the order of days in the month. This means that the first shot will be for 1st January, the next 2nd January, and so on.

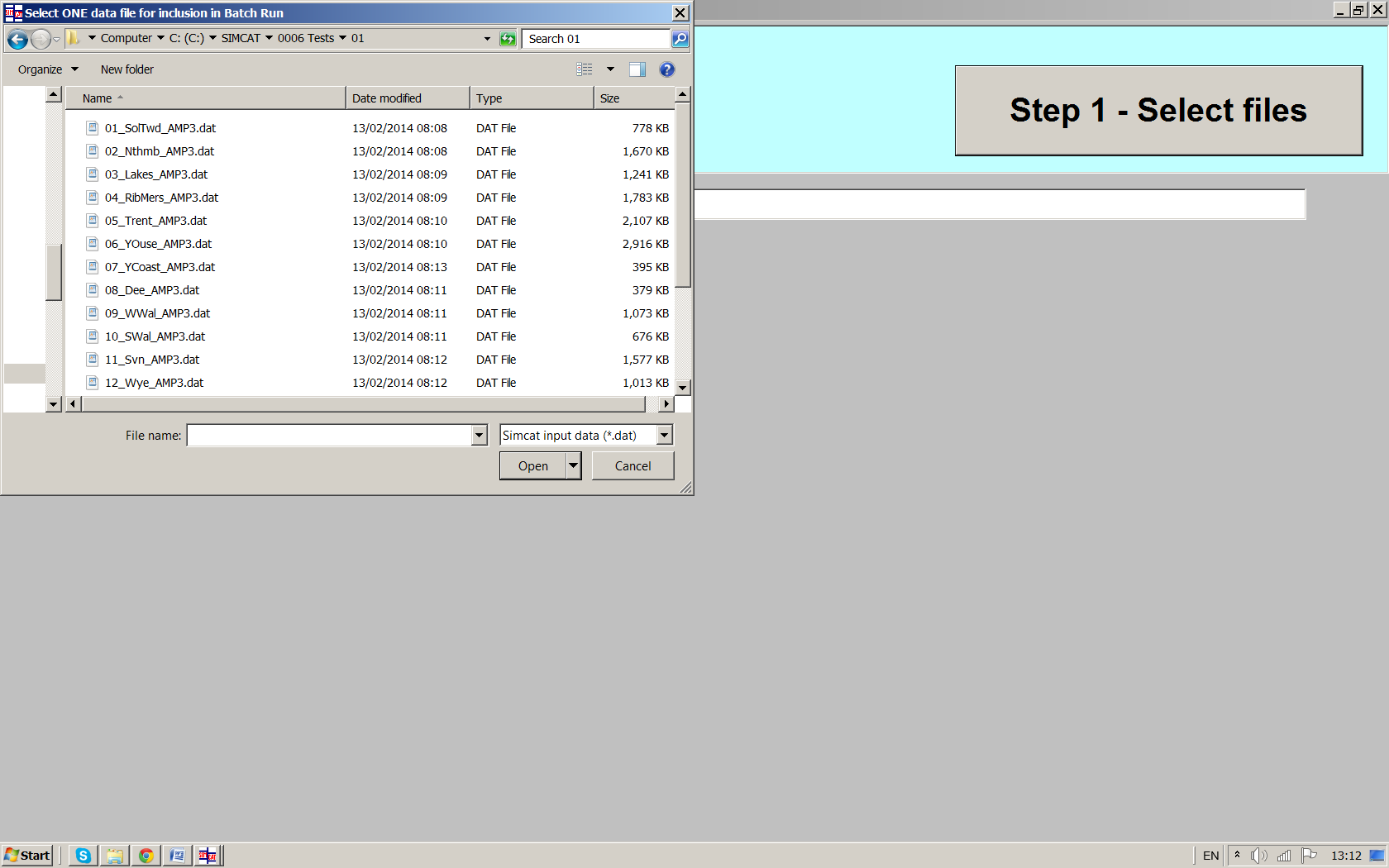
### This will be done by including a day-to-day autoregressive component so that the shot assigned for a date is related to that for the shots for the previous dates. This provides a facility to model time-series data. This could be important in calculating the effects on river water quality of opportunities for the real time control of discharge loads.

# BATCH RUNS

### We have set up an option by which any number of models can be run one after another and a summary produced that covers them all. This is called Batch Mode. You can gain access through the menu item on SIMCAT’s started screen. This is titled “Batch Run”. When you click this you see the following screen:



Click on Step 1 and move to the folder that holds the set of DAT files. Click on one of these files:



### 

### Click on “Step 2”, select a type of run such as Type 0, and click Step 3. The DAT files listed in the left-side window are run in sequence.

## Batch options for Gap Filling

### Also included at the bottom of the screen are some check-box options for the runs. These are labelled: ‘Renew Gap Filling; ‘Force Gap Filling’; etc. These save time when you run several large data files in a Batch Run. These options are:

Renew gap-filling – if this box is checked SIMCAT will run all the base models in mode 6. Mode 6 involves: gap-filling of river flows; gap-filling of river water quality; then a full run of all the gap-filling models.

Force gap-filling – if this box is checked SIMCAT will force Gap Filling of river flows and secure a match with specified observed flows even if the SIMCAT data-file itself does not specify this in the data you put together for features (§154, §144).

# APPENDIX 1: HOW SIMCAT WORKS

## Introduction

### We start with a discussion of water quality standards. We then look at the process of mixing a discharge with a river. This introduces the technique of Monte-Carlo Simulation.

## River Quality Standards

Why do we use as standards, summary statistics like the annual mean and annual 90-percentile? Why is the annual mean so important?

* Its status is enmeshed in law
* It defines the water quality standards for all our rivers
* It is the simplest way to ensure that a standard is correct and sensible[[6]](#footnote-6)
* It represents the spread and structure that defines variations in water quality[[7]](#footnote-7)
* We can spend less on monitoring because our data are less variable that, say, for river flow
* It allows an unbiased assessment of success and failure on a local or national scale
* It promotes correct methods to calculate action to protect water quality
* It means that we can do all the following tasks with the same data:
* Define national and regional targets
* Assess progress towards meeting such targets
* Define the RED points on maps that need attention
* Decide the action we need to take on these
* Confirm the action has worked.

The use of a summary statistic such as the annual mean or an annual 90-percentile is a welcome opportunity that stems from the data on concentrations of pollutants and their link to damage to the environment and water resources. The annual mean (and similar annual statistics) are well-suited as a simple and most helpful form of water quality target. A particular value of the annual mean can embrace and define an acceptable risk of killing fish.

The usefulness of the annual mean has its heart in observations, noted over the years, of the results of looking at histograms of concentrations of pollutant measured at points in rivers across the country. For a particular pollutant these histograms tend towards a similar shape and fatness – something like a log-normal distribution.

This means that the annual mean (or an annual percentile) acts as a summary of the full distribution. It is a single number that represents a range of the underlying values from small to large. It also embraces how the values are correlated with one another, or with river flow or the time of the year.

This facility allows us to extract maximum information from a low number of sample results. It also allows simple and correct calculations of compliance with standards and with national targets, and simple and correct calculations of things like permit limits for discharges.

Taking action to improving the annual mean at a point in a river has the result that the full distribution of concentrations is dragged to better values. As the mean is improved, all the other values will reduce, along with a risk in the occurrence of peak values thought to cause damage such as killing fish.

This use of the annual mean is demonstrated and set up though the comparison of annual means with for thousands of healthy or damaged rivers.

These properties of the annual mean lie behind the types of actions used to protect or to plan improvements to water quality, particularly those actions linked to the construction of the infrastructure and treatment works needed to protect the downstream river.

It may be that a more complex standard is advocated – one that defines sets of concentrations, their durations in days or hours, and the return periods of such events – one a month, one every five years etc. These standards are seldom necessary in terms of the precision provided by data and sampling.

They also require more complex models than SIMCAT – methods that defines the hour-by-hour or day-to-day variations of quality through the months of several years. Such standards must also retain the ability to provide unbiased estimates of summary statistics such as the annual mean.

## Mixing a Single Discharge with a River

### When a discharge enters a river, it is mixed with river water at a rate which depends on factors like the type of outfall, the river flow, tur­bulence in the river, and the nature of the river bed. The mixing process may be complex:

##### if the discharge is denser than river water it may tend to hug the bottom

##### a warm discharge may tend to rise to the surface

##### if the discharge enters one side of the river the pollution may stream down that side of the river for some distance

##### sediments may settle on to the river bed at low river flow only to be picked up again when river flow increases.

### In nearly all cases we can ignore these complications. One reason for this is that the biggest uncertainties lie in the use of sampling to measure water quality. The resulting errors dominate the process of taking decisions.

### Enormous simplification follows if we can allow some sort of *Mixing Zone*, and as­sume complete mixing downstream of this.

### So much so that it makes sense (both for the calculations and the environment) to obtain good and rapid mixing by the choice of outfall arrangements.

### The mixing of a discharge with a river is described by the *Mass Balance Equation*:

|  |
| --- |
|  |

where:

* F is the river flow upstream of the discharge;
* C is the concentration of pollutant in the river upstream of the discharge;
* f is the flow of the discharge;
* c is the concentration of pollutant in the discharge; and,
* T is the concentration of pollutant downstream of the discharge.

### Equation [1] is believable because it is based on the *Principle of Con­servation of Mass*. If the values of F, C, f and c refer to the same instant of time, we can calculate a value of T.

### The commonly used standards for rivers are annual means, and annual 90-percentiles (or 95-percentiles). The river will be protected to the required degree of reliability so long as, say, the (90-percentile) concentration is exceeded for no more than 10% of the time.

### Similarly, discharge standards are defined technically as annual means or annual percentiles.

### A single application of Equation [1] cannot be used to calculate the limits on discharges needed to meet river targets. In principle we have to simulate a range of data and time that can provide an unbiased and reasonably precise estimate of the annual mean. One way of doing this is to create a model that simulates several years of the conditions experienced in a river.

This is a demanding and time-consuming process. Fortunately, it can be done by the much simpler process of **Monte Carlo Simulation**. This is the simplest way of correctly calculating the relationship between summary statistics of the quality of rivers and pollution. It also calculates the errors in such calculations.

### Monte-Carlo Simulation is the simplest way of calculating correctly the relation between the mean and percentile values of T and the mean and percentile values of discharge quality.

## Monte Carlo Simulation

### In this, a value for each of the variables F, C, f and c is plucked randomly from the statistical distribution of possible values.

### A value for T is calculated from each set of values of F, C, f and c using Equation [1]. The sequence of selection and mass balance is repeated until enough values of T have been calculated to define its distribution. Each value of T (or each value of F, C, f or c) is called a **shot**. Routine calculations use 500 sets of shots.

### It is common to assume that F, C, f and c fol­low the Log-Normal distribution but other distributions can be used within SIMCAT, including non-parametric distributions. You can also introduce all the correlations between F, C, f and c (Appendix S, §62).

## Data

### You need data that characterise the distributions of the variables F, C, f and c. In most cases, the data can be presumed to be Log-normal. This means that two summary statistics will define the complete distribution. Any two statistics may be used, so it is best to use those readily available. These are:

◼ River flow: mean and 5-percentile;

◼ Upstream river quality: mean and standard deviation;

◼ Discharge flow: mean and standard deviation; and,

◼ Discharge quality: mean and standard deviation

## River Quality Targets

### The river target is usually an annual mean, an annual 90-percentile or an annual 95-percentile although any other percen­tiles can be used. Often the target will be the boundary which defines a declared Target Class. Or it may be some other water quality standard defined to protect a use of the river, or a standard required to comply with a Directive.

## Why a Model?

### When a river receives lots of discharges, the decisions at one can depend on the choices to be made at those upstream. For such rivers, the cal­culations can be complex and time-consuming because we have to compute, for example, how river quality upstream of one discharge is affected by the decisions we may make at the upstream discharges.

### It is therefore attractive to provide an automatic method of doing all the calculations for an entire catchment in one go. Not only does this save time, it helps plan improvements to river quality that are optimal in terms of their call on finance.

## How SIMCAT Works

### SIMCAT's calculations start at the upstream end of the river. Packages of shots are extracted from each of the distributions of flow and quality, and start a journey which will take them all the way downstream.

### Even if several hundred shots are used, there remains a small error in that the derived values may not quite reproduce the values of the mean and standard deviation that you specified as input data. SIMCAT eliminates this error by making a small, systematic adjustment to the values of the shots.

### At any point where discharge enters the rivers, SIMCAT uses the Mass Balance Equation to mix the sets of shots for the flow and quality of the dis­charge with the shots for the flow and quality of the upstream river. This gives the shots for river flow and quality downstream of the discharge.

### These shots are adjusted to take account of effects like diffuse sources of pollution (for example §69) and natural purification (Appendix R) as the river flows downstream. They will then define the upstream quality for any subsequent discharge.

### At a confluence, SIMCAT has to remember the quality of the river and divert its attention to the top of the new tributary. The sets of shots for the tributary are processed down to the confluence, at which point the sets of shots for the main river and tributary are mixed together using the Mass Balance Equation.

### At abstractions the values of flow associated with the shots may be reduced according to the scale and type of abstraction.

### In this manner, SIMCAT crunches its way down the river, perhaps dealing with hundreds of kilometres of river and dozens of tributaries and dis­charges. Water quality, as assessed by the values of the shots, is cal­culated down the whole length.

## Sampling Error

### As a rule, the biggest source of error in taking decisions is **Sam­pling Error** – the uncertainty caused by sampling that is not continuous over several years. We must take account of Sampling Error, if not directly within SIMCAT then afterwards when we use the results to take deci­sions.

### Sampling Error should also make us think hard about the time we devote to details. There may be little merit in researching the intimate details of the in-river processes which affect water quality, or in iden­tifying the subtleties in the input probability distributions. All this has little point if the effect on results is a lot smaller than the size of the Sampling Error.

### In SIMCAT, Sampling Error is modelled directly. This means that SIMCAT will calculate not only that the mean BOD is, say, 6.1 mg/l, but also give a range, say, 4.9 to 7.5 mg/l.

### If it were vital to guarantee a mean BOD in the river of 5.0 mg/l, we should need to work out the measures needed to reduce the **Pessimistic Confidence Limit**, 7.5 mg/l to 5.0 mg/l.

### If, in contrast, it were vital that we waste no money, then we should calculate the measures needed to reduce the **Optimistic Confidence Limit**, 4.9 mg/l, to 5.0 mg/l. (In this particular case we spend nothing - the Optimistic Confidence Limit is already less than 5.0 mg/l).

### The procedure for modelling Sampling Error is as follows.

### Each water quality Summary Statistic used as data will have been calculated from a particular number of samples. These numbers are given to SIMCAT as data. SIMCAT uses them, with the data on pollution loads, to calculate a quantity called the Effective Sampling Rate (EFR).

### As the calculations progress, SIMCAT will be working out the quality of river water at all points along the river length. At the same time, SIMCAT computes values of the EFR, using the fol­lowing Equation, for each point of inflow of pollution:



### In this Equation, l and L are the loads of pollution in the mixing streams, and n and N are the numbers of sample for the quality data for each stream. Often these numbers will be the values of the EFR calculated for upstream points. In effect then, the EFR is a running, load-weighted, average number of samples.

### The reason for calculating the EFR is that a knowledge of the number of samples allows us to estimate confidence limits and confidence of class (§**T**) (and a knowledge of such confidence shows the risk of taking wrong decisions).

## Gap-filling

### When you put together the data for a catchment you will be very lucky if the results of your first run of SIMCAT agree with the measurements you have obtained from your flow gauges and monitoring sta­tions. You will need to make adjustments in order to secure a fit. This process is called **Calibration**.

### When the Model has been calibrated you can think about using the Model to predict the effect of new discharges and new permit conditions.

### SIMCAT can calibrate automatically. This reduces the time taken to produce results. Without the automation, calibration will be done by the Trial-and-Error adjustment of rate con­stants and other data. (It can also be done this way with SIMCAT by repeated runs using Mode 0). When done by Trial-and-Error, calibration can take ages.

### As implied above, SIMCAT includes equations to describe processes like Natural Purification and Diffuse Sources. Gap-filling can be used in place of these, or to mop up any shortfall in the results of applying them. Gap-filling is seldom deployed by users of SIMCAT.

### Gap-filling takes the following steps:

### SIMCAT feeds in extra river flows so that the its results are the same as the distributions measured at flow gauges - the extra flows are added as a function of river length.

### You will have told SIMCAT, in your data file, what quality to assign to the extra flows; and, using its equations for modelling the river's capacity to purify (or pollute!) itself, SIMCAT calculates a network of empirical constants and adjustments that will reproduce exactly the distributions of water quality recorded at monitoring sta­tions.

### SIMCAT's method of calibration is best illustrated by describing what happens when SIMCAT comes across a monitoring station. First, SIMCAT compares its own results with the quality distribution measured at the monitoring station.

### Next, SIMCAT computes a set of adjustments that would produce exact agreement. It then retreats upstream to the previous monitoring station and repeats the calculations, this time putting in the adjustments as a function of river length or of Time-of-Travel.

### Once back at the original monitoring station, the newly calculated quality is compared with the required distribution. For simple adjust­ments based on linear relations with river length, the agreement will be exact.

### For more complex adjustments, like those involving exponential terms, the agreement will be less than exact. A second set of adjustments is calculated and tested as before by re-tracing the journey down to the monitoring station. This cycle is repeated until a set of adjustments is found which gives exact agreement.

### Two points will now be evident. First, SIMCAT is not embarrassed to use different rate constants for different parts of the catchment. Nor is SIMCAT concerned that separate constants are used for each of the shots.

### The empirical aspect of Gap-filling is justified by the dominating influence of Sampling Error. Sampling Error fogs the data and makes it impossible to work out an explanation of river behaviour solely in terms of physical mechanisms like mixing and chemical decay.

### SIMCAT stores the adjustments calculated by Gap-filling in two files called *filename*.FCL and *filename*.QCL. For the *What-If* Simulations (of Run Types 4, 7, 8 and 9), the adjustments in these files are picked up and applied.

Run Types 7, 8 and 9 calculate action to meet targets. If SIMCAT detects files .FCL and .QCL, these runs will incorporate Gap-filling. Otherwise they will not.

## Automatic Calculation of the Standards for Discharges

### To calculate the discharge standard needed to achieve a river quality standard, the SIMCAT compares the river quality target with the value of the calculated distribution of T. If these values are nearly equal, the discharge quality distribution used to compute T gives the required discharge standard. Otherwise SIMCAT adjusts the discharge distribu­tion and the entire calculation repeated.

### Further adjust­ments and repeats are made until SIMCAT finds the discharge quality distribution that gives the required river quality distribution. This is passed downstream. In this way SIMCAT can work down the catchment, calculating the permit conditions required for all discharges.

# APPENDIX 2: RIVER CHEMISTRY

## Exponential Decay

### Exponential decay is used to model things like Biochemical Oxygen Demand and Am­monia.

### A commonly used model for handling degradable pollutants is *First-Order* Exponential Decay. Here the rate of loss of pollutant is proportional to the concentration of the pollutant as in:

### 

where [C] is the concentration and *k* is a *Rate Constant*. This equation can be integrated to give:

### 

where C0 is the concentration at time t = 0.0

This equation is used by SIMCAT for determinands of Type 2. The Global Rate Constant is entered with the determinand data (§**E**). The River Chemistry Switch needs to be set to 1 (§33). If the determinand is Type 1, for example for conservative pollutants like chloride, no decay occurs even if a Global Rate Constant is entered, or if values are entered for Reaches.

### Rate Constants and the values of C0 are specified by the user in the data-file (§52). If necessary the Rate Constants can differ for each Reach (§72) or they can be calculated (or refined) by Gap Filling (§6).

## Dissolved Oxygen

### The Dissolved Oxygen regime is modelled by the equation:

### 

where D is the oxygen deficit at time, t, k is the Rate Constant for the loss of the BOD, C is the remaining oxygen demand at time t and R is the *Reaeration Coefficient*.

This equation is used by SIMCAT for determinands of type 3. The Global Rate Constant is entered with the determinand data (§**E)**. This can be over-written for individual Reaches. The River Chemistry Switch needs to be set to 1 (§33). If the determinand is Type 1, for example for This equation is used by SIMCAT for determinands of type 2.

### The oxygen deficit, D, is the amount by which the Dissolved Oxygen is less than the concentration giving a saturated solution. This Saturation Value, S, is calculated by[[8]](#footnote-8):



where T is the temperature in degrees Centigrade.

## Time of Travel

### The value of the time, t, required for the equations in § 0 and §0 is calcu­lated using equations of the form:

### 

where v is the velocity of river flow and F is the river flow. The time of travel, t, is obtained by dividing distance by the velocity, v.

The values of the constants, a and b, are specified with the data for Reaches in the data-file (§71)

## Temperature

### The Rate Constants are presumed to depend on temperature and temperature is presumed correlated with river flow (coefficient = -0.6):

### 

where RF is the Random Normal Deviate for river flow, R an initial Ran­dom Normal Deviate for temperature, and RT is the final deviate for Tempera­ture, T.

### Rate Constants are adjusted for temperature. For the decay of the BOD:

### 

### For the decay of Ammonia:

### 

### For Reaeration:

### 

where the suffices indicate the temperature for which the values of k and r apply.

### The Rate Constant for the decay of the BOD increases with the BOD con­centration:

### 

where C is the concentration of BOD.

# APPENDIX 3: CORRELATION

### In SIMCAT, Normal Random Deviates, N, are used to calculate values for variables like river flow, for instance, by assuming a Log Normal Dis­tribution. For example, the river flow, F, is:

### 

where m and s are the mean and standard deviation of the logarithms of the values of F.

### For two correlated variables, river flow, F and effluent flow, f, we need pairs of Normal Random Deviates. Call these L and N. Before using N and L in Equation [1], the correlation between F and C is imposed by cal­culating M where:

### 

where φ is the correlation coefficient between M and N. Values of F and C are then calculated from Equation [1] as:

### 

### 

### The value of φ lies between zero and unity. It may be estimated from real data because it is the same as the correlation coefficient produced by linear regression of the logarithm of F on the logarithm of f. To demonstrate this, we note that the correlation coefficient, R, is defined as:

### 

### Where X is the logarithm of F, Y is logarithm of Y and the summations cover all the pairs of values of X and Y.

### Substituting for X and Y, using the above equations, and noting that the means of M and N are zero, gives:

### 

This is the definition of the correlation coefficient between M and N.

# APPENDIX 4: CONFIDENCE LIMITS

## Method of Calculation

### We use the standard **Parametric Method** (**Method of Moments**, described below) to estimate confidence limits around percentiles.

## Normal Distributions: percentiles

### Given the mean, m, and the standard deviation, s, anestimate of the 10-percentile is q in:



### For the 5-percentile, we use 1.6449 instead of 1.2816. Similarly an estimate of the 95-percentile is q in:



### For the 95-percentile, we use 1.2815 instead of 1.6449 and for the 99-percentile we use 2.3263.

## Confidence of failure of mean standards

To calculate confidence limits about the mean we first compute the standard error, *se*, as:



The upper and lower confidence limits, *C1* and *C2*, are then calculated using the t-statistics for the required confidence limits, usually the 5 and 95% confidence limits:

*C1 = m – T0 \* se*

*C2 = m + T0 \* se*

The confidence that the mean, *m*, has failed its target is calculated by reversing this calculation and calculating the t-statistic *Tx* for the difference between the mean and the target:

*Tx = (target – m) / se*

We then use the value *Tx* to compute the confidence limit for *m* that is represented by the target. This gives the confidence that the target was met or exceeded.

## Normal Distributions: confidence of failure of percentile standards

## Log-normal Distributions: percentiles

### The values of m and s are converted to the values for the logarithms of the data using the **Method of Moments**:





### M and S stand for estimates of the mean and standard deviation of the logarithms of the data. The characters, *ln*, denote the natural logarithm.

### The Face-value estimate of the 90-percentile is then:



.

### To calculate confidence limits we replace the factor of 1.2816 or 1.6449 with, ***t0*** a value which depends on the sampling rate. The values of ***t0*** are given by:



### where f is the number of degrees of freedom, in this case n-1, where n is the number of samples. Also, in this equation:



and *z* is the Standard Normal Deviate: 1.6445 for the 95-percentile and 1.2815 for the 90-percentile and 2.3263 for the 99-percentile.

### The value of *λ* approximates to the Standard Normal Deviate for the confidence limit used to define the Optimistic Confidence Limit. For 95% confidence, *λ* approximates to 1.6445. The true value of *λ* is calculated more precisely as a function of *f* and *z*.

## References

N L Johnson and B L Welch (1939). *Applications of the Non-central t-Distribution*. Biometrika, 31, 362-389.

E S Pearson and H O Hartley (1972).  *Biometrika Tables for Statisticians*. Volume II. Cambridge University Press.

# APPENDIX 5: SOFTWARE

## General

### SIMCAT is provided as a file called SIMCAT157.CAB and a file called Setup.EXE. The program is installed by double-clicking on Setup.EXE.

### When you install, the default is that SIMCAT is placed in the folder C:/PROGRAM FILES/SIMCAT 15.7.

### SIMCAT is an executable file called SIMCAT157.EXE. It uses another executable file SIMCATF157.EXE and the various other files you can see stored in C:/PROGRAM FILES/SIMCAT 15.7.

### The core of SIMCAT is written in FORTRAN but with communications to the screen in VISUAL BASIC. The FORTRAN source is 60,000 lines of code in 400 Subroutines held on 28 files.

### The FORTRAN source code has been created within the INTEL FORTRAN Composer (2019) FORTRAN. The VISUAL BASIC is Visual Basic Version 6.0 or Visual Studio,

## Maximum Sizes for Data

### SIMCAT 15.7 is sized for the following. The numbers can be changed on request:

|  |  |
| --- | --- |
| Item | Number |
| Reaches | 4,999 |
| Features | 19,999 |
| Sets of River Flow Data | 10,999 |
| Sets of River Quality Data | 19,999 |
| Sets of Data on Discharges | 10,999 |
| Number of back-tracked discharges | 1,700 |
| Number of back-tracked sub-catchments | 900 |
| Monte Carlo Shots | 5,000 |
| Maximum number of determinands | 10 |
| Sets of River Quality Targets | 50 |
| Monitoring Stations | 1,999 |
| Non-parametric Distributions | 9,000 |
| Data items for each non-parametric distribution | 100,000 |
| Sets of monthly data | 9,000 |
| Bifurcations | 400 |
| Flow Gauges | 1,999 |

# COPY OF A SIMCAT DATA FILE

**======================================================================0**

**======= Test data file for SIMCAT: EG.DAT (25/11/18) =====0**

**======================================================================0**

**======= Lines beginning with '====' are notes explaining the data 0**

**======= Such lines are not used by SIMCAT and may be removed from 0**

**======= the data-file without affecting the calculations ... 0**

**======================================================================0**

**======= The following sets of data (Data-Sets) are required: 0**

**======= [1] General 0**

**======= [2] Determinands 0**

**======= [3] Reaches 0**

**======= [4] River Flow 0**

**======= [5] River Quality 0**

**======= [6] Effluent Flow and Quality 0**

**======= [7] River Quality Targets 0**

**======= [8] Intermittent Discharges 0**

**======= [9] Features 0**

**======================================================================0**

**======= For sets [4], [5] and [6] extra data will be needed if the 0**

**======= more unusual distributions are selected. These will take the 0**

**======= form of extra data files called ANYNAME.NPD. 0**

**======= 0**

**======= In the following notes the term, River Chemistry, refers to 0**

**======= the effect of the fixed set of Rate Constants defined below 0**

**======= in the Data-Sets for Determinands and Reaches. These can be 0**

**======= used with the equations written into SIMCAT to model changes 0**

**======= in river quality. 0**

**======================================================================0**

**======= A descriptive title follows ... 0**

**======================================================================0**

**Set of data to illustrate the SIMCAT User Manual ... EG.DAT**

**======================================================================1**

**========[1] General Data =============================================1**

**======================================================================1**

**1 Set to 1 to add monthly structure to all annual flow data 1**

**======= Set to zero otherwise. This will be reset to 1 if monthly 1**

**======= data (types 5 or 8) are entered. 1**

**======= Set to 2 never impose monthly structure on annual flow data 1**

**0 percentage of class used in Mode 9 (the default is 50) 1**

**0 set to 1 to exclude output for non-effluent features 1**

**======================================================================1**

**======= In Mean Mode the calculated values of the mean quality will 1**

**======= be output to the screen ... 1**

**======= In 95, 90 or 99-percentile Mode the calculated values of the 1**

**======= corresponding percentiles will be output to the screen 1**

**======= All any of these summary statistics are calculated by SIMCAT 1**

**======= can be plotted etc ... 1**

**======================================================================1**

**1 set to 1 for Mean Mode; 0 for 95-percentile mode; or set as 2 1**

**======= for 90-percentile mode; 3 for 90-percentile mode =============1**

**365 number of shots (minimum is 5; maximum is 5000) 1**

**11.2 3.0 -0.6 river water temperature ... mean, SD, correlation 1**

**'m3/d' units for river and effluent flow (4 characters in quotes) 1**

**======================================================================1**

**1 set to 1 to insert Diffuse Sources specified for Reaches 1**

**1 set to 1 to include River Chemistry 1**

**0 set to 1 for Auto-Interpolation between Features 1**

**======================================================================1**

**======= [2] Determinand ==============================================2**

**======================================================================2**

**======= The code number for each determinand is defined by its order 2**

**======= in the list ... the first is code number 1 etc 2**

**======= There is one line of data for each determinand ... 2**

**======= Each line holds the following items: 2**

**======= (a) defines the type of determinand and the method of 2**

**======= handling River Chemistry and Gap-filling(GF) 2**

**======= The types are: 2**

**======= 1: the determinand is conservative; also, all the 2**

**======= corrections calculated by Gap Filling will be 2**

**======= be applied as a linear function of river length 2**

**======= 2: losses calculated by GF will be applied as an 2**

**======= exponential function of river length; gains will be 2**

**======= linear 2**

**======= 3: Dissolved Oxygen; it is assumed that the second and 2**

**======= third pollutants in the list are BOD and Ammonia 2**

**======= respectively; the Gap Filling corrections 2**

**======= corrections are as for type 2 2**

**======= 4: (or any other number) the determinand will be 2**

**======= excluded from the run 2**

**======= 5: partitioned determinands 2**

**======= (b) the name of the determinand 2**

**======= (c) the short name for the determinand 2**

**======= The names BOD, DO, DOX, AMM, NH4, NH4+ and NH4N are 2**

**======= special and trigger the hard-wired decay rates and 2**

**======= temperature coefficients for BOD, Dissolved Oxygen and 2**

**======= Ammonia 2**

**======= (d) the unit of measurement 2**

**======= (e) the global rate constant (reciprocal days) 2**

**======= (f) the minimum quality achievable by exponential decay with 2**

**======= the rate constants listed above for (e) 2**

**======= (g) the quality of the diffuse inflows added by Gap Filling 2**

**======= Filling when fitting river flows 2**

**======= (h) the minimum quality allowed by extrapolation of the 2**

**======= extra exponential decay introduced by Gap Filling 2**

**======================================================================2**

**======= The following variables (i),(j) and (l) are used as 2**

**======= constraints by Modes 7 - 9. They are mean concentrations 2**

**======================================================================2**

**======= (i) the worst permissible effluent quality (annual mean) 2**

**======= (j) the best feasible effluent quality (annual mean) 2**

**======= (k) a definition of good effluent quality (annual mean) 2**

**======= a negative value excludes the determinand from 2**

**======= calculations 2**

**======================================================================2**

**======= (l) summary statistic used to define river targets: 2**

**======= 1, 2, 3 for mean, 95-percentile and 90-percentile 2**

**======= 4 and 5 for the 5 and 10-percentile 2**

**======= 6 for the 99-percentile 2**

**======= (m) partition coefficient (optional) 2**

**======= A positive value means the standard is total dissolved 2**

**======= plus solid. A negative sign is a code that the standard 2**

**======= applies to dissolved. 2**

**========b===========c======d====e====f=====g====h=====i===j====k==l===m**

**1 'Chloride...' ' Cl' 'mg/l' 0.00 0.0 35.0 20.0 0.0 0.0 0.0 1**

**2 'B.O.D......' ' BOD' 'mg/l' 1.20 1.0 1.0 0.8 500.0 3.0 20.0 3**

**2 'Ammonia....' ' Amm' 'mg/l' 3.00 0.0 0.0 0.0 35.0 2.0 10.0 3**

**3 'Diss.Oxygen' ' DO' 'mg/l' 2.00 0.0 0.0 0.0 0.0 7.0 2.0 5**

**2 'Phosphate..' ' PO4' 'mg/l' 0.05 0.0 0.05 0.0 8.0 0.2 0.0 1**

**\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* indicator of the end of the determinand data \*\*\*\*\*\*\*\*\*2**

**======================================================================3**

**======= Section [3] Reaches ==========================================3**

**======================================================================3**

**======= For each Reach the following are given: 3**

**======= (a) the code number 3**

**======= (b) the name 3**

**======= (c) length (km) 3**

**======================================================================3**

**======= There are two ways of defining how reaches are connected 3**

**======= In the newer version (no longer preferred): 3**

**======= (d) defines the next downstream reach 3**

**======= (e) and (f) are dummy values 'set as x' and not used by 3**

**======= SIMCAT 3**

**======================================================================3**

**======= The older version is now preferred because of developments 3**

**======= for things like lakes and bifurcations. In this (d), (e) and 3**

**======= (f) define the sequence in which the Reaches will be 3**

**======= processed: 3**

**======= 0,x,0 ... the NEXT Reach will be a branch to Reach 3**

**======= number z 3**

**======= x,0,0 ... the NEXT Reach will be a straight 3**

**======= continuation to Reach number z 3**

**======= z,y,x ... the NEXT Reach, number x, will be formed by 3**

**======= mixing z and y 3**

**======================================================================3**

**======= (g) the flow data-set for any diffuse inflow 3**

**======= (h) the quality data-set for these diffuse inflows 3**

**======= (i) term a for the velocity/discharge relation 3**

**======= (j) term b for the velocity/discharge relation 3**

**======================================================================3**

**======= Then follows an optional line of data on rate constants, for 3**

**======= the reach - one constant for each determinand in the order 3**

**======= the determinands are entered above (2) 3**

**======= If non-zero, these replace any global values set in the 3**

**======= determinand data (at section [C]) 3**

**======= To replace the global value with zero enter '-1.0' 3**

**======================================================================3**

**======= Then follows an optional line of data for Temperature for 3**

**======= the reach. This set replaces any global values set in the 3**

**======= general data (in section [1]). 3**

**======================================================================3**

**======= Then follows an optional line of data for Suspended Solids 3**

**======= for the reach. This set replaces values hard wired within 3**

**======= SIMCAT. 3**

**======================================================================3**

**======= Then follows an optional line of data on river quality 3**

**======= targets and class limits for the reach. These replace values 3**

**======= entered in section [7] which are invoked in the data on 3**

**======= Features in Section [8]. 3**

**=========b==================c===d==e==f====g===h======i===j===========3**

**1 'Upper Ouse' 16.0 0 2 0 10 11 33.0 0.6**

**0.00 0.00 0.00 0.00 0.00**

**2 'River Avon' 12.0 1 2 3 10 11 1.0 1.0**

**0.00 0.00 0.00 0.00 0.00**

**3 'Middle Ouse' 2.0 0 4 0 10 11 1.0 1.0**

**0.00 0.00 0.00 0.00 0.00**

**4 'Black Brook' 10.0 3 4 5 10 11 1.0 1.0**

**0.00 0.00 0.00 0.00 0.00**

**5 'Lower Ouse ' 8.0 0 0 0 10 11 1.0 1.0**

**0.00 0.00 0.00 0.00 0.00**

**\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* indicator of the end of the Reach data \*\*\*\*\*\*\*\*\*\*\*\*\*3**

**======================================================================4**

**======= Section [4] River Flow =======================================4**

**======================================================================4**

**======= The River Flow Data-Sets follow: 4**

**======= There is one line for each data-set: For each line: 4**

**======= (a) the code number of the data-set that will be referred 4**

**======= in the data on Features (8) and Reaches (3) 4**

**======= (b) the code number of type of distribution: 4**

**======= (for Feature Types 7 and 9 only zero, 1 or 2 can be used 4**

**======= 0 - constant, uniform flow 4**

**======= 1 - flow follows the Normal Distribution 4**

**======= 2 - the Log-Normal Distribution 4**

**======= 3 - a Three-Parameter Log-Normal Distribution 4**

**======= 4 - non-parametric distribution 4**

**======= 5 - monthly data - distribution for each month 4**

**======= 8 - monthly structure 4**

**======================================================================4**

**======= For distribution types 4 and 5 the items (c),(d) and 4**

**======= (e) below do not appear. Instead we show the name 4**

**======= of data file holding the data for these distributions. 4**

**======= For example: 'npar.npd' (Note the need to use this 4**

**======= type of quotation marks) 4**

**======================================================================4**

**======= (c) the mean flow; except when used by: 4**

**======= Feature Type 7 (abstractions): the abstracted flow 4**

**======= Feature Type 9 (river regulation): zero 4**

**======= Distribution Type 3: the mean of transformed data 4**

**======= (d) the 95-percentile low flow: except when used by: 4**

**======= Feature Type 7 (abstractions): the Hands-Off Flow 4**

**======= Feature Type 9 (river regulation): a Maintained Flow 4**

**======= (e) the shift parameter for distribution types 3: 4**

**======= for Distribution Type 0, 1, 2: zero or blank 4**

**======= (f) reserved for a non-standard correlation coefficient 4**

**======= (g) the name of the site. This is used only for help with 4**

**======= preparing the DAT file. It is not needed by SIMCAT. 4**

**===========c=====d======e=======f=============g=======================4**

**1 3 28.0 4.80 -3.0 -9.9 'Head of Upper Ouse'**

**2 2 4.0 1.20 0.0 -9.9 'Head of River Avon'**

**3 3 1.0 0.20 0.1 -9.9 'Head of Black Brook'**

**4 2 30.0 6.00 0.0 -9.9 'Upper Ouse at Pig Farm'**

**5 2 2.0 0.40 0.0 -9.9 'Ouse Stream'**

**6 2 15.0 5.00 0.0 -9.9 'Avon at Valley Bottom'**

**8 2 0.0 0.00 0.0 -9.9 'Middle Ouse Station'**

**9 2 84.0 13.00 0.0 -9.9 'Ouse at New Mill'**

**10 2 1.0 0.07 0.0 -9.9 'Diffuse inflow'**

**11 2 1.0 0.10 0.0 -9.9 'Flow Adjustment'**

**12 2 0.0 3.00 0.0 -9.9 'Avon Regulation'**

**16 2 100.0 15.00 0.0 -9.9 'Ouse Stream'**

**17 2 0.0 40.00 0.0 -9.9 'Regulation'**

**18 2 82.0 0.00 0.0 -9.9 'Abstraction'**

**\*\*\*\*\*\*\*\*\*\*\* indicator of the end of the list of river flow data \*\*\*\*\*\*4**

**======================================================================5**

**======= Section [5] River Quality ====================================5**

**======================================================================5**

**======= The River Quality Data-Sets follow. For each Data-Set 5**

**======= there is a line of data for each determinand. 5**

**======================================================================5**

**======= For each line the following items are required: 5**

**======= (a) the code number of the data-set that will be referred 5**

**======= in the data on Features (8) and Reaches (3) 5**

**======= (b) the code number for the determinand. 5**

**======= (This is defined by its order in the above list of 5**

**======= determinands (2) ... the first is code number 1 etc) 5**

**======= (c) the code number of type of distribution: 5**

**======= (for Feature types 7 and 9: this is zero, 1 or 2) 5**

**======= 0 - constant, uniform concentration 5**

**======= 1 - concentration follows the Normal Distribution 5**

**======= 2 - the Log-Normal Distribution 5**

**======= 3 - a Three-Parameter Log-Normal Distribution 5**

**======= 4 - non-parametric distribution 5**

**======= 5 - monthly data - a distribution for each month 5**

**======================================================================5**

**======= For distribution types 4,5,8 and 9 the items (d),(e) and 5**

**======= (f) below do not appear. Instead is shown the name of 5**

**======= the data file holding the data for the distribution. 5**

**======= For example: 'npar.npd' (Note the need for this type of 5**

**======= quotation marks) 5**

**======================================================================5**

**======= 8 - monthly structure 5**

**======= 6 - as 1 but the data (d) and (e) refer to loads 5**

**======= 7 - as 2 but the data (d) and (e) refer to loads 5**

**======= 9 - non-parametric distribution of loads 5**

**======= 10 - a power-curve distribution for concentrations 5**

**======= 11 - a power-curve distribution for loads 5**

**======================================================================5**

**======= (d) the mean concentration 5**

**======= (e) the standard deviation 5**

**======= (f) the shift parameter for distribution types 3 5**

**======= for Distribution Type 0, 1 or 2: zero or blank 5**

**======= (g) reserved for a non-standard correlation coefficient 5**

**======= (h) number of samples used to compute the mean 5**

**======= (i) the name of the site (this is used for 5**

**======= identification. It is not needed by SIMCAT) 5**

**======================================================================5**

**======= For the power curves (10) and (11) items (f), (g) and (h) 5**

**======= become: 5**

**======= (f) the power index 5**

**======= (g) the base concentration (specified as a percentage of the 5**

**======= mean 5**

**======= (h) the cut off percentile (values below this are set to 5**

**======= zero) 5**

**======= (g) reserved for a non-standard correlation coefficient 5**

**======= (h) number of samples used to compute the mean 5**

**======= (i) the name of the site (this is used for 5**

**======= identification. It is not needed by SIMCAT) 5**

**=====b==c======d======e====f=======g===h=======i======================5**

**1 1 1 35.00 4.60 0.0 -9.9 30 'Head of Upper Ouse'**

**1 2 3 1.90 0.90 -0.5 -9.9 30 ''**

**1 3 2 0.05 0.05 0.0 -9.9 30 ''**

**1 4 1 9.00 1.50 0.0 -9.9 30 ''**

**1 5 2 0.07 0.07 0.0 -9.9 30 ''**

**2 1 2 35.00 4.60 0.0 -9.9 30 'Head of River Avon'**

**2 2 2 1.80 0.90 -0.5 -9.9 30 ''**

**2 3 2 0.07 0.10 0.0 -9.9 30 ''**

**2 4 1 9.00 1.50 0.0 -9.9 30 ''**

**2 5 2 0.09 0.09 0.0 -9.9 30 ''**

**3 1 2 35.00 4.60 0.0 -9.9 30 'Head of Black Brook'**

**3 2 3 1.90 1.00 0.5 -9.9 30 ''**

**3 3 2 0.04 0.04 0.0 -9.9 30 ''**

**3 4 3 9.00 1.00 0.0 -9.9 30 ''**

**3 5 2 0.05 0.05 0.0 -9.9 30 ''**

**4 1 1 33.60 4.60 0.0 -9.9 12 'Upper Ouse at Pig Farm'**

**4 2 2 2.00 0.80 0.0 -9.9 12 ''**

**4 3 2 0.00 0.00 0.0 -9.9 12 ''**

**4 4 1 8.80 1.20 0.0 -9.9 12 ''**

**4 5 2 0.10 0.10 0.0 -9.9 12 ''**

**5 1 2 36.00 4.20 0.0 -9.9 30 'Ouse Stream'**

**5 2 2 1.20 3.50 0.0 -9.9 26 ''**

**5 3 2 0.70 0.60 0.0 -9.9 30 ''**

**5 4 1 5.20 2.00 0.0 -9.9 26 ''**

**5 5 2 0.10 0.50 0.0 -9.9 30 ''**

**6 1 2 42.90 7.10 0.0 -9.9 30 'Black Brook'**

**6 2 2 2.00 1.00 0.0 -9.9 30 ''**

**6 3 2 0.04 0.04 0.0 -9.9 30 ''**

**6 4 1 8.80 1.00 0.0 -9.9 30 ''**

**6 5 2 0.05 0.06 0.0 -9.9 30 ''**

**7 1 2 50.00 5.70 0.0 -9.9 0 'Temply Station'**

**7 2 2 3.90 2.10 0.0 -9.9 0 ''**

**7 3 2 0.10 0.10 0.0 -9.9 0 ''**

**7 4 1 7.20 2.10 0.0 -9.9 0 ''**

**7 5 2 0.25 0.20 0.0 -9.9 26 ''**

**8 1 2 50.00 5.70 0.0 -9.9 26 'Middle Ouse Station'**

**8 2 2 3.90 2.10 0.0 -9.9 26 ''**

**8 3 2 0.30 0.30 0.0 -9.9 26 ''**

**8 4 1 7.20 2.10 0.0 -9.9 26 ''**

**8 5 2 0.11 0.80 0.0 -9.9 26 ''**

**9 1 2 53.00 5.30 0.0 -9.9 26 'Ouse at New Mill'**

**9 2 2 4.10 2.40 0.0 -9.9 26 ''**

**9 3 2 0.30 0.20 0.0 -9.9 30 ''**

**9 4 1 8.10 2.40 0.0 -9.9 26 ''**

**9 5 2 0.25 0.20 0.0 -9.9 26 ''**

**10 1 2 46.00 4.90 0.0 -9.9 12 'Avon at Valley Bottom'**

**10 2 2 3.90 2.20 0.0 -9.9 12 ''**

**10 3 2 0.50 0.50 0.0 -9.9 12 ''**

**10 4 1 5.90 2.20 0.0 -9.9 12 ''**

**10 5 2 1.15 0.80 0.0 -9.9 12 ''**

**11 1 1 10.00 2.00 0.0 -9.9 36 'Diffuse inflows'**

**11 2 2 0.50 0.20 0.0 -9.9 36 ''**

**11 3 2 0.00 0.00 0.0 -9.9 36 ''**

**11 4 1 8.80 0.00 0.0 -9.9 36 ''**

**11 5 2 0.05 0.05 0.0 -9.9 36 ''**

**14 1 2 90.00 6.00 0.0 -9.9 36 'Diffuse inflows'**

**14 2 2 60.00 40.00 0.0 -9.9 36 ''**

**14 3 2 40.00 5.00 0.0 -9.9 36 ''**

**14 4 1 0.00 0.00 0.0 -9.9 36 ''**

**14 5 1 4.00 4.00 0.0 -9.9 36 ''**

**\*\*\*\*\*\*\*\*\* indicator of end of the list of river quality data \*\*\*\*\*\*\*\*\*5**

**======================================================================6**

**======= Section [F] Effluent Flow & Quality ==========================6**

**======================================================================6**

**======= Effluent Flow and Quality Data-Sets follow. For each Data-Set 6**

**======= there is a line for the flow and a line for each determinand 6**

**======= each determinand in turn: 6**

**======= For each line the following are entered: 6**

**======= (a) the code number of the data-set (this will be referred 6**

**======= to in the data on Feature (8) 6**

**======= (b) the code number for the determinand (zero for flow) 6**

**======= (c) the code number of type of distribution: 6**

**======= 0 - constant, uniform values 6**

**======= 1 - a Normal Distribution 6**

**======= 2 - the Log-Normal Distribution 6**

**======= 3 - a Three-Parameter Log-Normal Distribution 6**

**======= 4 - non-parametric distribution 6**

**======= 5 - monthly data - distribution for each month 6**

**======= For distribution types 4,5 and 9 the items (d),(e) and 6**

**======= (f) below do not appear. Instead is shown the name of 6**

**======= the data file holding the data for the distribution. 6**

**======= For example: 'npar.npd' (Note the need for this type of 6**

**======= quotation marks) 6**

**======= 6 - as 2 but the data (d) and (e) refer to loads 6**

**======= 7 - as 5 but the data in the data file refer to loads 6**

**======= 8 - monthly structure 6**

**======= 9 - non-parametric distribution of loads 6**

**======= (d) the mean value 6**

**======= (e) the standard deviation 6**

**======= (f) the shift parameter for distribution types 3: for 6**

**======= Distribution Type 0, 1 or 2: zero or blank 6**

**======= (g) reserved for non-standard correlation coefficient 6**

**======= (h) number of samples used to compute the mean 6**

**======= (i) the name of the discharge. This is used for 6**

**======= identification. It is not needed by SIMCAT 6**

**======================================================================6**

**======= The following types of Feature use effluent data: 6**

**======================================================================6**

**======= 3 - sewage works or sewage discharge 6**

**======= 5 - industrial effluent discharge 6**

**======= 12 - intermittent discharge 6**

**======= 15 - start point for diffuse pollution 6**

**======= (effluent type) 6**

**======= 40 - start point for aggregated CSOs 6**

**======= 42 - start point for aggregated sewage works 6**

**======= 60 - other point sources 6**

**======= 61 - private wastewaters 6**

**======b=c=========d========e=====f========g===h=====i=================6**

**1 0 2 4.00 1.80 1.00 -9.9 365 'Wellington STW'**

**1 1 2 91.50 8.20 0.00 -9.9 30 ''**

**1 2 2 35.00 30.00 20.00 -9.9 56 ''**

**1 3 2 15.00 9.00 0.00 -9.9 55 ''**

**1 4 2 0.50 0.20 0.00 -9.9 56 ''**

**1 5 2 4.50 2.20 0.00 -9.9 56 ''**

**2 0 2 2.50 0.80 0.00 -9.9 365 'Brickton STW'**

**2 1 2 95.00 4.60 0.00 -9.9 30 ''**

**2 2 2 35.00 30.00 0.00 -9.9 56 ''**

**2 3 2 15.00 9.00 0.00 -9.9 55 ''**

**2 4 2 1.00 0.50 0.00 -9.9 56 ''**

**2 5 2 4.50 2.20 0.00 -9.9 56 ''**

**3 0 2 2.00 0.70 0.00 -9.9 365 'Appleford STW'**

**3 1 2 95.00 4.60 0.00 -9.9 30 ''**

**3 2 3 17.00 9.00 4.00 -9.9 56 ''**

**3 3 2 15.00 9.00 0.00 -9.9 55 ''**

**3 4 3 2.00 1.20 0.00 -9.9 56 ''**

**3 5 2 1.50 2.20 0.00 -9.9 56 ''**

**4 0 2 0.10 0.10 0.00 -9.9 365 'Allied Industries'**

**4 1 1 380.00 22.00 0.00 -9.9 10 ''**

**4 2 2 80.00 50.00 0.00 -9.9 10 ''**

**4 3 2 0.00 0.00 0.00 -9.9 10 ''**

**4 4 2 0.00 0.00 0.00 -9.9 10 ''**

**4 5 2 4.50 2.20 0.00 -9.9 56 ''**

**6 0 4 'inter.npd' -9.9 365 'New Mill Storm Overflows'**

**6 1 2 60.00 4.60 0.00 -9.9 30 ''**

**6 2 3 163.00 30.00 4.00 -9.9 26 ''**

**6 3 2 20.00 6.00 0.00 -9.9 27 ''**

**6 4 3 0.00 0.00 0.00 -9.9 28 ''**

**6 5 2 2.50 2.20 0.00 -9.9 56 ''**

**8 0 2 1.00 0.40 0.00 -9.9 365 'Diffuse Source'**

**8 1 2 91.00 12.60 0.00 -9.9 30 ''**

**8 2 2 61.00 30.00 0.00 -9.9 56 ''**

**8 3 2 15.00 9.00 0.00 -9.9 55 ''**

**8 4 2 1.00 0.50 0.00 -9.9 56 ''**

**8 5 2 4.50 2.20 0.00 -9.9 56 ''**

**\*\*\*\*\*\*\*\*\*\*\*\* indicator of end of effluent flow and quality data \*\*\*\*\*\*6**

**======================================================================7**

**======= Section [6] River Quality Targets ============================7**

**======================================================================7**

**======= The data sets for River Quality Targets follow. There is one 7**

**======= line for each set. It contains: 7**

**======= (a) a code number to be cited in the Feature data below (8) 7**

**======================================================================7**

**======= The targets follow. These are defined as the statistics 7**

**======= entered above (as item (l)) within data on Determinands (1) 7**

**======================================================================7**

**======= If the Determinand data contain no such definition, these 7**

**======= standards are defined as the statistic set up above (Set 0) 7**

**======= as the definition of Mean Mode 7**

**======================================================================7**

**======= (b-k) the targets for up to 10 determinands. Zero indicates 7**

**======= that no target is to be applied. 7**

**======================================================================7**

**======= These targets will be over-written by any targets that have 7**

**======= been specified above with the data for individual Reaches (3) 7**

**======================================================================7**

**======= Negative values specified for (a) are taken as defining a 7**

**======= system of classification. (The positive value of (a) is still 7**

**======= used as a target within the data on Features). 7**

**======= This classification is over-written by any classification 7**

**======= entered for particular reaches with the Reach Data (3) 7**

**======a======b======c======d======e======f======g======h======i=======7**

**1 0.00 5.00 1.50 0.00 0.10**

**2 0.00 8.00 3.00 0.00 0.10**

**3 250.00 5.00 1.50 0.00 0.10**

**\*\*\*\*\*\*\*\*\* indicator of the end of data on river quality targets \*\*\*\*\*\*7**

**======================================================================8**

**======= Section [I] Features =========================================8**

**======================================================================8**

**======= The Data-Sets for Features follow. There is one line for 8**

**======= each feature. Each line holds: 8**

**======= (a) the name of the Feature 8**

**======= (b) the code for the type of Feature, these are: 8**

**======= 1 - monitoring station 8**

**======= 2 - stream or tributary 8**

**======= 3 - sewage works or sewage discharge 8**

**======= 4 - river flow gauge 8**

**======= 5 - industrial effluent discharge 8**

**======= 6 - plotting point 8**

**======= 7 - abstraction (of flow) 8**

**======= 8 - weir 8**

**======= (must be at head of Reach) 8**

**======= 9 - river flow regulation point 8**

**======= (switched on only in Modes 3-8) 8**

**======= 10 - upstream river boundary 8**

**======= 11 - bifurcation 8**

**======= (must be at head of Reach) 8**

**======= 12 - intermittent discharge 8**

**======= 13 - start point for diffuse pollution 8**

**======= (river type) 8**

**======= 14 - end point for diffuse pollution 8**

**======= 15 - start point for diffuse pollution 8**

**======= (effluent type) 8**

**======= 16 - end point for diffuse pollution 8**

**======= 17 - a feature that has no flow, eg. a future 8**

**======= effluent discharge in a current model 8**

**======= Allow "what-if" runs based on gap-filled 8**

**======= model 8**

**======= 18 - an abstraction which removes a set 8**

**======= distribution of flow feature. A sort 8**

**======= of negative discharge. The 8**

**======= distribution to be abstracted is 8**

**======= entered with the river flow data sets 8**

**======= 19 - as 18 but the distribution to be 8**

**======= abstracted is entered with the effluent 8**

**======= data sets 8**

**======= 20 - bifurcation (first arm) 8**

**======= distribution to be abstracted to second 8**

**======= arm is entered as a river flow data set 8**

**======= (feature must be at head of Reach) 8**

**======= 21 - bifurcation (second arm) 8**

**======= distribution to be diverted to this 8**

**======= arm is entered as a river flow data set 8**

**======= (Feature must be at head of the Reach) 8**

**======= 22 - bifurcation (first arm) 8**

**======= the distribution to be abstracted 8**

**======= to second arm (23) is entered with 8**

**======= the effluent data sets 8**

**======= (Feature must be at head of the Reach) 8**

**======= 23 - bifurcation (second arm) 8**

**======= the distribution to be diverted to this 8**

**======= arm (23) is entered with the effluent 8**

**======= data sets (the feature must be at the 8**

**======= head of a Reach) 8**

**======= 24 - boundary of a sub-catchment 8**

**======= 25 - start point for agricultural livestock 8**

**======= 26 - end point for agricultural livestock 8**

**======= 27 - start point for agricultural arable 8**

**======= 28 - end point for agricultural arable 8**

**======= 29 - start point for highway runoff 8**

**======= 30 - end point for highway runoff 8**

**======= 31 - start point for urban runoff 8**

**======= 32 - end point for urban runoff 8**

**======= 33 - start point for atmospheric deposition 8**

**======= 34 - end point for atmospheric deposition 8**

**======= 35 - start point for natural background 8**

**======= 36 - end point for natural background 8**

**======= 37 - start point for septic tanks 8**

**======= 38 - end point for septic tanks 8**

**======= 39 - point discharge from mine water 8**

**======= 40 - start point for aggregated CSOs 8**

**======= 41 - end point for aggregated CSOs 8**

**======= 42 - start point for aggregated sewage works 8**

**======= 43 - end point for aggregated sewage works 8**

**======= 44 - flow into a lake 8**

**======= 45 - flow from a lake 8**

**======= 46 - start point for - diffuse mines 8**

**======= 47 - end point for - diffuse mines 8**

**======= 48 - start for - birds, boats and angling 8**

**======= 49 - end point - birds, boats and angling 8**

**======= 50 - start for - "user defined type" 8**

**======= 51 - end point - "user defined type" 8**

**======= 52 - start for - "user defined type" 8**

**======= 53 - end point - "user defined type" 8**

**======= 54 - start for - "user defined type" 8**

**======= 55 - end point - "user defined type" 8**

**======= 56 - start for - "user defined type" 8**

**======= 56 - end point - "user defined type" 8**

**======= 58 - start for - "user defined type" 8**

**======= 59 - end point - "user defined type" 8**

**======= 60 - other point sources 8**

**======= 61 - private wastewaters 8**

**======================================================================8**

**======= (c) the code number of the Reach on which the 8**

**======= Feature is located (Set 2) 8**

**======= (d) distance from the head of the reach (km) 8**

**======= (except for Feature Type 11 where it defines 8**

**======= the fraction of flow passing down the 8**

**======= bifurcation) 8**

**======= (e) the code number of the river flow Data-Set 8**

**======= (discharged from Feature Types 2 & 13) 8**

**======= (recorded at Feature Type 4) 8**

**======= (abstracted at Feature Type 7 or 18) 8**

**======= (for feature types 20 and 21 where this 8**

**======= is the Reach number that provides flow data 8**

**======= at the end of the Reach for the bifurcation) 8**

**======= (f) the code number for the river quality 8**

**======= Data-Set(4) or the effluent flow/quality 8**

**======= Data-Set(5) (non-zero for Feature Types 2,3,5, 8**

**======= 13 and 15, 19) 8**

**======= (data-set for quality produced by Weir(8) 8**

**======= (for feature types 20 and 21 where this 8**

**======= the river flow data set giving flow for the 8**

**======= bifurcation) 8**

**======= (for feature types 22 and 22 where this 8**

**======= the discharge data set giving flow for the 8**

**======= bifurcation) 8**

**======= (g) the code number of any river flow Data-Set to 8**

**======= be fitted by Gap-filling. Prefixing a minus 8**

**======= sign will suppress downstream extrapolation 8**

**======================================================================8**

**======= (h) the code number of any river quality Data-Set 8**

**======= to be fitted by SIMCAT Gap-filling. 8**

**======= Prefixing a minus sign will suppress downstream 8**

**======= extrapolation. 8**

**======= For Feature Type 8 the code number for this 8**

**======= river quality Data-Set defines quality 8**

**======= downstream of the Weir. 8**

**======================================================================8**

**======= Defining the Feature to be at the Head of a 8**

**======= Reach will suppress upstream interpolation. 8**

**======================================================================8**

**======= (i) the code number for any Data-set of river 8**

**======= quality targets specified above in Set 7. 8**

**======= If a Reach Target is in Set 3 this target will 8**

**======= be replaced by that Reach Target. 8**

**======= If value is 999 for a discharge, its quality 8**

**======= will not be tuned to achieve any target 8**

**======= If value is -ve the target will be retained 8**

**======= despite the presence of Reach Targets (Set 3) 8**

**======================================================================8**

**======= (j) user notes such as grid reference for GIS (not 8**

**======= required by SIMCAT but often helpful to users) 8**

**===========a=======================b==c=====d===e===f==g==h=i====j====8**

**'Head of Upper Ouse' 10 1 0.0 1 1 0 0 0**

**'Pig Farm Gauging Station' 4 1 4.0 4 0 4 0 0**

**'Ouse Stream' 2 1 6.0 5 1 0 0 0**

**'Wellington STW' 3 1 8.0 0 1 0 0 3**

**'Middle Ouse Monitoring Station' 1 1 14.0 0 8 0 8 0**

**'Head of River Avon' 10 2 0.0 2 2 0 0 0**

**'Avon Regulation' 9 2 1.0 12 11 0 0 0**

**'Brickton STW' 3 2 3.0 0 2 0 0 1**

**'Valley Bottom Monitoring Station' 1 2 9.0 0 10 0 10 0**

**'Valley Bottom Gauging Station' 4 2 9.0 6 0 6 0 0**

**'Allied Industries' 5 3 1.0 0 4 0 0 3**

**'Head of Black Brook' 10 4 0.0 3 3 0 0 0**

**'Black Brook Monitoring Station' 1 4 2.0 0 6 0 6 0**

**'Appleford STW' 3 4 3.0 0 3 0 0 2**

**'Intermittent' 12 4 6.1 0 4 0 0 3**

**'Avon Stream' 2 5 1.0 16 1 0 0 0**

**'NM Monitoring Station' 1 5 1.5 0 9 0 9 0**

**'NM Flow Gauging Station' 4 5 2.0 9 0 9 0 0**

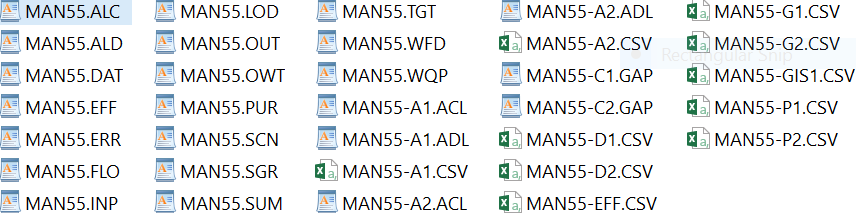
**'Storm Overflow' 12 5 4.0 0 6 0 0 0**

**'Abstraction' 7 5 7.0 18 0 0 0 0**

**\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* indicator of end of all data \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\***

# SIMCAT OUTPUT FILES

### SIMCAT creates lots of output files. These can be inspected using a Word Processor or your Text Editor or they can be printed. Files of the type .CSV can be picked up with things like EXCEL. The list of files produced for 5 determinands is shown below. These will all reside in the same folder as your SIMCAT data file:



### The names of some of the files are shown below. The term 'name' is the stem of the name of the data-file entered on the screen. For the test data, *EG*.DAT, the output files will be called *EG.*OUT, *EG.*SCN, etc. Examples of the files *EG.*SCN, *EG.*LOD and *EG.*OWT are given in this Appendix.

|  |  |
| --- | --- |
| apportionment of loads from sub-catchments | *name* .ALC |
| apportionment of loads from discharges | *name* .ALD |
| a report on errors or peculiarities in data uncovered by SIMCAT | *name* .ERR |
| a report of effluent discharges | *name* .EFF |
| a report on river flows | *name* .FLO |
|  | *name* .INP |
| a report on loads | *name* .LOD |
| the detailed output | *name* .OUT |
| smaller version of .OUT | *name* .OWT |
| a report on natural purification and diffuse pollution | *name* .PUR |
| a copy of the output displayed on the screen | *name* .SCN |
| file for use in SIMCAT's graph plotting | *name* .SGR |
| a report on sources and sinks of pollution | *name* .SUM |
| a report on compliance with river quality standards | *name* .TGT |
| a report on classification under the Water Framework Directive | *name* .WFD |
| a file use for reports on water quality planning | *name* .WQP |
|  |  |
| a file of data that can be taken up into a Geographical Information System and used to display SIMCAT’s results as maps | *name-GIS1*.CSV |
| data on effluents and the standards needed to meet river targets | *name-EFF*.CSV |
|  |  |
| a working file used by Gap-filling of river flows | *name* .FCL |
| a working file used by Gap-filling of river quality | *name* .QCL |
|  |  |
| apportionment of contributions to concentrations from discharges | *name .*ACD |
| and from contributions to concentrations from sub-catchments | *name .*ACC |
|  |  |
| apportionment for each determinand: A1, A2, etc |  |
| apportionment of loads from sub-catchments | *name*-A1.ACL |
| apportionment of loads from discharges | *name*-A1.ADL |
| apportionment of loads from discharges (comma-separated-data) | *name*-A1.CSV |
| apportionment of contributions to concentrations from discharges | *name*-A1.ACD |
|  |  |
| output files for each determinand: C1, C2, etc |  |
|  | *name*-C1.GAP |
| output files for each determinand: D1, D2, etc |  |
|  | *name*-D1.CSV |
|  | *name*-D1.MON |
|  |  |
| output files on effluent discharges for particular determinand: |  |
| effluent discharges | *name*-EFF.CSV |
|  |  |
| output files for each determinand: G1, G2, etc |  |
| file for use in SIMCAT's graph plotting | *name*-G1.CSV |
|  |  |
| Simplified output on apportionment from discharges: P1, P2, etc |  |
| apportionment for determinand 1 ... etc | *name*-P1.CSV |

## Copy of the Output File EG.SCN for Run Type 0

**-----------------------------------------------------------------------------**

**SIMCAT Model for Planning River Water Quality ... Date: 06/12/2018**

**Version 15.7 (Tony Warn 25/11/18) ... Time: 11.37**

**-----------------------------------------------------------------------------**

**Set of data to illustrate the SIMCAT User Manual ... EG.DAT**

**-----------------------------------------------------------------------------**

**Number of Shots - 365**

**-----------------------------------------------------------------------------**

**Run type = 0 (Basic Simulation)**

**-----------------------------------------------------------------------------**

**-----------------------------------------------------------------------------**

**Copy of information displayed on the screen ...**

**-----------------------------------------------------------------------------**

**-----------------------------------------------------------------------------**

**\*\*\* Your SIMCAT data is set up to expect monthly structured data**

**\*\*\* No such data have been specified ...**

**\*\*\* Monthly structure will still be imposed on annual flow data**

**\*\*\* Change the setting to zero to suppress this ...**

**-----------------------------------------------------------------------------**

**--------------------------------------------------------------------------------------------**

**Dist Flow Cl BOD Amm DO PO4**

**(km) m3/d mg/l mg/l mg/l mg/l mg/l**

**---- mean mean mean mean mean mean**

**--------------------------------------------------------------------------------------------**

**Head of Upper Ouse 0.0 28.0 35.0 1.90 .0500 9.00 .0700**

**Head of Upper Ouse 0.0 28.0 35.0 1.90 .0500 9.00 .0700**

**Pig Farm Gauging Station 4.0 32.0 32.6 1.66 .0331 9.34 .0676**

**Measured river flow 30.0**

**Ouse Stream 6.0 36.0 31.7 1.59 .0288 9.44 .0669**

**Wellington STW 8.0 42.0 39.3 6.32 2.12 8.27 .693**

**--------------------------------------------------------------------------------**

**Form of standard ... mean Q90 Q90 Q10 mean**

**Targets for river quality 250.0 5.00 1.50 - .100**

**Downstream river quality 39.3 12.7 4.37 7.13 .693**

**--------------------------------------------------------------------------------**

**Middle Ouse Monitoring Station 14.0 48.0 36.6 4.57 1.13 8.46 .633**

**================================================================================**

**... observed mean values 50.0 3.90 .300 7.20 .110**

**... observed 95 or 5-percentiles 59.9 7.87 .834 3.75 .400**

**================================================================================**

**End of Reach: Upper Ouse 16.0 50.0 35.9 4.17 .939 8.55 .615**

**% Errors in mean 6% 17% 19% 4% 20%**

**Head of River Avon 0.0 4.00 35.0 1.80 .0700 9.00 .0900**

**Head of River Avon 0.0 4.00 35.0 1.80 .0700 9.00 .0900**

**Avon Regulation 1.0 5.34 28.7 1.46 .0490 9.02 .0792**

**Brickton STW 3.0 9.84 45.7 11.4 4.47 6.69 1.39**

**--------------------------------------------------------------------------------**

**Form of standard ... mean Q90 Q90 Q10 mean**

**Targets for river quality - 5.00 1.50 - .100**

**Downstream river quality 45.7 20.7 8.05 5.54 1.39**

**--------------------------------------------------------------------------------**

**Valley Bottom Monitoring Statio 9.0 15.8 35.8 7.20 2.36 7.43 1.03**

**================================================================================**

**... observed mean values 46.0 3.90 .500 5.90 1.15**

**... observed 95 or 5-percentiles 54.5 8.06 1.39 2.28 2.65**

**================================================================================**

**Valley Bottom Gauging Station 9.0 15.8 35.8 7.20 2.36 7.43 1.03**

**Measured river flow 15.0**

**End of Reach: River Avon 12.0 18.8 32.9 5.99 1.79 7.70 .920**

**% Errors in mean 7% 21% 17% 5% 15%**

**Mix to form Middle Ouse 16.0 68.8 35.0 4.71 1.18 8.31 .698**

**Allied Industries 17.0 69.9 35.6 4.79 1.11 8.34 .699**

**--------------------------------------------------------------------------------**

**Form of standard ... mean Q90 Q90 Q10 mean**

**Targets for river quality 250.0 5.00 1.50 - .100**

**Downstream river quality 35.6 8.63 1.99 6.92 .699**

**--------------------------------------------------------------------------------**

**End of Reach: Middle Ouse 18.0 70.9 35.4 4.65 1.04 8.37 .693**

**% Errors in mean 7% 15% 15% 4% 15%**

**Head of Black Brook 0.0 1.00 35.0 1.90 .0400 9.00 .0500**

**Head of Black Brook 0.0 1.00 35.0 1.90 .0400 9.00 .0500**

**Black Brook Monitoring Station 2.0 3.00 20.6 1.08 .0154 9.07 .0500**

**================================================================================**

**... observed mean values 42.9 2.00 .0400 8.80 .0500**

**... observed 95 or 5-percentiles 55.5 3.89 .111 7.16 .151**

**================================================================================**

**Appleford STW 3.0 6.00 52.8 8.16 6.71 5.87 .721**

**--------------------------------------------------------------------------------**

**Form of standard ... mean Q90 Q90 Q10 mean**

**Targets for river quality - 8.00 3.00 - .100**

**Downstream river quality 52.8 14.8 13.0 3.93 .721**

**--------------------------------------------------------------------------------**

**Intermittent 6.1 9.20 46.9 6.87 4.23 6.73 .607**

**--------------------------------------------------------------------------------**

**Form of standard ... mean Q90 Q90 Q10 mean**

**Targets for river quality 250.0 5.00 1.50 - .100**

**Downstream river quality 46.9 12.5 8.35 4.67 .607**

**--------------------------------------------------------------------------------**

**End of Reach: Black Brook 10.0 13.1 38.8 5.00 2.67 7.45 .482**

**% Errors in mean 12% 16% 21% 6% 34%**

**Mix to form Lower Ouse 18.0 84.0 35.8 4.69 1.28 8.24 .662**

**Avon Stream 19.0 185.0 35.5 3.16 .587 8.66 .349**

**NM Monitoring Station 19.5 185.5 35.4 3.13 .571 8.69 .348**

**================================================================================**

**... observed mean values 53.0 4.10 .300 8.10 .250**

**... observed 95 or 5-percentiles 62.1 8.64 .677 4.15 .621**

**================================================================================**

**NM Flow Gauging Station 20.0 186.0 35.3 3.10 .555 8.72 .347**

**Measured river flow 84.0**

**Storm Overflow 22.0 190.1 35.3 3.68 .604 8.79 .350**

**--------------------------------------------------------------------------------**

**Form of standard ... mean Q90 Q90 Q10 mean**

**Targets for river quality - - - - -**

**Downstream river quality 35.3 5.04 1.01 7.46 .350**

**--------------------------------------------------------------------------------**

**Abstraction 25.0 - 35.0 3.44 .515 8.93 .345**

**End of Reach: Lower Ouse 26.0 - 25.1 2.49 .339 9.20 .186**

**% Errors in mean 13% 47% 55% 5% 19%**

**----------------------------------------------------------------------------------------**

**Number of WARNINGS about data: 1**

**Check the .ERR file for details ...**

**#####################################################**

## Copy of the Output File EG.OWT for Run Type 0

**-----------------------------------------------------------------------------**

**SIMCAT Model for Planning River Water Quality ... Date: 06/12/2018**

**Version 15.7 (Tony Warn 25/11/18) ... Time: 11.37**

**-----------------------------------------------------------------------------**

**Set of data to illustrate the SIMCAT User Manual ... EG.DAT**

**-----------------------------------------------------------------------------**

**Number of Shots - 365**

**-----------------------------------------------------------------------------**

**Run type = 0 (Basic Simulation)**

**-----------------------------------------------------------------------------**

**=============================================================================**

**THE MAIN CALCULATIONS FOLLOW ...**

**=============================================================================**

**Calculations for the first reach ... Upper Ouse**

**=============================================================================**

**Calculated summary statistics for temperature ... Mean = 11.2 Deg**

**Standard deviation = 3.00 Deg**

**==============================================================================================================**

**Calculation for the reach named: Upper Ouse Reach Number 1**

**==============================================================================================================**

**Length of Reach: 16.0 km Flow at head of Reach: Mean = 28.0 m3/d**

**95-percent exceedence = 4.80 m3/d**

**90% exceedence = 6.46 m3/d**

**99% exceedence = 2.56 m3/d**

**==============================================================================================================**

**Calculated summary statistics for temperature ... Mean = 11.2 Deg**

**Standard deviation = 3.00 Deg**

**==============================================================================================================**

**River quality at the head of the Reach named: Upper Ouse**

**==============================================================================================================**

**Chloride... Mean = 35.0 mg/l (34-36)**

**Standard deviation = 4.60 mg/l**

**90-percentile = 41.1 mg/l (39-44)**

**95-percentile = 43.3 mg/l (41-47)**

**99-percentile = 45.4 mg/l (42-50)**

**--------------------------------------------------------------------------------------------------------------**

**B.O.D...... Mean = 1.90 mg/l (1.6-2.2)**

**Standard deviation = .899 mg/l**

**90-percentile = 3.09 mg/l (2.6-3.9)**

**95-percentile = 3.87 mg/l (3.3-4.9)**

**99-percentile = 5.49 mg/l (4.5-7.4)**

**--------------------------------------------------------------------------------------------------------------**

**Ammonia.... Mean = .0500 mg/l (0.035-0.065)**

**Standard deviation = .0495 mg/l**

**90-percentile = .0992 mg/l (0.073-0.151)**

**95-percentile = .132 mg/l (0.093-0.216)**

**99-percentile = .292 mg/l (0.21-0.50)**

**--------------------------------------------------------------------------------------------------------------**

**Diss.Oxygen Mean = 9.00 mg/l (8.5-9.5)**

**Standard deviation = 1.50 mg/l**

**10-percentile = 6.99 mg/l (6.2-7.5)**

**5-percentile = 6.69 mg/l (5.8-7.3)**

**1-percentile = 5.58 mg/l (4.5-6.3)**

**--------------------------------------------------------------------------------------------------------------**

**Phosphate.. Mean = .0700 mg/l (0.049-0.091)**

**Standard deviation = .0705 mg/l**

**90-percentile = .160 mg/l (0.123-0.234)**

**95-percentile = .202 mg/l (0.147-0.323)**

**99-percentile = .416 mg/l (0.30-0.71)**

**--------------------------------------------------------------------------------------------------------------**

**==============================================================================================================**

**Classification at the head of the Reach called Upper Ouse**

**==============================================================================================================**

**....... Confidence of class (%) .......**

**==============================================================================================================**

**High Good Moderate Poor Bad Class boundaries ...................... Statistic**

**==============================================================================================================**

**==============================================================================================================**

**==============================================================================================================**

**Stretch: Upper Ouse From the start of the Reach ...**

**==============================================================================================================**

**==============================================================================================================**

**Stretch: Upper Ouse from: Head of Upper Ouse to Pig Farm Gauging Station**

**==============================================================================================================**

**==============================================================================================================**

**Classification at: Pig Farm Gauging Station Feature: 2 Reach: 1**

**--------------------------------------------------------------------------------------------------------------**

**Location: 4.0 km downstream from the head of the Reach called Upper Ouse**

**==============================================================================================================**

**....... Confidence of class (%) .......**

**==============================================================================================================**

**High Good Moderate Poor Bad Class boundaries ...................... Statistic**

**==============================================================================================================**

**==============================================================================================================**

**--------------------------------------------------------------------------------------------------------------**

**Pig Farm Gauging Station Feature No 2 Reach No 1**

**--------------------------------------------------------------------------------------------------------------**

**LOCATION: 4.0 km downstream from the head of the Reach called Upper Ouse**

**--------------------------------------------------------------------------------------------------------------**

**Flow in river just upstream ... Mean = 32.0 m3/d**

**95% exceedence = 5.08 m3/d**

**90% exceedence = 6.92 m3/d**

**99% exceedence = 2.68 m3/d**

**=============================================================================**

**=============================================================================**

**Observed flow in the river ... Mean = 30.0 m3/d**

**95-percentile low flow = 6.00 m3/d**

**=============================================================================**

**Chloride... Mean = 32.6 mg/l (31-34)**

**Standard deviation = 4.25 mg/l**

**90-percentile = 38.0 mg/l (36-40)**

**95-percentile = 40.3 mg/l (38-43)**

**99-percentile = 42.7 mg/l (40-47)**

**--------------------------------------------------------------------------------------------------------------**

**B.O.D...... Mean = 1.66 mg/l (1.45-1.87)**

**Standard deviation = .705 mg/l**

**90-percentile = 2.60 mg/l (2.3-3.2)**

**95-percentile = 3.21 mg/l (2.8-4.0)**

**99-percentile = 4.38 mg/l (3.7-5.7)**

**--------------------------------------------------------------------------------------------------------------**

**Ammonia.... Mean = .0331 mg/l (0.023-0.043)**

**Standard deviation = .0324 mg/l**

**90-percentile = .0673 mg/l (0.050-0.101)**

**95-percentile = .0888 mg/l (0.064-0.144)**

**99-percentile = .186 mg/l (0.134-0.318)**

**--------------------------------------------------------------------------------------------------------------**

**Diss.Oxygen Mean = 9.34 mg/l (9.0-9.7)**

**Standard deviation = 1.13 mg/l**

**10-percentile = 7.91 mg/l (7.4-8.3)**

**5-percentile = 7.58 mg/l (6.9-8.0)**

**1-percentile = 6.69 mg/l (5.9-7.2)**

**--------------------------------------------------------------------------------------------------------------**

**Phosphate.. Mean = .0676 mg/l (0.049-0.087)**

**Standard deviation = .0637 mg/l**

**90-percentile = .144 mg/l (0.111-0.209)**

**95-percentile = .188 mg/l (0.139-0.292)**

**99-percentile = .385 mg/l (0.29-0.63)**

**--------------------------------------------------------------------------------------------------------------**

**==============================================================================================================**

**Stretch: Upper Ouse from: Pig Farm Gauging Station to Ouse Stream**

**==============================================================================================================**

**==============================================================================================================**

**Classification at: Ouse Stream Feature: 3 Reach: 1**

**--------------------------------------------------------------------------------------------------------------**

**Location: 6.0 km downstream from the head of the Reach called Upper Ouse**

**==============================================================================================================**

**....... Confidence of class (%) .......**

**==============================================================================================================**

**High Good Moderate Poor Bad Class boundaries ...................... Statistic**

**==============================================================================================================**

**==============================================================================================================**

**--------------------------------------------------------------------------------------------------------------**

**Ouse Stream Feature No 3 Reach No 1**

**--------------------------------------------------------------------------------------------------------------**

**LOCATION: 6.0 km downstream from the head of the Reach called Upper Ouse**

**--------------------------------------------------------------------------------------------------------------**

**Flow in river just upstream ... Mean = 34.0 m3/d**

**95% exceedence = 5.22 m3/d**

**90% exceedence = 7.15 m3/d**

**99% exceedence = 2.74 m3/d**

**=============================================================================**

**River quality just upstream of tributary ...**

**--------------------------------------------------------------------------------------------------------------**

**Chloride... Mean = 31.5 mg/l (30-33)**

**Standard deviation = 4.13 mg/l**

**90-percentile = 37.0 mg/l (35-39)**

**95-percentile = 38.7 mg/l (37-42)**

**99-percentile = 41.6 mg/l (39-46)**

**--------------------------------------------------------------------------------------------------------------**

**B.O.D...... Mean = 1.57 mg/l (1.38-1.75)**

**Standard deviation = .630 mg/l**

**90-percentile = 2.38 mg/l (2.1-2.9)**

**95-percentile = 2.95 mg/l (2.6-3.6)**

**99-percentile = 3.94 mg/l (3.3-5.1)**

**--------------------------------------------------------------------------------------------------------------**

**Ammonia.... Mean = .0274 mg/l (0.019-0.036)**

**Standard deviation = .0272 mg/l**

**90-percentile = .0567 mg/l (0.042-0.085)**

**95-percentile = .0739 mg/l (0.053-0.120)**

**99-percentile = .162 mg/l (0.117-0.274)**

**--------------------------------------------------------------------------------------------------------------**

**Diss.Oxygen Mean = 9.47 mg/l (9.2-9.8)**

**Standard deviation = 1.01 mg/l**

**10-percentile = 8.22 mg/l (7.7-8.6)**

**5-percentile = 7.81 mg/l (7.2-8.2)**

**1-percentile = 7.15 mg/l (6.4-7.6)**

**--------------------------------------------------------------------------------------------------------------**

**Phosphate.. Mean = .0666 mg/l (0.049-0.085)**

**Standard deviation = .0609 mg/l**

**90-percentile = .141 mg/l (0.109-0.203)**

**95-percentile = .183 mg/l (0.137-0.281)**

**99-percentile = .372 mg/l (0.28-0.60)**

**--------------------------------------------------------------------------------------------------------------**

**Flow discharged from tributary: Mean = 2.00 m3/d**

**Number of data set: 5 95% exceedence = .400 m3/d**

**-----------------------------------------------------------------------------**

**Chloride... Mean = 35.0 mg/l**

**Standard deviation = 4.60 mg/l**

**B.O.D...... Mean = 1.90 mg/l**

**Standard deviation = .900 mg/l**

**Ammonia.... Mean = .0500 mg/l**

**Standard deviation = .0500 mg/l**

**Diss.Oxygen Mean = 9.00 mg/l**

**Standard deviation = 1.50 mg/l**

**Phosphate.. Mean = .0700 mg/l**

**Standard deviation = .0700 mg/l**

**-----------------------------------------------------------------------------**

**-----------------------------------------------------------------------------**

**Flow in river just downstream ... Mean = 36.0 m3/d**

**95% exceedence = 5.62 m3/d**

**-----------------------------------------------------------------------------**

**--------------------------------------------------------------------------------------------------------------**

**River quality d/s of tributary ...**

**--------------------------------------------------------------------------------------------------------------**

**Chloride... Mean = 31.7 mg/l (31-33)**

**Standard deviation = 3.92 mg/l**

**90-percentile = 36.8 mg/l (35-39)**

**95-percentile = 38.4 mg/l (37-41)**

**99-percentile = 41.0 mg/l (39-45)**

**--------------------------------------------------------------------------------------------------------------**

**B.O.D...... Mean = 1.59 mg/l (1.39-1.78)**

**Standard deviation = .643 mg/l**

**90-percentile = 2.41 mg/l (2.1-2.9)**

**95-percentile = 2.97 mg/l (2.6-3.7)**

**99-percentile = 4.04 mg/l (3.4-5.2)**

**--------------------------------------------------------------------------------------------------------------**

**Ammonia.... Mean = .0288 mg/l (0.020-0.037)**

**Standard deviation = .0284 mg/l**

**90-percentile = .0597 mg/l (0.045-0.089)**

**95-percentile = .0753 mg/l (0.053-0.123)**

**99-percentile = .170 mg/l (0.124-0.287)**

**--------------------------------------------------------------------------------------------------------------**

**Diss.Oxygen Mean = 9.44 mg/l (9.2-9.7)**

**Standard deviation = .940 mg/l**

**10-percentile = 8.28 mg/l (7.8-8.6)**

**5-percentile = 7.93 mg/l (7.4-8.3)**

**1-percentile = 7.32 mg/l (6.6-7.8)**

**--------------------------------------------------------------------------------------------------------------**

**Phosphate.. Mean = .0669 mg/l (0.049-0.085)**

**Standard deviation = .0613 mg/l**

**90-percentile = .142 mg/l (0.110-0.204)**

**95-percentile = .184 mg/l (0.138-0.283)**

**99-percentile = .376 mg/l (0.28-0.61)**

**--------------------------------------------------------------------------------------------------------------**

**==============================================================================================================**

**Classification d/s of: Ouse Stream Feature: 3 Reach: 1**

**--------------------------------------------------------------------------------------------------------------**

**Location: 6.0 km downstream from the head of the Reach called Upper Ouse**

**==============================================================================================================**

**....... Confidence of class (%) .......**

**==============================================================================================================**

**High Good Moderate Poor Bad Class boundaries ...................... Statistic**

**==============================================================================================================**

**==============================================================================================================**

**==============================================================================================================**

**Stretch: Upper Ouse from: Ouse Stream to Wellington STW**

**==============================================================================================================**

**==============================================================================================================**

**Classification at: Wellington STW Feature: 4 Reach: 1**

**--------------------------------------------------------------------------------------------------------------**

**Location: 8.0 km downstream from the head of the Reach called Upper Ouse**

**==============================================================================================================**

**....... Confidence of class (%) .......**

**==============================================================================================================**

**High Good Moderate Poor Bad Class boundaries ...................... Statistic**

**==============================================================================================================**

**==============================================================================================================**

**--------------------------------------------------------------------------------------------------------------**

**Assessment of compliance with standards u/s of Wellington STW**

**--------------------------------------------------------------------------------------------------------------**

**Chloride... Mean standard = 250.0 mg/l**

**Test statistic = 30.9 mg/l (30-32)**

**Confidence that the standard was failed = 0.000 per cent**

**--------------------------------------------------------------------------------------------------------------**

**B.O.D...... 90-percentile standard = 5.00 mg/l**

**Test statistic = 2.26 mg/l (2.0-2.7)**

**Confidence that the standard was failed = 0.000 per cent**

**--------------------------------------------------------------------------------------------------------------**

**Ammonia.... 90-percentile standard = 1.50 mg/l**

**Test statistic = .0520 mg/l (0.039-0.079)**

**Confidence that the standard was failed = 0.000 per cent**

**--------------------------------------------------------------------------------------------------------------**

**Phosphate.. Mean standard = .100 mg/l**

**Test statistic = .0660 mg/l (0.048-0.084)**

**Confidence that the standard was failed = 0.157 per cent**

**--------------------------------------------------------------------------------------------------------------**

**--------------------------------------------------------------------------------------------------------------**

**Wellington STW Feature No 4 Reach No 1**

**--------------------------------------------------------------------------------------------------------------**

**LOCATION: 8.0 km downstream from the head of the Reach called Upper Ouse**

**--------------------------------------------------------------------------------------------------------------**

**Flow in river just upstream ... Mean = 38.0 m3/d**

**95% exceedence = 5.76 m3/d**

**90% exceedence = 7.90 m3/d**

**99% exceedence = 3.02 m3/d**

**=============================================================================**

**River quality just upstream of effluent discharge ...**

**--------------------------------------------------------------------------------------------------------------**

**Chloride... Mean = 30.9 mg/l (30-32)**

**Standard deviation = 3.85 mg/l**

**90-percentile = 35.8 mg/l (34-38)**

**95-percentile = 37.1 mg/l (35-40)**

**99-percentile = 40.3 mg/l (38-44)**

**--------------------------------------------------------------------------------------------------------------**

**B.O.D...... Mean = 1.50 mg/l (1.33-1.68)**

**Standard deviation = .579 mg/l**

**90-percentile = 2.26 mg/l (2.0-2.7)**

**95-percentile = 2.72 mg/l (2.4-3.3)**

**99-percentile = 3.66 mg/l (3.1-4.7)**

**--------------------------------------------------------------------------------------------------------------**

**Ammonia.... Mean = .0241 mg/l (0.017-0.031)**

**Standard deviation = .0243 mg/l**

**90-percentile = .0520 mg/l (0.039-0.078)**

**95-percentile = .0640 mg/l (0.045-0.106)**

**99-percentile = .149 mg/l (0.109-0.251)**

**--------------------------------------------------------------------------------------------------------------**

**Diss.Oxygen Mean = 9.56 mg/l (9.3-9.8)**

**Standard deviation = .859 mg/l**

**10-percentile = 8.53 mg/l (8.1-8.8)**

**5-percentile = 8.13 mg/l (7.6-8.5)**

**1-percentile = 7.63 mg/l (7.0-8.0)**

**--------------------------------------------------------------------------------------------------------------**

**Phosphate.. Mean = .0660 mg/l (0.049-0.083)**

**Standard deviation = .0589 mg/l**

**90-percentile = .137 mg/l (0.106-0.196)**

**95-percentile = .176 mg/l (0.131-0.270)**

**99-percentile = .363 mg/l (0.27-0.58)**

**--------------------------------------------------------------------------------------------------------------**

**=============================================================================**

**Flow discharged from works: Set: 1 Type: 2 Wellington STW**

**=============================================================================**

**Flow discharged as effluent: Annual mean = 4.00 m3/d**

**Standard Deviation = 1.80 m3/d**

**=============================================================================**

**Shift = 0 m3/d**

**=============================================================================**

**-----------------------------------------------------------------------------**

**Chloride... Mean = 91.5 mg/l**

**Standard deviation = 8.20 mg/l**

**-----------------------------------------------------------------------------**

**B.O.D...... Mean = 35.0 mg/l**

**Standard deviation = 30.0 mg/l**

**-----------------------------------------------------------------------------**

**Ammonia.... Mean = 15.0 mg/l**

**Standard deviation = 9.00 mg/l**

**-----------------------------------------------------------------------------**

**Diss.Oxygen Mean = .500 mg/l**

**Standard deviation = .200 mg/l**

**-----------------------------------------------------------------------------**

**Phosphate.. Mean = 4.50 mg/l**

**Standard deviation = 2.20 mg/l**

**-----------------------------------------------------------------------------**

**Flow in river just downstream ... Mean = 42.0 m3/d**

**95% exceedence = 8.13 m3/d**

**-----------------------------------------------------------------------------**

**-----------------------------------------------------------------------------**

**River quality ...**

**-----------------------------------------------------------------------------**

**Chloride... Mean = 39.3 mg/l (37-41)**

**Standard deviation = 6.96 mg/l**

**90-percentile = 48.7 mg/l (46-53)**

**95-percentile = 52.1 mg/l (49-58)**

**99-percentile = 65.5 mg/l (61-73)**

**--------------------------------------------------------------------------------------------------------------**

**B.O.D...... Mean = 6.32 mg/l (4.9-7.8)**

**Standard deviation = 5.73 mg/l**

**90-percentile = 12.7 mg/l (10.1-17.4)**

**95-percentile = 17.4 mg/l (13.5-24.7)**

**99-percentile = 30.5 mg/l (23-47)**

**--------------------------------------------------------------------------------------------------------------**

**Ammonia.... Mean = 2.12 mg/l (1.7-2.6)**

**Standard deviation = 1.81 mg/l**

**90-percentile = 4.37 mg/l (3.5-5.8)**

**95-percentile = 6.19 mg/l (5.0-8.4)**

**99-percentile = 9.89 mg/l (7.5-14.8)**

**--------------------------------------------------------------------------------------------------------------**

**Diss.Oxygen Mean = 8.27 mg/l (8.0-8.6)**

**Standard deviation = .985 mg/l**

**10-percentile = 7.13 mg/l (6.7-7.5)**

**5-percentile = 6.60 mg/l (6.0-7.0)**

**1-percentile = 5.14 mg/l (4.4-5.6)**

**--------------------------------------------------------------------------------------------------------------**

**Phosphate.. Mean = .693 mg/l (0.56-0.82)**

**Standard deviation = .524 mg/l**

**90-percentile = 1.22 mg/l (0.98-1.63)**

**95-percentile = 1.63 mg/l (1.29-2.24)**

**99-percentile = 2.99 mg/l (2.3-4.3)**

**--------------------------------------------------------------------------------------------------------------**

**==============================================================================================================**

**Classification d/s of: Wellington STW Feature: 4 Reach: 1**

**--------------------------------------------------------------------------------------------------------------**

**Location: 8.0 km downstream from the head of the Reach called Upper Ouse**

**==============================================================================================================**

**....... Confidence of class (%) .......**

**==============================================================================================================**

**High Good Moderate Poor Bad Class boundaries ...................... Statistic**

**==============================================================================================================**

**==============================================================================================================**

**--------------------------------------------------------------------------------------------------------------**

**Assessment of compliance d/s of Wellington STW**

**--------------------------------------------------------------------------------------------------------------**

**Chloride... Mean standard = 250.0 mg/l**

**Test statistic = 39.3 mg/l (37-41)**

**Confidence that the standard was failed = 0.000 per cent**

**--------------------------------------------------------------------------------------------------------------**

**B.O.D...... 90-percentile standard = 5.00 mg/l**

**Test statistic = 12.7 mg/l (10.0-17.4)**

**Confidence that the standard was failed = 100.000 per cent**

**--------------------------------------------------------------------------------------------------------------**

**Ammonia.... 90-percentile standard = 1.50 mg/l**

**Test statistic = 4.37 mg/l (3.5-5.9)**

**Confidence that the standard was failed = 100.000 per cent**

**--------------------------------------------------------------------------------------------------------------**

**Phosphate.. Mean standard = .100 mg/l**

**Test statistic = .693 mg/l (0.56-0.83)**

**Confidence that the standard was failed = 100.000 per cent**

**--------------------------------------------------------------------------------------------------------------**

**==============================================================================================================**

**Stretch: Upper Ouse from: Wellington STW to Middle Ouse Monitoring Station**

**==============================================================================================================**

**==============================================================================================================**

**Classification at: Middle Ouse Monitoring Station Feature: 5 Reach: 1**

**--------------------------------------------------------------------------------------------------------------**

**Location: 14.0 km downstream from the head of the Reach called Upper Ouse**

**==============================================================================================================**

**....... Confidence of class (%) .......**

**==============================================================================================================**

**High Good Moderate Poor Bad Class boundaries ...................... Statistic**

**==============================================================================================================**

**==============================================================================================================**

**--------------------------------------------------------------------------------------------------------------**

**Middle Ouse Monitoring Station Feature No 5 Reach No 1**

**--------------------------------------------------------------------------------------------------------------**

**LOCATION: 14.0 km downstream from the head of the Reach called Upper Ouse**

**--------------------------------------------------------------------------------------------------------------**

**Flow in river just upstream ... Mean = 48.0 m3/d**

**95% exceedence = 8.61 m3/d**

**90% exceedence = 11.6 m3/d**

**99% exceedence = 5.71 m3/d**

**=============================================================================**

**Calculated river quality at this monitoring point ...**

**--------------------------------------------------------------------------------------------------------------**

**Chloride... Mean = 36.6 mg/l (35-39)**

**Standard deviation = 7.12 mg/l**

**90-percentile = 45.8 mg/l (43-50)**

**95-percentile = 49.6 mg/l (46-55)**

**99-percentile = 63.2 mg/l (58-72)**

**--------------------------------------------------------------------------------------------------------------**

**B.O.D...... Mean = 4.57 mg/l (3.8-5.4)**

**Standard deviation = 3.20 mg/l**

**90-percentile = 8.56 mg/l (7.1-11.0)**

**95-percentile = 11.3 mg/l (9.2-14.9)**

**99-percentile = 18.5 mg/l (14.6-26.0)**

**--------------------------------------------------------------------------------------------------------------**

**Ammonia.... Mean = 1.13 mg/l (0.92-1.34)**

**Standard deviation = .814 mg/l**

**90-percentile = 2.10 mg/l (1.7-2.7)**

**95-percentile = 2.76 mg/l (2.2-3.7)**

**99-percentile = 4.57 mg/l (3.6-6.5)**

**--------------------------------------------------------------------------------------------------------------**

**Diss.Oxygen Mean = 8.46 mg/l (8.1-8.8)**

**Standard deviation = 1.11 mg/l**

**10-percentile = 7.00 mg/l (6.5-7.4)**

**5-percentile = 6.23 mg/l (5.6-6.7)**

**1-percentile = 4.63 mg/l (3.8-5.2)**

**--------------------------------------------------------------------------------------------------------------**

**Phosphate.. Mean = .633 mg/l (0.51-0.76)**

**Standard deviation = .490 mg/l**

**90-percentile = 1.13 mg/l (0.90-1.51)**

**95-percentile = 1.50 mg/l (1.18-2.08)**

**99-percentile = 2.83 mg/l (2.2-4.1)**

**--------------------------------------------------------------------------------------------------------------**

**==============================================================================================================**

**Observed river quality at this monitoring point ...**

**==============================================================================================================**

**Chloride... Mean = 50.0 mg/l (48-52)**

**Log-normal 90-percentile = 57.5 mg/l (55-61)**

**Log-normal 95-percentile = 59.9 mg/l (57-64)**

**Log-normal 99-percentile = 64.7 mg/l (61-71)**

**=============================================================================**

**B.O.D...... Mean = 3.90 mg/l (3.2-4.6)**

**Log-normal 90-percentile = 6.56 mg/l (5.4-8.6)**

**Log-normal 95-percentile = 7.87 mg/l (6.4-10.8)**

**Log-normal 99-percentile = 11.1 mg/l (8.6-16.7)**

**=============================================================================**

**Ammonia.... Mean = .300 mg/l (0.20-0.40)**

**Log-normal 90-percentile = .617 mg/l (0.45-0.97)**

**Log-normal 95-percentile = .834 mg/l (0.59-1.41)**

**Log-normal 99-percentile = 1.47 mg/l (0.96-2.89)**

**=============================================================================**

**Diss.Oxygen Mean = 7.20 mg/l (7.9-6.5)**

**Normal 10-percentile = 4.51 mg/l (3.4-5.3)**

**Normal 5-percentile = 3.75 mg/l (2.4-4.6)**

**Normal 1-percentile = 2.31 mg/l (0.61-3.40)**

**=============================================================================**

**Phosphate.. Mean = .110 mg/l (0.000-0.368)**

**Log-normal 90-percentile = .194 mg/l (0.09-0.57)**

**Log-normal 95-percentile = .400 mg/l (0.17-1.41)**

**Log-normal 99-percentile = 1.56 mg/l (0.6-7.9)**

**=============================================================================**

**==============================================================================================================**

**Stretch: Upper Ouse from: Middle Ouse Monitoring Station to the end of the Reach**

**==============================================================================================================**

**==============================================================================================================**

**End of reach number 1 (Upper Ouse )**

**==============================================================================================================**

**River quality at the end of the Reach ...**

**--------------------------------------------------------------------------------------------------------------**

**Chloride... Mean = 35.9 mg/l (34-38)**

**Standard deviation = 7.15 mg/l**

**90-percentile = 45.1 mg/l (42-50)**

**95-percentile = 48.9 mg/l (45-55)**

**99-percentile = 62.5 mg/l (57-71)**

**--------------------------------------------------------------------------------------------------------------**

**B.O.D...... Mean = 4.17 mg/l (3.5-4.9)**

**Standard deviation = 2.80 mg/l**

**90-percentile = 7.78 mg/l (6.5-9.9)**

**95-percentile = 10.2 mg/l (8.5-13.4)**

**99-percentile = 15.6 mg/l (12.4-21.9)**

**--------------------------------------------------------------------------------------------------------------**

**Ammonia.... Mean = .939 mg/l (0.76-1.11)**

**Standard deviation = .688 mg/l**

**90-percentile = 1.79 mg/l (1.47-2.32)**

**95-percentile = 2.26 mg/l (1.8-3.1)**

**99-percentile = 3.82 mg/l (3.0-5.5)**

**--------------------------------------------------------------------------------------------------------------**

**Diss.Oxygen Mean = 8.55 mg/l (8.2-8.9)**

**Standard deviation = 1.13 mg/l**

**10-percentile = 7.02 mg/l (6.5-7.4)**

**5-percentile = 6.22 mg/l (5.6-6.6)**

**1-percentile = 4.60 mg/l (3.8-5.1)**

**--------------------------------------------------------------------------------------------------------------**

**Phosphate.. Mean = .615 mg/l (0.49-0.74)**

**Standard deviation = .480 mg/l**

**90-percentile = 1.10 mg/l (0.88-1.47)**

**95-percentile = 1.46 mg/l (1.15-2.03)**

**99-percentile = 2.78 mg/l (2.2-4.0)**

**--------------------------------------------------------------------------------------------------------------**

**==============================================================================================================**

**River flow at the end of the Reach ... Mean = 50.0 m3/d**

**95-percent exceedence = 8.77 m3/d**

**90% exceedence = 11.8 m3/d**

**99% exceedence = 5.75 m3/d**

**==============================================================================================================**

**==============================================================================================================**

**Classification at the end of the Reach called Upper Ouse**

**--------------------------------------------------------------------------------------------------------------**

**Location: 16.0 km from the head of the Reach**

**==============================================================================================================**

**....... Confidence of class (%) .......**

**==============================================================================================================**

**High Good Moderate Poor Bad Class boundaries ...................... Statistic**

**==============================================================================================================**

**==============================================================================================================**

**=====================================================**

**CALCULATIONS COMPLETED FOR THIS REACH ... 1**

**Name of reach: Upper Ouse**

**=====================================================**

**=====================================================**

**BRANCH TO THE NEXT REACH ... 2**

**River Avon**

**=====================================================**

# NOTES IN PREPARATION

## Back-tracking of sub-catchments

### In this process the loads added within each of the individual sub-catchments is tracked all the way down the river to the sea.

### Whenever a Feature 24 (§163 - the Sub-catchment Boundary) is encountered, SIMCAT will have summed all the inputs from all the sources from all lengths of rivers upstream of the Sub-catchment Boundary that have not been collected already under Sub-catchment Boundary further upstream.

### By placing features of 24 at the end of particular Reaches, the entire catchment can be broken up into sub-catchments or “water bodies” of the required size.

### The details of the contribution from each Sub-catchment are now written to the files of monthly data (MON and CSV) in terms of the net load from each Sub-catchment, the length of river within each Sub-catchment, and the load per kilometre added by each Sub-catchment.

### The “net load” is the load added in the Sub-catchment, altered by any specified losses from subsequent abstractions, diversions or decay, and by any effects calculated for Gap Filling.

### At each point in the catchment SIMCAT produces a breakdown of the:

### loads from all types of discharge and all types of diffuse pollution

### contributions from each individual upstream point discharge

### contribution from each upstream sub-catchment

### contributions from each Sub-catchment of all types of pollution.

1. Source Apportionment Geographical Information System [↑](#footnote-ref-1)
2. Water quality standards must be defined as summary statistics like means and percentiles in order to assess compliance and calculate properly the action needed to achieve them. This is a minimum technical requirement on how standards are defined. It relies on the fact that the statistical distributions of pollutants usually have similar shapes in nearly all rivers. This means that such a distribution can be represented by a single number such as a 90-percentile. [↑](#footnote-ref-2)
3. Gap-filling is the automatic adjustment of SIMCAT's calculations of river flow and river quality so that perfect agreement is reached with the summary statistics recorded at river flow gauges and monitoring stations. This shows gaps in sources and sinks of pollution that are being modelled. [↑](#footnote-ref-3)
4. SAGIS: Source Apportionment Geographical Information System [↑](#footnote-ref-4)
5. This point is fundamental to the most effective and successful rounds of water quality planning. [↑](#footnote-ref-5)
6. It is the right thing to do in terms of the “science of taking decision” – ensuring that we demonstrate that our decisions are correct and essential [↑](#footnote-ref-6)
7. It is a welcome opportunity that stems from the data on concentrations of pollutants and their link to damage to the environment and water resources. The annual mean (and similar annual statistics) are well-suited as a simple and most helpful form of water quality target. A particular value of the annual mean can embrace and define an acceptable risk of killing fish [↑](#footnote-ref-7)
8. *Water Pollution Research Laboratory (1957): G.A.Truesdale and A.L.H Gameson. The Solubility of Oxygen in Saline Water. Etrait du Journal do Conseil International pour l'Exploration de la Mer. Vol.xxii, No.2, 1957.* [↑](#footnote-ref-8)