



Water Use

Supporting Guidance (WAT-SG-03)

Data Analysis and River Quality Planning Model

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Update Summary

Version	Description
v1.0	First issue for Water Use reference using approved content from the following documents: <i>SG02 - Modelling Continuous discharges to rivers.doc</i>
v2.0	<i>Consent</i> renamed <i>Licence</i> , New base template applied, links to docs revised for new SEPA website, Nov 2008
v3.0	Expired CMS links reviewed and updated.
v4.0	New document created from content in WAT-SG-02 v3 and with new title to reflect data analysis purpose. WAT-SG-02 v4 now focusses on latest modelling techniques.

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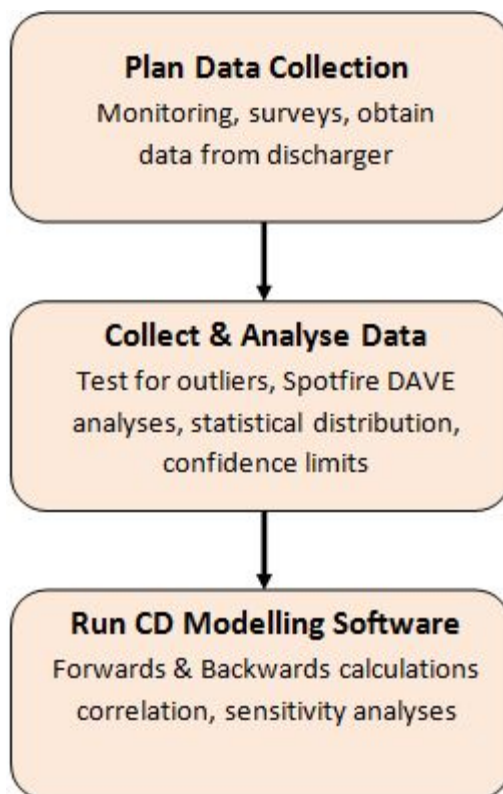
1. Process Flow Summary

In any modelling exercise it is important to maintain an audit trail detailing sources of all data used, assumptions and key decisions.

If in doubt about any aspect of data handling and/or modelling, particularly when the quality of data is poor or decisions could significantly affect capital expenditure for a proposed discharge, contact ESIU (Environmental and Spatial Informatics Unit) for advice and assistance.

The process can be summarised as follows:

Figure 1 Process Summary



2. Data Collection and Analysis

Plan ahead to ensure sufficient data of adequate quality is available, particularly if significant capital expenditure rests on decisions arising from modelling outputs. Ideally, the minimum data set is 36 data points over 3-4 years to enable statistically robust analyses. If this cannot be achieved due to time or resource constraints and data is required for input to CD modelling software there are alternative options for deriving input data, see CD Model Data Requirements.

However, this may introduce considerable error and the model outputs should always be tested for sensitivity, as described in Sensitivity Analysis.

It is good practice to undertake a statistical assessment of raw data to produce more robust summary statistics prior to any CD modelling exercise. Data should be tested for outliers and *Spotfire DAVE Chemistry* used to check data distribution, correlation and identify temporal trends.

Refer to section 9 for a practical example.

An audit trail detailing sources of data, assumptions and key decisions taken must be maintained throughout the determination process. This will also help plan monitoring and data collection for any future review of licence. In order to keep a clear record it is helpful to save each time series graph as the data set is manipulated e.g. the time period is restricted and outliers removed. These can be copied and pasted into a Word or Powerpoint file. Spreadsheet output files from CD modelling should also be saved.

2.1 Screening Data For Outliers

Data should be screened for unusual values. High data values can have a very significant influence on summary statistics being produced, especially the arithmetic average or mean. Outliers result from a variety of reasons including data entry errors. If this is suspected the data should be traced back through the National Environmental Monitoring System (NEMS) in liaison with relevant chemistry personnel.

Spotfire DAVE Chemistry includes an automated test for outliers which can be automatically removed. The time-series plot can be used to identify values above (or below) a specified threshold and automatically screened from the dataset using 'Min' or 'Max'. This creates a new determinand for analysis with the suspected outliers removed.

Exclusion of any value from a data set needs to be justified, therefore, decisions and reasons for excluding any data should be documented in the audit trail. When exclusion of an outlier is debatable, summary statistics should be obtained including and excluding the outlier(s) and the CD model run and tested for sensitivity using both sets of statistics.

2.2 Rules for Identifying Outliers

Discharge Quality

1. Remove all unrepresentative results. For example, samples obtained:
 - a) during adverse operating conditions including 'unusual situations' as defined by licence conditions
 - b) as a result of an accident/vandalism/unforeseeable acts by a 3rd party
 - c) during periods of impeded plant performance/prolonged equipment failures.
2. Circumspect analytical results may be queried by a discharger. Check inspection reports and letters from the discharger, minutes of meetings etc., and remove data results if suspicions are justified.
3. Compare sample determinand results, for example, a STW with an NH₄-N of 2mg/l is unlikely to have a BOD of 50 mg/l.
4. Identify any suspected outliers from local knowledge of the effluent and the type of treatment process, e.g. a sewage treatment works should not produce a BOD of 400mg/l (unless it's a bulking activated sludge plant or the plant is hit by a trade effluent discharge). Calculate the summary statistics with and without the suspected outliers to check whether significantly different summary statistics are produced.

River Quality

1. Check for atypical parameter results.
2. Check results on the same day for samples on the same river (pollution incident).
3. Check for unusual events (1 in 100 years storm).
4. Check for poor quality discharges upstream.
5. Check pollution incident reports on complaints/incident register.

2.3 Use of Spotfire DAVE Chemistry

This section provides an introduction to the basic considerations that need to be made when undertaking preliminary data analyses. It does not cover operation of the software or data input to the software package. Advice on these issues is in the guidance on *Spotfire DAVE Chemistry*.

2.3.1 Testing For Temporal Trends

Summary statistics for CD mass balance modelling should represent the current and near future conditions in the watercourse and discharge, i.e. the period for which the authorisation will be granted. It is important, therefore, to

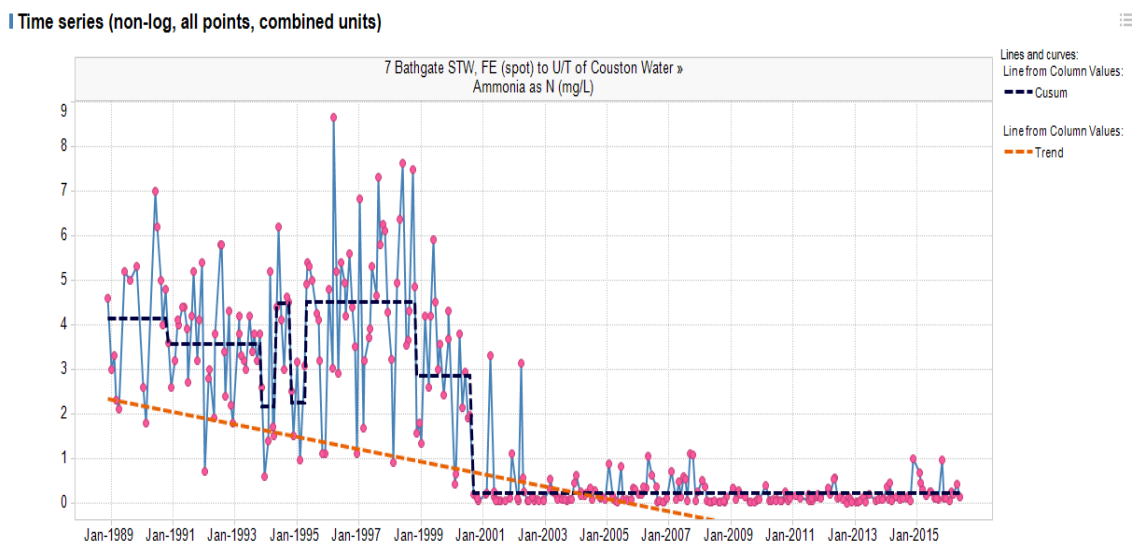
examine data sets for temporal trends so that only the most recent, representative data is used to produce the required summary statistics.

Within *Spotfire DAVE Chemistry*, the CUSUM (cumulative summation) analysis routine under the Sample statistics tab is used to undertake temporal trend analysis.

CUSUM is a valuable diagnostic technique for separating periods over which a determinand has different underlying mean levels. First, the deviations of the data values from some suitable target value are calculated. The CUSUM then consists of a plot of the cumulative sum of those deviations against an observation number. Changes in mean level (often difficult to spot in a time series plot because of the scatter between successive observations) are transformed by the CUSUM into changes in slope which are much easier to detect.

CUSUM analysis is designed to look for step changes in a data series, not gradual changes. This means that even if any temporal change is a slow gradual effect, it can only be represented by a series of steps.

Figure 2 CUSUM analysis



If the data is suspected of following a gradual change over time, the predicted change over the period of interest, e.g. the design life of the discharge, should ideally be taken account of when undertaking any modelling. Log-Normally distributed data can be transformed to normally distributed data using the 'Log data' option under the data analysis tab.

If CUSUM analysis indicates that there have been statistically significant changes in mean levels of the determinand over the period of interest, then only the most recent data (data for the last time-step period) should be used to produce summary statistics for CD mass balance modelling. This is done by using the Date Range option on the menu. This will create a new determinand covering only the period of interest.

Advice on temporal trend analysis of data sets can be obtained from the Environmental and Spatial Informatics Unit.

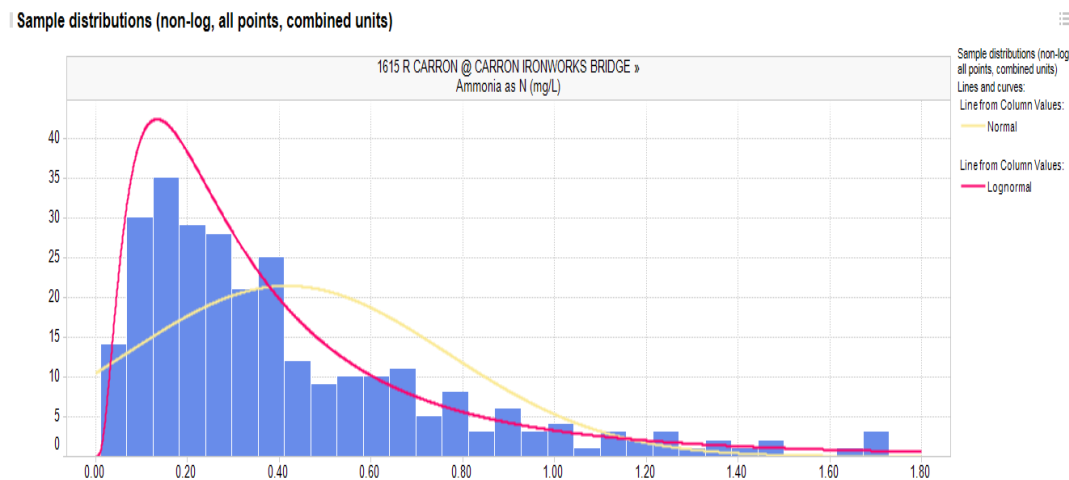
2.3.2 Data Distribution

The CD mass balance modelling software assumes, by default, that the distributions of the variables (i.e. upstream river flow and quality and discharge flow and quality) are log-normal. If this is not the case and the model is particularly sensitive to the assumption and/or the situation being looked at is an important one, then other distributions can be used by defining them non-parametrically.

The normal distribution is widely used in statistics. It is bell-shaped, unbounded in both directions and can be defined by two parameters, the mean and standard deviation of the population.

The log-normal distribution is so-called because the logarithms of the population values have a normal distribution. The log-normal distribution is not symmetrical but positively skewed, that is, the right-hand tail extends further and contains more values than the left. Also, the left-hand tail is bounded by zero meaning that the log-normal translation is appropriate for populations which cannot have zero or negative values.

Figure 3 Distribution Plot



Spotfire DAVE Chemistry can be used to examine the data distribution. The most basic approach is to plot a histogram of the data and assess its shape visually. However, *Spotfire DAVE Chemistry* also has the option to test the 'goodness of fit' of normal and log-normal distributions to the underlying data. The result is a histogram with 'fitted' curves superimposed, together with a summary box stating whether the fit is 'poor' or 'not poor'.

The fit will only be pronounced as being poor if the statistical test shows that it is unlikely (with a default significance level of at least 5%) that the data are derived from such a distribution. It is, therefore, possible that both normal and log-normal distributions could provide 'not poor' fits to the data. If this is the case the % significance level will give an indication of which is better, but for

the purposes of CD mass balance modelling the log-normal assumption is adequate. The smaller the % significance level, the greater is the likelihood that the data is not derived from that particular underlying distribution.

Sometimes the data does not fit a defined distribution – *Spotfire DAVE Chemistry* will say ‘poor’ to both log-normal and normal model fits. There are two options for handling this:

1. In most cases, it will be acceptable to assume that the data’s distribution is log-normal, as long as the shape of the histogram is essentially log-normal-shaped: that is, the data is right-skewed such that there are a few high values to the right-hand side, the majority of the data is to the left-hand side, and there are no data values of zero or less than zero. Determinands such as BOD and ammonia are usually found to be log-normally distributed when measured in surface waters.
2. In cases where the model is sensitive to the parameter in question and/or has particularly significant consequences in terms of capital outlay or environmental risk, a non-parametric distribution should be used. This entails feeding the full raw dataset (instead of mean and standard deviation summary statistics) into the Monte Carlo Mass Balance software, using the ‘Non-parametric data’ button at the bottom of the Base Data screen. If in doubt, assess the difference between both approaches, i.e. assuming log-normality and using a non-parametric data file.

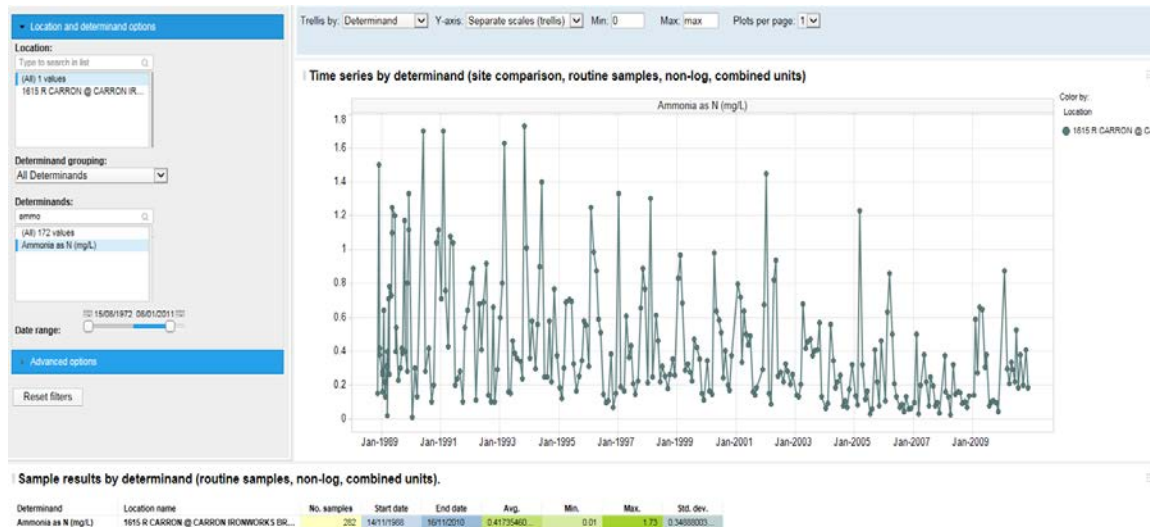
2.3.3 Producing Summary Statistics

Summary statistics are produced by *Spotfire DAVE Chemistry*, (*Figure 4*). The statistics required for Combined Distribution Modelling are the mean, standard deviation, 90%ile and possibly 95%ile. If the percentile values are required, *Spotfire DAVE Chemistry* allows the user to define how these are to be calculated:

- by assuming some underlying distribution – **parametric**
- by not assuming an underlying data distribution - **non-parametric**

Spotfire DAVE Chemistry uses non-parametric methods.

Figure 4 Summary Statistics



2.3.4 Confidence Intervals For Summary Statistics

Spotfire DAVE Chemistry can be used to calculate confidence intervals for summary statistics to illustrate the underlying uncertainty in defining any parameter by spot sampling. It is recommended that upper and lower confidence limits are used in a manual sensitivity exercise. This will demonstrate the range of outcomes i.e. worst case using the upper confidence limit and, if giving the benefit of doubt to the discharger, the optimistic outcome using the lower tier confidence limit.

Within *Spotfire DAVE Chemistry*, confidence intervals under the Sample Distributions tab.

Figure 5 shows that the 95% confidence interval about the 90%ile ranges from 0.807 to 1.070. The 'best estimate' is 0.922. It is useful to see the effect of using 0.807 and 1.070 rather than 0.922 in the CD mass balance modelling exercise.

In general, the fewer data points in the dataset, the lower the certainty will be about the final summary statistics. There is no universal 'rule of thumb' for a minimum number of samples needed to create summary statistics for Monte Carlo Effluent Quality Modelling. A minimum of one year's data is suggested – preferably 12 samples but 6 samples could suffice if these are spaced evenly across the year. However, the main issue in terms of the effluent modelling is the sensitivity of the model to summary statistics.

When running the model's sensitivity analysis, if the results flag up that the model is more than 10% sensitive to a change in any input data, the summary statistic should be revisited to ensure that the best possible estimate of the value has been made. For example, if the model is sensitive to the mean upstream concentration, and this mean estimate is from 7 data points which occurred after a CUSUM step change, it may be advisable to go

further back in time to the penultimate step change and take the mean value from this date up until the present date.

Figure 5 Statistical Confidence Summary

Lognormal distribution quantile table

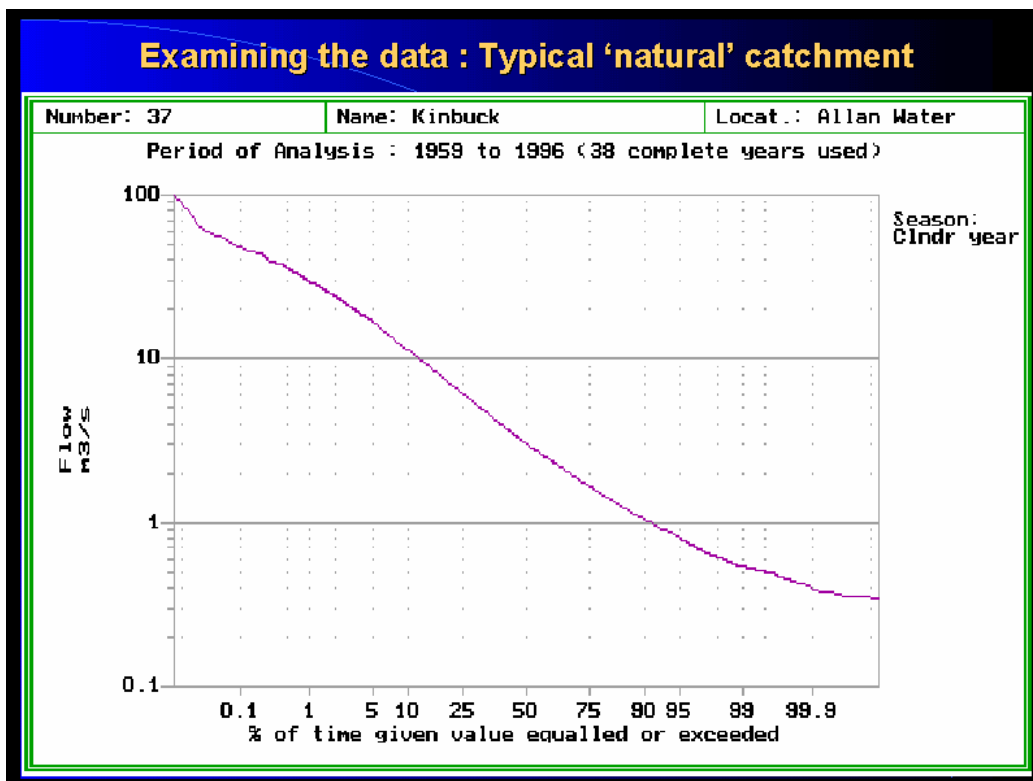
Location	Determina...	Percent	Lower conf. limit	Quantile	Upper conf. limit
1615 R CARRON @ CARRON IRONWORKS BRIDGE	Ammonia as N (mg/L)	5.00	0.058	0.068	0.079
		10.00	0.081	0.094	0.108
		90.00	0.807	0.922	1.070
		95.00	1.096	1.273	1.510

3. CD Model Data Requirements

3.1 Upstream River Flow

The standard flow duration curve for a given river can provide an indication of whether the flow regime is **parametric** or **non-parametric**. A graph of river flow regime is plotted with log flow on the y-axis and % time flow equalled or exceeded on the x-axis with a normal probability scale. If the flow is log-normally distributed then the resulting curve is a straight line. Flow duration curves from a **natural** catchment and a **regulated** catchment are shown respectively in *Figure 6* and *Figure 7*.

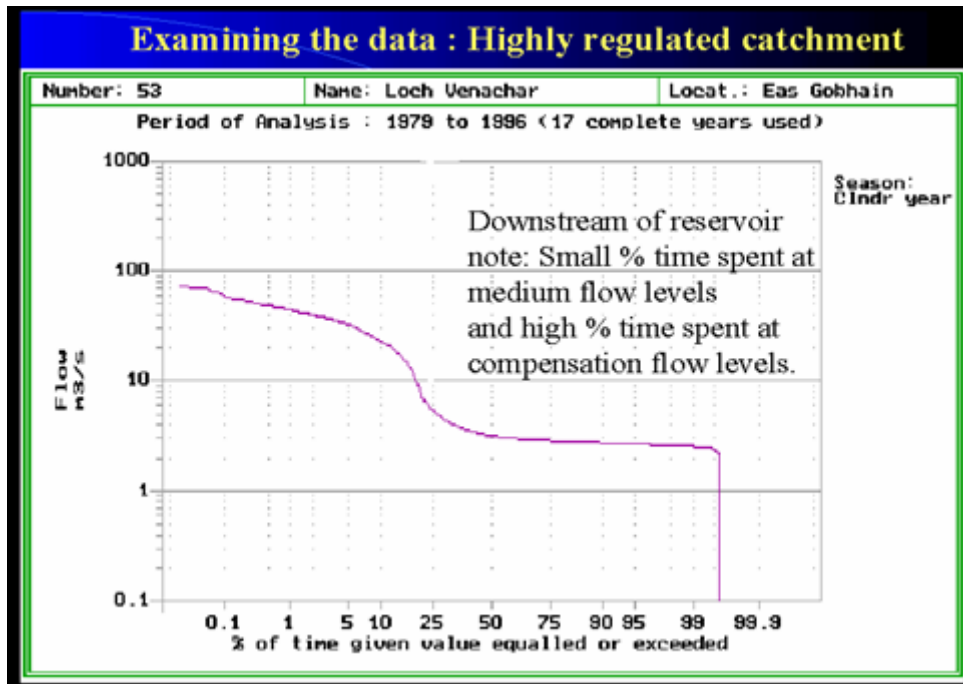
Figure 6 Natural Catchment



Rivers not subject to flow regulation or abstraction activity can be assumed to have natural flow regimes and the upstream river flow distribution is defined by the mean flow and the 95% exceedance flow¹.

¹ The 95% exceedance flow is a low flow. It is the flow which is exceeded for 95% of the year, or other specified time period and is effectively the 5%ile. Hydrologists call it the Q95 flow.

Figure 7 Regulated Catchment



In most cases, there will not be any continuous flow record available and the hydrology department should be able to advise on the most reliable method for estimating the required flow statistics. This may include short term deployment of flow monitoring equipment, spot gauging/s and theoretical calculations, depending on the sensitivity of the discharge.

Ideally, where there is continuous flow measurement data available from a gauging station, these two summary statistics should be derived from the flow record of instantaneous values i.e. data at 15 minute intervals. If this is not readily available a record of Daily Mean Flows (DMFs) may be used. This might be the case where DMFs need to be estimated from records from a neighbouring gauging station.

The CD model should represent the current and foreseeable circumstances for the authorised life span of the discharge being considered. Therefore, summary statistics (mean and Q95) derived from a gauging station record spanning the last 30 years may not always be the most appropriate figures to use. This is especially true where historical changes in the catchment may have affected the water balance. For example, closure of a mine which contributed a significant proportion of river flow from pumped minewaters or increased development resulting in higher consumptive abstractions. In such instances, it is appropriate to consider more recent records representative of current river flows.

3.2 Upstream River Quality

If there is no upstream water quality data then data from a comparable watercourse should be considered. If this is not available the value of obtaining data will have to be considered. For example, in the case of a low

significance discharge and insensitivity of the CD model to upstream quality there is little merit in targeting sampling resources to improve the accuracy and precision of summary statistics. It may suffice to assume that the quality lies 60% of the way through the classification range and that the standard deviation is 1/3rd of the mean.

NB Face-value class means the class of the watercourse based on just that one determinand, but not the overall class which may be lower due to other determinands. Refer to section 9.2.1 for more information on data collection.

Sometimes data from historic/disused monitoring points may need to be used. These sites can be identified using GIS by adding the Monitoring Theme. Spottfire DAVE can also be a useful tool for quick screening of data. See section 9 for a worked example.

If there is little or no upstream data but a good data set for a downstream site, together with historical data for the discharge, then it is possible to use the CD mass balance modelling software to back-calculate upstream quality. This can then be used to look at the effect of changes to the discharge or the introduction of another discharge.

It may be necessary to take account of natural purification, decay, uptake or transformation of the determinand concerned when the nearest sampling point is some distance upstream. Contact the *Environmental and Spatial Informatics Unit* for advice.

Effects of tributaries and other discharges entering the watercourse between the nearest upstream water quality sampling point and the proposed discharge point may need to be considered by undertaking CD modelling in a piecemeal manner. Alternatively, catchment models such as SIMCAT and QUASAR may be more suited for complex studies, see Catchment Models.

3.3 Discharge Flow

This is often the least well defined variable, either due to a lack of historic data for an existing discharge, or, in the case of a new discharge, estimates can only be derived from design criteria, e.g. population equivalents/number of houses for STWs discharges. Assuming log-normal distribution, the summary statistics required are the mean and standard deviation.

Where flow data is unavailable the following rule of thumb may be applied:

Mean flow = 1.5 x design dry weather flow (DWF)

SD of flow = 1/3 of the mean

DWF = (PG + I + E), where

P = population

G = per capita consumption (typically 150 l/h/d)

I = infiltration*

E = trade effluent.

*Always use accurate information for infiltration whenever this is available.
For larger catchments infiltration should be measured, not estimated.

3.4 Discharge Quality

Data requirements for this variable depend upon whether a forward' or 'backward' calculation is being undertaken.

Forwards

To calculate the downstream impact of a defined discharge the current discharge quality needs to be defined as accurately as possible. The summary statistics required are the mean and either the standard deviation or the 95%ile effluent quality.

Backwards

To calculate the discharge quality required to meet a given water quality standard downstream, a measure of the variability of the effluent quality about its mean value is required. This is calculated as the ratio of the standard deviation to the mean discharge quality. In statistical terms this is referred to as the 'Coefficient of Variation', but it can be thought of as a measure of variability.

It is only the ratio of the mean to standard deviation that is important for modelling the required discharge quality. For example, entering a mean of 2 and a standard deviation of 1 will give the same results (allowing for small differences due to the Monte-Carlo process) as entering a mean of 20 and a standard deviation of 10. The Coefficient of Variation is 0.5 in both cases. Where there is no historic data available or improved treatment is to be provided, resulting in more consistent performance, data providing the coefficient of variation for a similar type of treatment works may be used.

3.5 Downstream River Quality

It is useful to undertake a simple model validation exercise to ensure the predicted downstream concentration is comparable with that measured in the field if there is an existing discharge with historical data, together with upstream and downstream river quality data,. The downstream data required are the mean and 90%ile river quality. It is particularly important to undertake model calibration where downstream river quality data is more reliable than upstream data, e.g. more samples available for downstream site.

If the model produces results comparable with field measurements it is reasonable to assume that the input data is valid. However, if there is a marked discrepancy between model output and field measurements reasons for the discrepancy should be investigated and model input data re-examined.

Table 1 Model and Field Result Discrepancies

Reason For Discrepancy	Examples
Unrepresentative points for field measurements	Distance u/s and d/s from discharge, natural purification and mixing, unidentified discharges
Sampling errors in field measurements analytical errors	Outliers, extreme events , analytical errors
Statistical uncertainties in field measurement	Confidence intervals, standard deviations and percentiles
Incorrect assumptions about input data	Greatest discrepancy lies with discharge flow and upstream quality

3.6 River Quality Target

If the CD Mass Balance model is being used in backwards mode a River Quality Target is required, defined as a percentile. The model will calculate the discharge quality standard required to just meet the percentile target value set downstream. No allowance is made for spare capacity or for other discharges and future development. Therefore, the percentile target value should reflect these issues where they are considered important. The target should not be set such that the discharge uses the full capacity available, as described in *WAT-RM-21: Allocation of Capacity and Protection of the Water Environment*. Section 2 of this current document summarises the approach.

4. Modelling Concepts and Calculations

The mixing of a discharge with a river is described by the **Mass-Balance Equation**:

$$T = \frac{FC + fc}{F + f}$$

where:

T = River concentration **after mixing**

F = Upstream river flow

C = Upstream river concentration

f = Discharge flow

c = Discharge concentration

The above equation, based on the principle of conservation of mass, assumes that mixing is instantaneous and complete. It is useful for assessing river quality at a fixed point in time, e.g. to demonstrate exceedance of a toxic threshold during a pollution incident, but it does not take account of variability in flows or quality. To do so, the distribution of F, f, C and c must be considered.

The Mass Balance equation may be used to obtain a crude estimate of the downstream impact in which case the following summary statistics should be used:

- 95%ile upstream flow
(i.e. this scenario assumes low river flow)
- Mean upstream concentration
- Discharge mean flow (1.5 x design dry weather flow)
- Mean discharge concentration

4.1 Monte-Carlo Simulation

Standard computer-based methodologies have been developed which allow calculation of mean and percentile values for T by combining distributions of flow and concentration using the Mass Balance equation. In Monte-Carlo simulation, a value for each of the variables F, C, f and c is plucked at random from a range of actual data or from possible values described by summary statistics, usually the mean and a percentile or the standard deviation. A value for T is calculated from each set of values of F, C, f and c using the Mass Balance Equation. This 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** **The software gives 1000 shots by default, but this should be increased to 5000 shots**) This can be fixed for all subsequent runs by right clicking and ensuring a yellow circle is present.

To calculate the discharge standard needed to achieve a 90%ile river quality standard, the programme compares the river quality target with the 90%ile 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 the discharge distribution percentile can be used to run Monte Carlo in reverse mode to predict the discharge quality required to achieve a pre-defined downstream water quality target.

4.1.1 Assumptions

It is important to recognise certain assumptions that are implicit in the Mass Balance CD modelling approach. These are related to the underlying form of the distributions of the variables, the correlations that exist between variables, and the assumption of full and instantaneous mixing.

Distribution

It is common to assume that F, C, f and c follow the Log-Normal distribution, because this is often the case, but other distributions can be used, if required. One advantage of assuming that the underlying distribution is Log-Normal, is that the complete population of possible values can be defined by only two numbers. One is the Mean (arithmetic average) and the other is a measure of the variability, typically the Standard Deviation or a percentile value (e.g. 90 or 95 percentile).

Correlation

The Monte-Carlo method allows all combinations of correlation to be introduced, if required. So, for example, river flow can be positively correlated with discharge flow, and/or upstream river quality could be negatively correlated with upstream river flow. However, unless there is good evidence that two variables are correlated, correlation should not be assumed for any combination of variables and all correlation coefficients should be set at zero (section 6.3).

Full Mixing

The Mass Balance equation assumes full mixing. In reality, immediate and complete mixing is rarely achieved as discharges enter watercourses at point sources, requiring processes of dispersion and diffusion to achieve full mixing throughout the water body. This means that the localised impact of a discharge may be more extreme than that predicted by Mass Balance which assumes dilution by the total upstream river flow. Equally, it may be the case that downstream monitoring data masks impacts caused by streaming effects within the mixing zone. This is particularly important if monitoring points are some distance downstream of existing or proposed discharges.

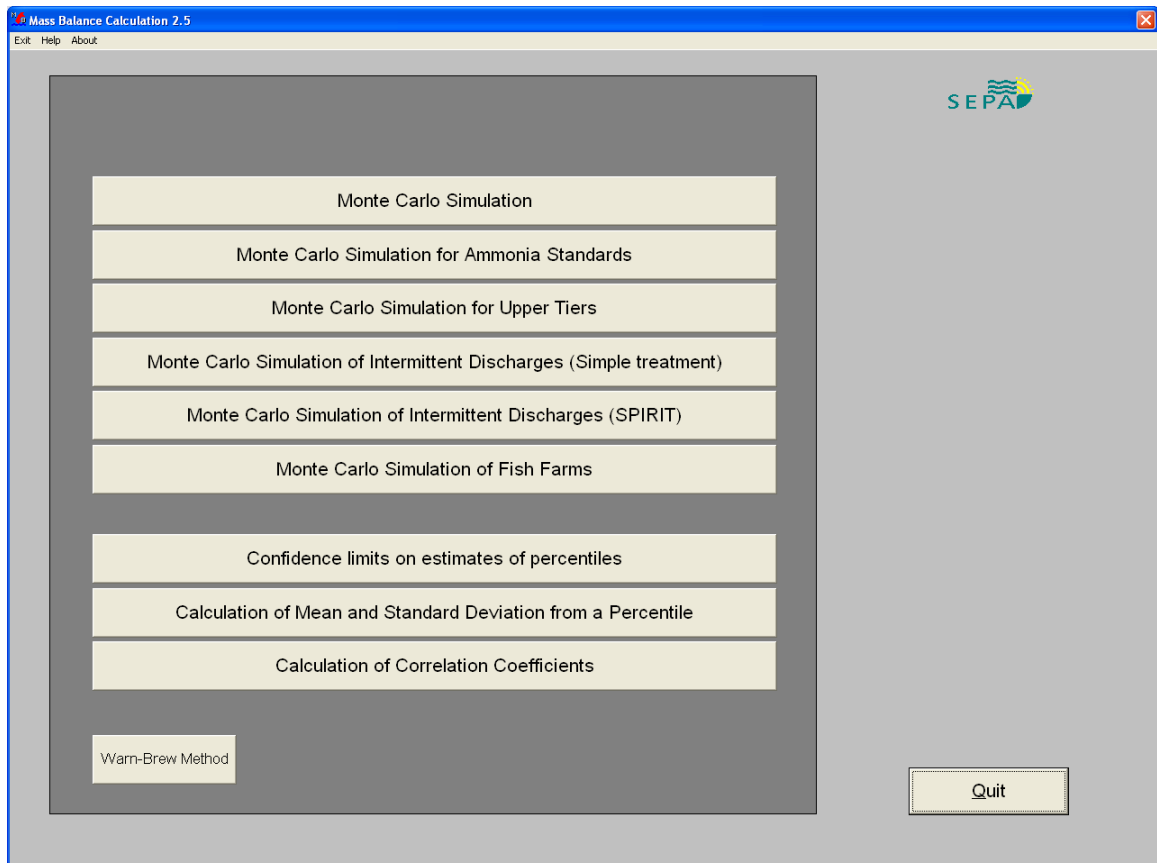
5. Using CD Mass Balance Modelling Software

Select the Mass Balance Calculation option/icon from the submenu or subfolder for *RQP (River Quality Planning)* to display the *Main Menu*, Fig 8.

5.1 Main Menu

Nine items are available grouped into 2 'families', the first of which is Monte Carlo simulations approach to CD modelling. It is the first of these 6 options which will be referred to in this section. The 'Monte Carlo Simulation' option is used most often since Environmental Quality Standards and targets are defined as percentiles or means (e.g., BOD and Total Ammonia standards are 90 percentiles, soluble reactive phosphate is defined as a mean). The second option 'Monte Carlo Simulation for Ammonia Standards' is used for unionised ammonia (section 7).

Figure 8 Main Menu



5.1.1 Monte Carlo Simulation Data Input

Monte Carlo Simulation has 2 modes of operation:

- **Forwards mode**
To calculate the downstream impact of a discharge

■ **Backwards mode**

To determine discharge flow and/or quality needed to meet the downstream River Quality Target.

Toggle between modes by selecting the appropriate button midway down the *Base Data* screen.

Figure 9 Backwards Mode

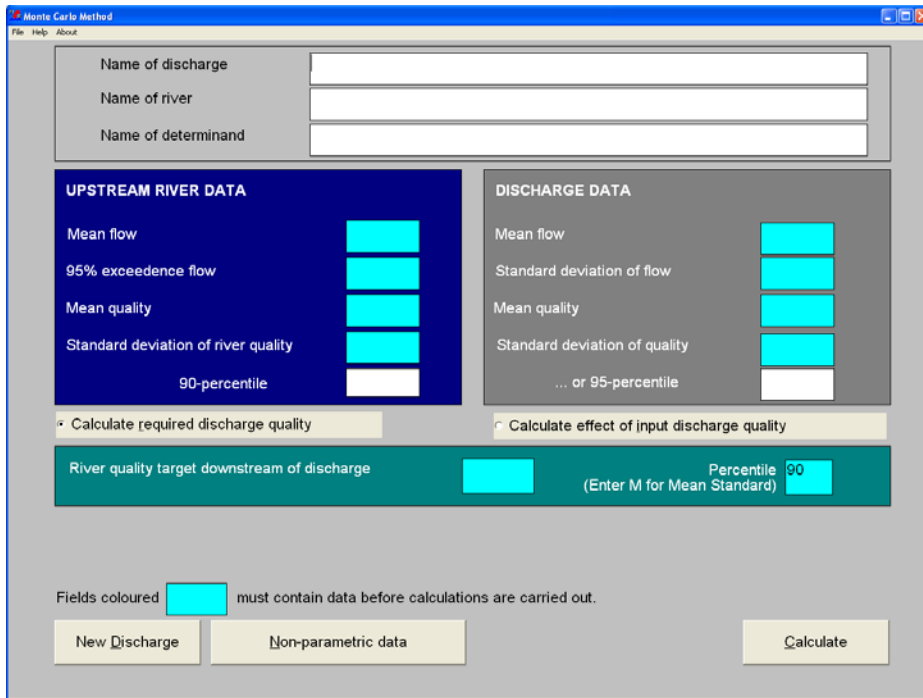
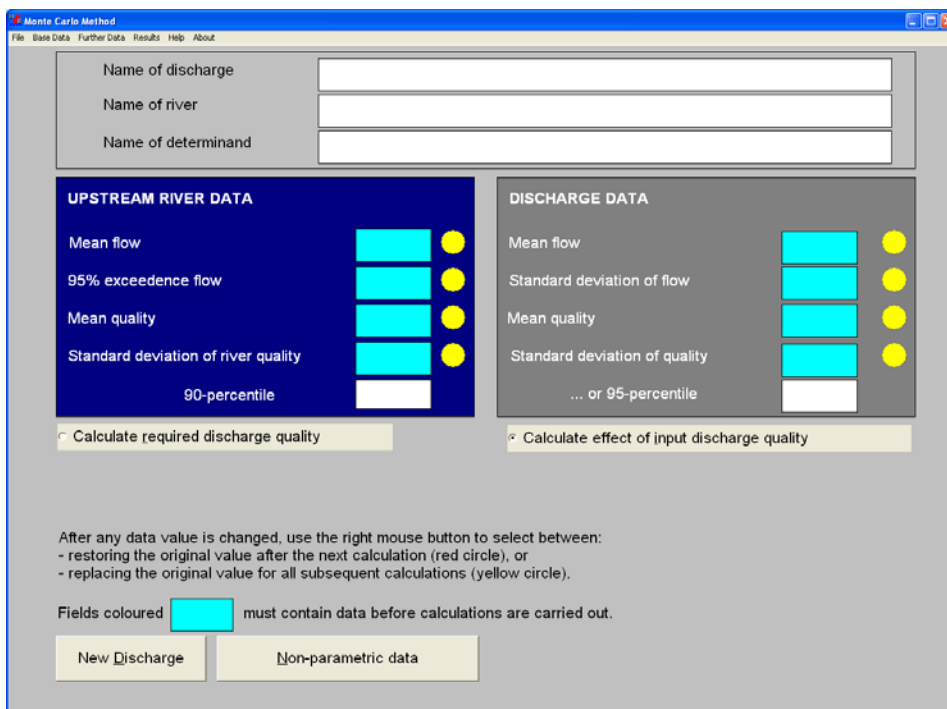


Figure 10 Forwards Mode



Compulsory Fields

Are highlighted in light blue and data must be entered before continuing. If the standard deviation is not known for the river quality and/or discharge quality the respective percentile can be entered and the standard deviation will be calculated automatically. All other data input fields are optional.

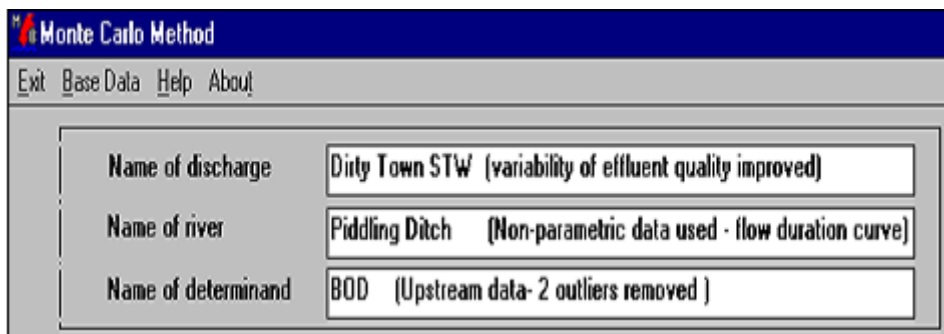
If no percentile is available a rule of thumb is that the standard deviation is 1/3 to 1/4 of the mean.

Data Entries

Can be changed at any time by highlighting the current data and overtyping the new value. A red circle adjacent to the field means that the change will apply for a single model run then revert to the original data value. A yellow circle means that the new value is fixed for all subsequent model runs until it is changed again. Right clicking over the data field toggles between red and yellow.

Time taken to enter meaningful descriptors in *Name of Discharge*, *Name of River* and *Name of Determinand* fields will make future reference to the outputs much easier, *Figure 11*).

Figure 11 Descriptor Fields



The screenshot shows a software window titled "Monte Carlo Method" with a menu bar containing "Exit", "Base Data", "Help", and "About". The main area contains three input fields:

Name of discharge	Dirty Town STW (variability of effluent quality improved)
Name of river	Piddling Ditch (Non-parametric data used - flow duration curve)
Name of determinand	BOD (Upstream data- 2 outliers removed)

A **non-parametric option** is available on the *Base Data* screen. If this method is selected an ASCII text file containing the raw data needs to be set up beforehand. For a small number of values (see example below) this can be produced using NOTEPAD, WORDPAD or EXCEL and saving as a text file. If the non-parametric datafile is to be generated from another datasource (e.g. Hydrology Database) then it may be necessary to create a file which can be read into EXCEL then manipulated and saved from EXCEL as a text file.

The software prompts for selection of the variable/s to be defined non-parametrically and identification of the respective data file(s) using a standard windows 'Open File' dialogue box. The data within the file needs to be structured such that the first number represents the number of data points followed by the data itself. The data should be representative and may be sample results or a summary of the data distribution such as equi-spaced points from a flow duration curve or other cumulative frequency distribution.

Table 2 Example Datafile

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 above data file example contains flow data comprising 14 data points which could be 14 field measurements of flow representing the complete record of measurements made at an infrequently gauged site, or, it could represent 14 equally spaced points (not in any order) extracted from the stations long term flow duration curve.

A data file containing river quality data might contain several years of spot sampling data for the determinand of interest. The data should be representative of current conditions.

5.2 Model Outputs

Once the data has been entered click *Calculate*.

This produces the *Results Screen* which looks similar for both backward (*Figure 12*) and forward (*Figure 13*) modes.

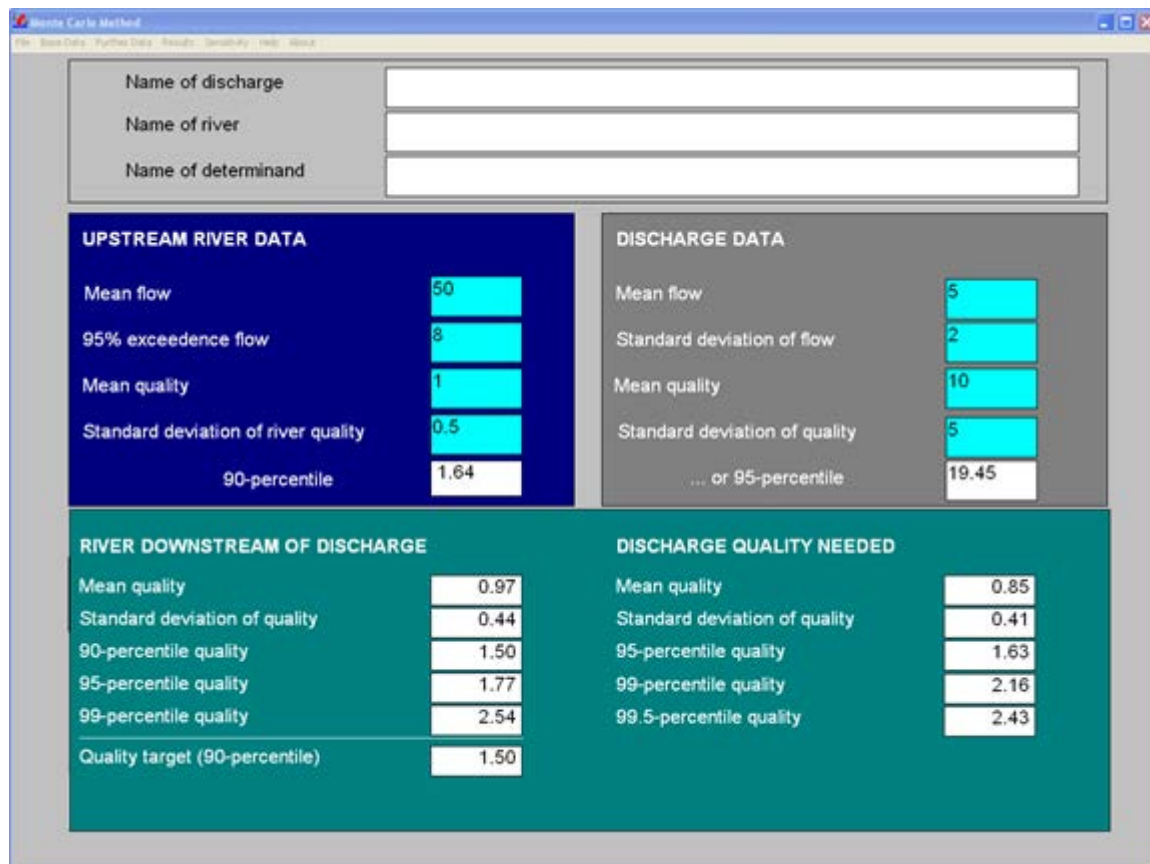
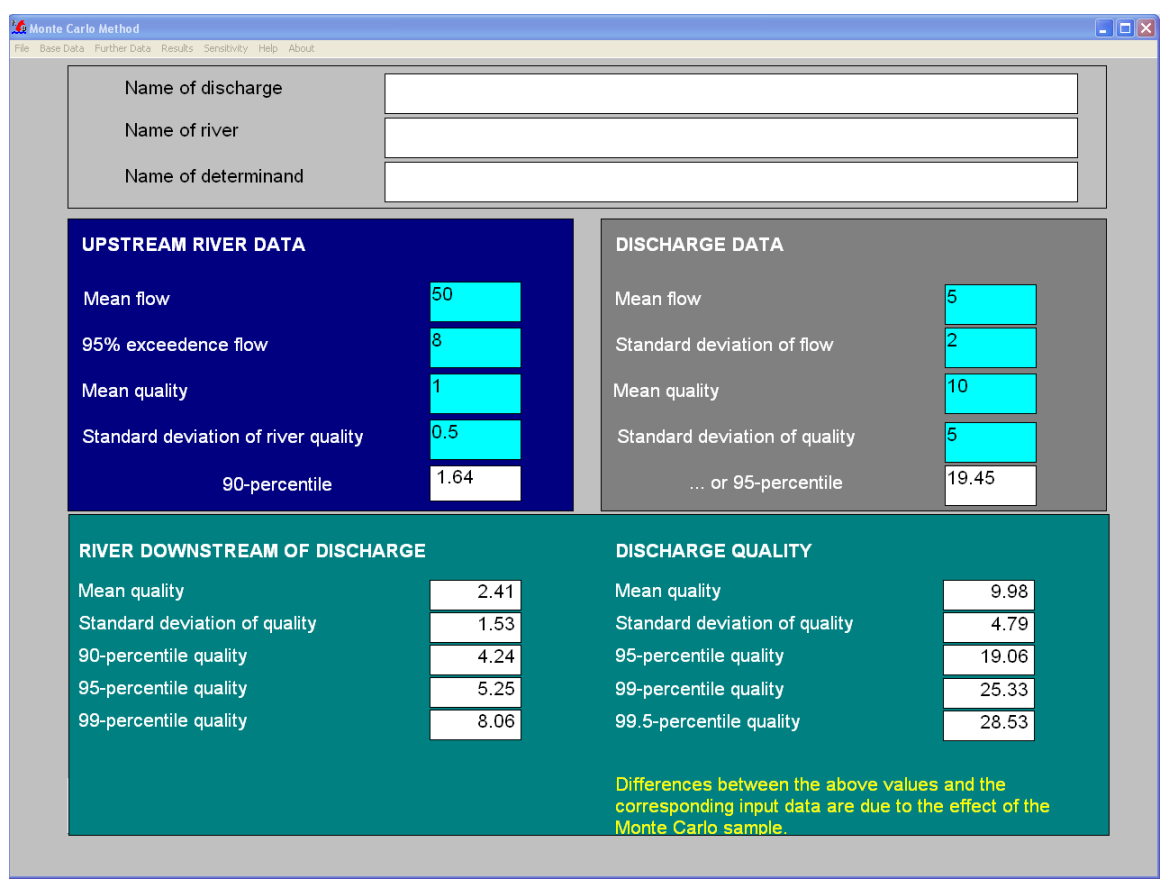
Figure 12 Backwards Output

Figure 13 Forwards Output



The results displayed should not be accepted at face value. The next step is to set the Correlation Coefficients then perform Sensitivity Analysis.

5.3 Correlation Coefficients²

Toggle to the *Further Data* screen from the menu bar, *Figure 14*. The default correlation coefficient between river flow and discharge flow is set at 0.6. This assumes that increased discharge flow is associated with increased river flow. **Unless analysis of survey data demonstrates correlation it should always be set to 0.** Similarly, all other correlation coefficients should be left at the default setting of 0 unless a data analysis suggests correlation. The Number of Shots should also be changed from 1000 to 5000 in this Further

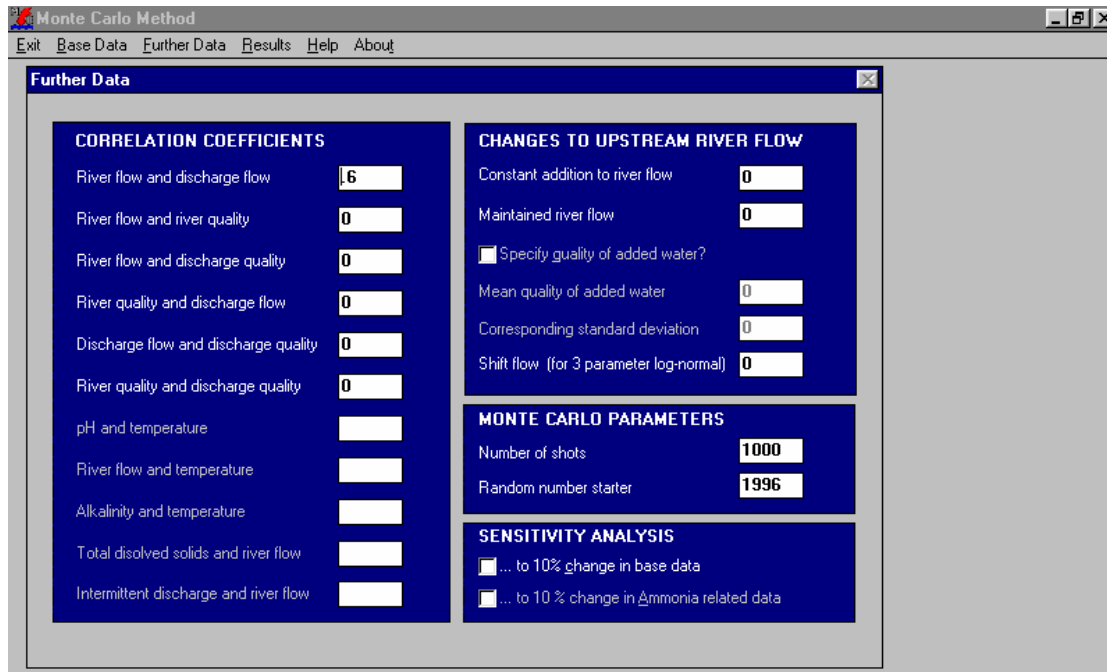
² When two variables x and y are unrelated, the correlation coefficient is zero. A positive correlation of +1 indicates that the two variables are perfectly related, such that any value of x corresponds to a unique value of y. It also indicates that values of x increase in magnitude in proportion to corresponding increases in y. A negative correlation indicates that one variable decreases in magnitude as the other increases. Correlation coefficients can therefore lie anywhere between -1 and +1. *ft

Correlation does not infer 'causality', i.e. it does not mean that an increase in x causes an increase in y. There may be numerous unknown influences causing correlation.

Scatter plots of variables provide a graphical means of assessing correlation. However, more precise methods are provided by AARDVARK software (WRc) or 'Calculation of Correlation Coefficients' Option in the CD modelling software.

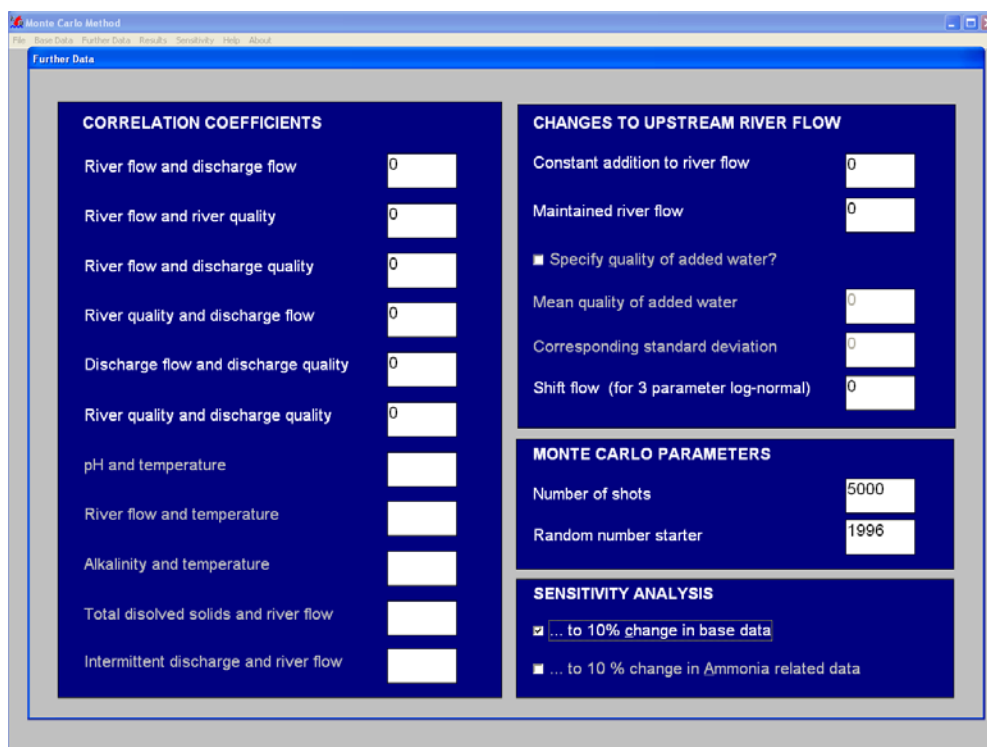
Data window, as shown in *Figure 15*. The correlation coefficient and the number of shots can be fixed for all subsequent runs by right clicking and ensuring a yellow circle is present.

Figure 14 Further Data Screen (default)



NOTE: This screen is not available until model has been run with base data

Figure 15 Further Data Screen (as required)



5.4 Sensitivity Analysis

Generally, the sensitivity of results to data is far smaller than the statistical errors associated with sampling programmes.

However, it is worth noting that;

- It is quicker to repeat a calculation to gauge sensitivity than to seek out and process input data to a prejudged impression of the required accuracy
- Sensitivity reflects real uncertainty about the decisions needed in order to achieve the river target. It is not a consequence of the method of calculation

Sensitivity analysis may be done manually, by changing entries for specific data, see Monte Carlo Simulation Data Input. Alternatively, check the *Sensitivity Analysis - 10% change in base data* option on the *Further Data* screen to adjust each variable automatically by $\pm 10\%$ (see *Figure 16*). Return to the *Base Data* screen and recalculate to display the *Sensitivity Analysis Results* Screen.

The automated sensitivity analysis changes the input parameters by 10% one at a time and recalculates the model output. It changes each input parameter by 10% in both directions (i.e. +10% and -10%) in order to evaluate which has the larger impact on the output. Only the larger impact is summarised in the results.

Figure 16 Sensitivity Results

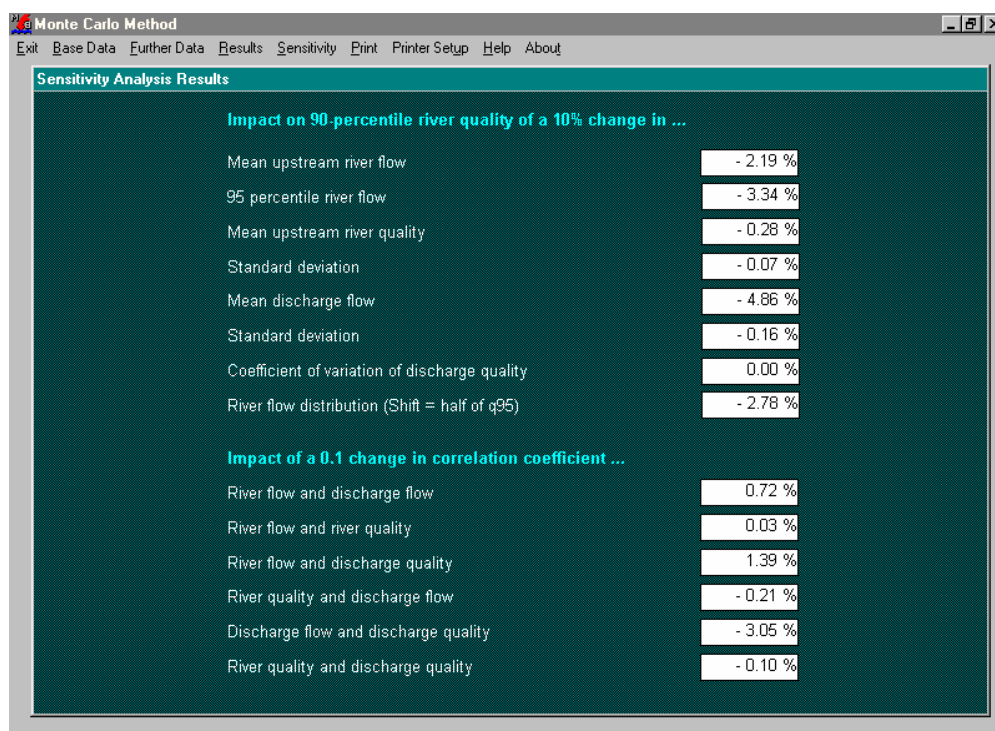


Figure 16 shows sensitivity of the 90%ile downstream river quality target to a 10% change in input parameters. In this case, the greatest effect is demonstrated by a 10% change in the mean discharge flow producing a change of 4.86% in the 90%ile river quality.

However, unless continuous flow monitoring data or a very large data set was used, the confidence limits around the mean discharge flow will be significant and the potential impact far greater.

Similarly, changing the mean upstream river flow by 10% changes the downstream 90%ile quality by only 2.19% but there may be great uncertainty about actual river flow and this must be considered when assessing sensitivity. The model should be re-run substituting the relevant parameters with both the upper and lower 95%ile confidence limits to produce the worst case and optimistic scenarios respectively.

Therefore, the significance of the sensitivity results depends on the robustness of the input data. This should be considered on a case specific basis, particularly where the discharge is environmentally significant or there are implications for capital outlay.

5.5 Model Calibration

Large uncertainties are associated with summary statistics for a limited sample set. These uncertainties often far outweigh any other deficiencies in the model. However, for an existing discharge, provided there is recent flow and quality data available for the discharge and the upstream and downstream river quality, it is worthwhile undertaking this exercise to establish whether model outputs are comparable to observed results.

Run the CD modelling software in 'forwards' mode, to determine whether recently measured downstream quality can be modelled using recent upstream and discharge data. If there are large discrepancies, even taking account of statistical uncertainties in summary statistics, then it implies that the data does not adequately represent processes going on in the vicinity of the discharge. Further examination of all potential sources of pollution and sampling data is recommended. Localised impacts from e.g. CSOs may be of particular significance, or the location of the sampling points in relation to the mixing zone for the discharge.

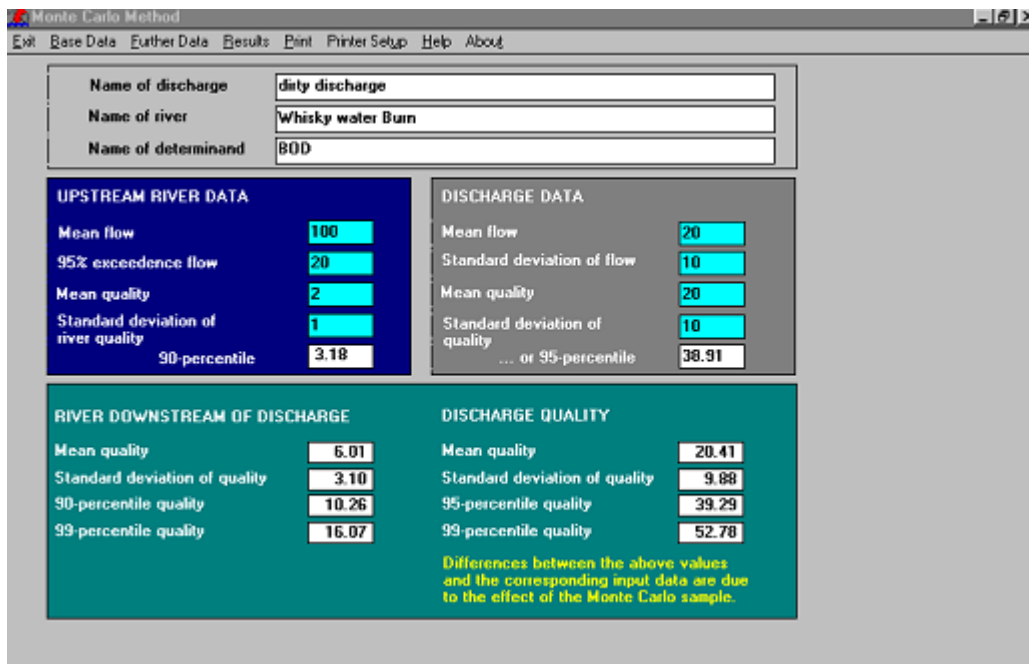
5.6 Forward Calculation of Downstream River Quality

The output comprises of statistics describing both the river quality downstream of the discharge and discharge quality. The latter is generated by Monte Carlo using the ratio of the mean and s.d. inputs and provides a check that the required effluent quality distribution has been produced. Any differences are due to the Monte Carlo sampling process. If these are unexpectedly large, then check that 5000 Monte Carlo shots have been specified in the *Further Data* screen.

The statistics describing the river downstream of the discharge are the mean, standard deviation, 90 percentile and 99 percentile. These can be compared against Water Quality Standards, WFD Classification scheme limits and the upstream river quality to assess the degree of impact.

In the example shown in *Figure 17* river mean BOD quality has increased from 2.0 to 6.01 mg/l and the 90%ile from 3.18 to 10.26 mg/l. For a receiving river waterbody of LHAT typology, this is a decline in face value class from High to Bad (LHAT = lowland high alkalinity).

Figure 17 Results Screen



5.7 Backward Calculation of Discharge Quality Required

The model outputs are statistics describing the distribution of discharge quality required to meet the specified River Quality Target. The model calculates a discharge quality distribution using all the capacity available and the output represents the impact after full mixing. Therefore, it is important to consider the length of the mixing zone and the percentage of the available capacity to be allocated to the discharge. The downstream target should be set in accordance with the guidelines described in *WAT-RM-21*.

The discharge quality is summarised by the mean, standard deviation, 95%ile and 99%ile statistics. Depending on the nature of the discharge being considered it may be necessary to assure oneself that the discharge can comply with these statistics. However, it is usually sufficient to ensure that the mean and 95%ile can be achieved.

6. Lower and Upper Tier Numeric Limits

The 95%ile result from the Backwards Modelling is used as the lower tier in the licence. The upper tier value should be set using the *Two-tier Multiplier Tables*. The multiplier used to calculate the upper tier value varies with the determinand being licensed and also with the lower tier value.

In *Figure 18* the mean discharge BOD quality of 7.88 mg/l and associated 95%ile of 15.17 mg/l need to be met in order to ensure the 90%ile downstream river quality target of 5mg/l is achieved.

The two tier licence limits would be a 95%ile of 15 mg/l and an upper tier of 50 mg/l.

For guidance on using lower and upper tier numeric limits refer to *WAT-SG-13: Municipal Sewage Treatment Works (STW)*.

Figure 18 BOD Determinands

The screenshot shows the 'Monte Carlo Method' software interface. The main window displays input and output data for a BOD determinand. The input fields are: Name of discharge: 'dirty discharge', Name of river: 'Whisky water Burn', and Name of determinand: 'BOD'. The output is organized into four panels: 'UPSTREAM RIVER DATA', 'DISCHARGE DATA', 'RIVER DOWNSTREAM OF DISCHARGE', and 'DISCHARGE QUALITY NEEDED'. Each panel contains a list of parameters with their corresponding values in input boxes.

UPSTREAM RIVER DATA		DISCHARGE DATA	
Mean flow	100	Mean flow	20
95% exceedence flow	20	Standard deviation of flow	10
Mean quality	2	Mean quality	20
Standard deviation of river quality	1	Standard deviation of quality	10
90-percentile	3.18	... or 95-percentile	38.91

RIVER DOWNSTREAM OF DISCHARGE		DISCHARGE QUALITY NEEDED	
Mean quality	3.29	Mean quality	7.88
Standard deviation of quality	1.32	Standard deviation of quality	3.82
90-percentile quality	5.00	95-percentile quality	15.17
99-percentile quality	7.14	99-percentile quality	20.38
Quality target (90-percentile)	5.00		

7. Calculation of Un-ionised Ammonia

WFD standards are based on Total Ammonia and the method described in section 6 should be used to derive Total Ammonia standards.

There is a different CD modelling tool for looking at the potential effects of un-ionised Ammonia. This is the second option on the *Mass Balance Calculation Main Menu* entitled Monte Carlo Simulation for Ammonia Standards (see Figure 8). This option is used for setting numeric licence limits for Total Ammonia based upon river quality standards for un-ionised ammonia.

Ammonia dissolved in water exists mostly in the ionised form, NH_4^+ , but some is present as un-ionised ammonia, NH_3 . It is the latter which is more toxic to fish and needs to be considered dependent on initial analysis for Total Ammonia using the standard Monte-Carlo Mass Balance option.

Within the Monte-Carlo Mass Balance Simulation for un-ionised Ammonia, there are two steps:

1. The downstream concentration of Total Ammonia is calculated using the Mass Balance equation.
2. The un-ionised Ammonia concentration is calculated using the result from Step 1 and river water chemistry data.

Figure 19 Monte-Carlo Simulation for Ammonia Standards

UPSTREAM RIVER DATA	
Mean flow	100
95% exceedence flow	20
Mean Total Ammonia	0.1
Standard deviation of Total Ammonia	0.1
90-percentile	0.21

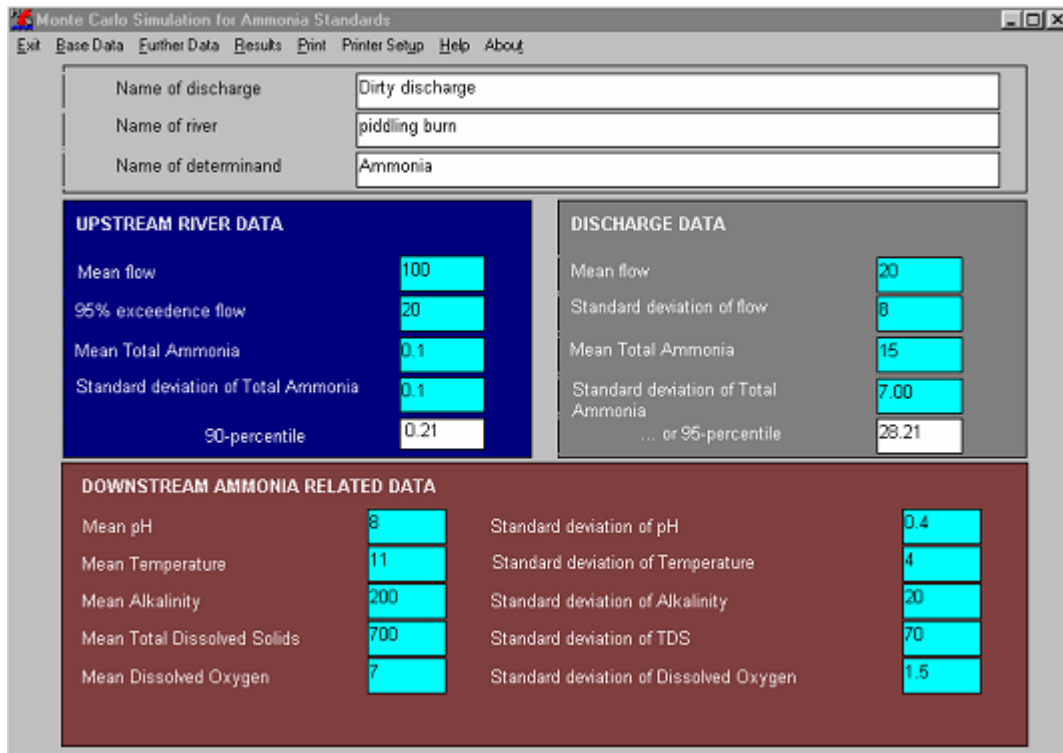
DISCHARGE DATA	
Mean flow	20
Standard deviation of flow	8
Mean Total Ammonia	15
Standard deviation of Total Ammonia	7.00
... or 95-percentile	28.21

Calculate required discharge quality Calculate effect of input discharge quality

River quality target downstream of discharge (> 0.1 for Total Ammonia; < 0.1 for Unionised Ammonia) 0.021 Percentile 95

Fields coloured must contain data before calculations are carried out.

Figure 20 Ammonia-Related Data input screen



UPSTREAM RIVER DATA		DISCHARGE DATA	
Mean flow	100	Mean flow	20
95% exceedence flow	20	Standard deviation of flow	6
Mean Total Ammonia	0.1	Mean Total Ammonia	15
Standard deviation of Total Ammonia	0.1	Standard deviation of Total Ammonia	7.00
90-percentile	0.21	... or 95-percentile	28.21

DOWNSTREAM AMMONIA RELATED DATA			
Mean pH	8	Standard deviation of pH	0.4
Mean Temperature	11	Standard deviation of Temperature	4
Mean Alkalinity	200	Standard deviation of Alkalinity	20
Mean Total Dissolved Solids	700	Standard deviation of TDS	70
Mean Dissolved Oxygen	7	Standard deviation of Dissolved Oxygen	1.5

The proportion of ammonia present in the un-ionised form depends on water chemistry, particularly pH and temperature. To calculate un-ionised river quality data for pH, Temperature, Alkalinity, Total Dissolved Solids and Dissolved Oxygen is required. This data is input from the 'Ammonia related data' screen, see *Figure 20*.

In the Monte-Carlo simulation, the calculation of unionised ammonia is done by extracting values from each of the distributions of pH, Temperature, Alkalinity, Total Dissolved Solids and Dissolved Oxygen (expressed as mg/l). These are variables used in equations describing water chemistry relationships to calculate the concentration of un-ionised ammonia corresponding to a total ammonia concentration. This provides an estimate of the distribution of un-ionised ammonia downstream of the discharge and hence estimates of the summary statistics, the mean and percentiles.

If there is a lack of data for Alkalinity, Total Dissolved Solids and Dissolved Oxygen the programme can be run with default values:

Table 3 Default Values for Monte Carlo Ammonia Standards Option

Determinand	Mean (mg/l)	Std. Deviation (mg/l)
Alkalinity	200	20
Total Dissolved Solids	700	70
Dissolved Oxygen	7.0	1.5

As with the standard CD Mass Balance software, the un-ionised ammonia modelling option requires data which characterise the distributions of the variables. The data, by default, are presumed to be Normal or Log-normal. This means that two summary statistics will define the complete distribution. However, non-parametric data can also be used. Temperature, pH, alkalinity, dissolved oxygen and total dissolved solids are all assumed to follow the Normal Distribution.

The input statistics are listed in *Table 4*.

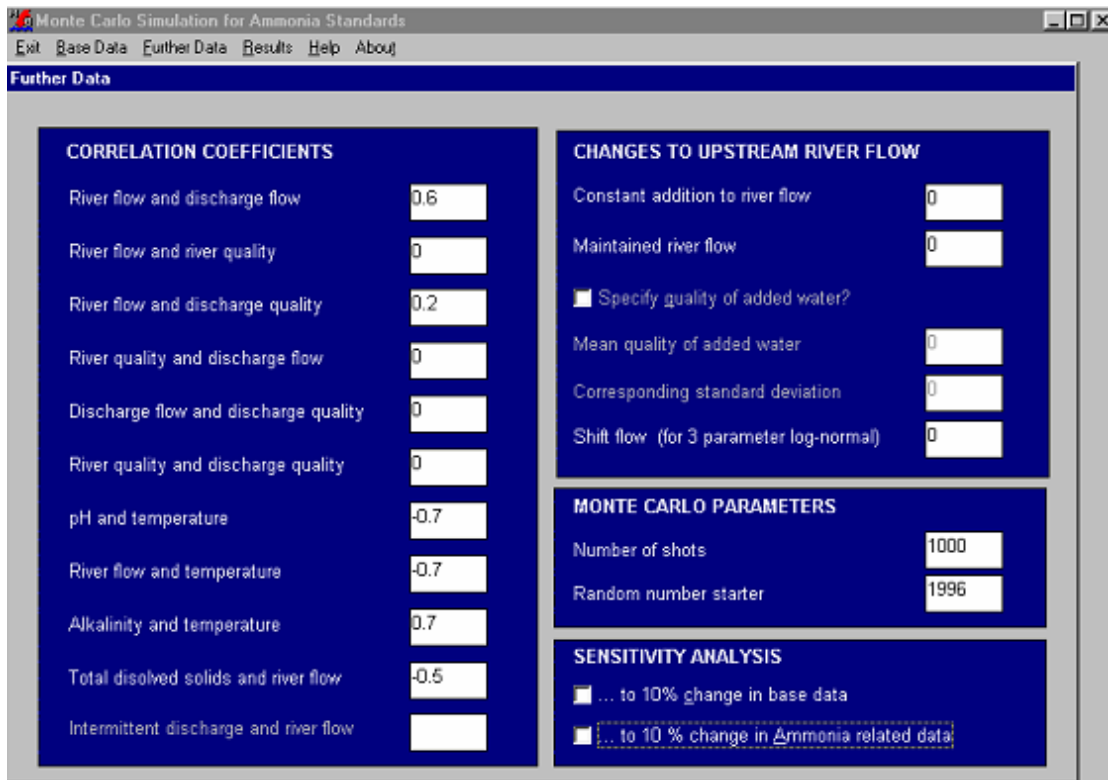
Table 4 Input Statistics

Upstream River		
River flow	Log-Normal	mean & 5-percentile
Total Ammonia	Log-Normal	mean & standard deviation
Discharge		
Discharge flow	Log-Normal	mean & standard deviation
Total Ammonia	Log-Normal	mean & standard deviation or 95%ile
Downstream River		
pH	Normal	mean & standard deviation
Temperature	Normal	mean & standard deviation
Alkalinity	Normal	mean & standard deviation
Total dissolved solids	Normal	mean & standard deviation
Dissolved Oxygen	Normal	mean & standard deviation
River Target		
Un-ionised Ammonia	Log-Normal	mean or percentile

If the software is being used to calculate the discharge quality then the downstream River Quality Target will need to be entered. If a river target which is larger than 0.1 mg/l is entered it will be interpreted as a standard for total ammonia and not as one for un-ionised ammonia. The software prompts the user as a reminder and enables switching between standards for both ammonia species.

In addition to the extra data requirements of the ammonia model, there are further correlations between variables which may need to be considered. For example, temperature is assumed to correlate with river flow. There is an additional sensitivity analysis option available from the *Further Data* screen which tests the sensitivity of results to the ammonia-related input data, *Figure 21*. It is recommended that both sensitivity options are selected.

Figure 21 Further Data for Ammonia Standards



Monte Carlo Simulation for Ammonia Standards
 Exit Base Data Further Data Results Help About

Further Data

CORRELATION COEFFICIENTS	
River flow and discharge flow	0.6
River flow and river quality	0
River flow and discharge quality	0.2
River quality and discharge flow	0
Discharge flow and discharge quality	0
River quality and discharge quality	0
pH and temperature	-0.7
River flow and temperature	-0.7
Alkalinity and temperature	0.7
Total dissolved solids and river flow	-0.5
Intermittent discharge and river flow	

CHANGES TO UPSTREAM RIVER FLOW	
Constant addition to river flow	0
Maintained river flow	0
<input checked="" type="checkbox"/> Specify quality of added water?	
Mean quality of added water	0
Corresponding standard deviation	0
Shift flow (for 3 parameter log-normal)	0

MONTE CARLO PARAMETERS	
Number of shots	1000
Random number starter	1996

SENSITIVITY ANALYSIS	
<input checked="" type="checkbox"/> ... to 10% change in base data	
<input checked="" type="checkbox"/> ... to 10 % change in Ammonia related data	

Output from the Monte Carlo simulation for Ammonia standards is identical to the standard Monte Carlo mass balance software, except statistics are displayed describing downstream river quality in terms of both total and un-ionised ammonia.

Figure 22 Results Screen Ammonia Standards

Monte Carlo Simulation for Ammonia Standards

Exit Base Data Further Data Results Print Printer Setup Help About

Name of discharge	Dirty discharge
Name of river	piddling burn
Name of determinand	Ammonia

RIVER DOWNSTREAM OF DISCHARGE		DISCHARGE QUALITY NEEDED	
Mean Total Ammonia	0.57	Mean Total Ammonia	2.33
Standard deviation	0.30	Standard deviation	1.04
90-percentile Total Ammonia	0.97	95-percentile Total Ammonia	4.21
Mean Unionised Ammonia	0.0078		
Standard Deviation	0.0069		
95-percentile Unionised Ammonia	0.0210		
Quality target (95-percentile)	0.0210		

In this example discharge quality, summarised by the mean, standard deviation and 95%ile Total Ammonia concentration, is that required to meet an un-ionised ammonia river quality target of 0.021 mg/l as a 95%ile.

8. Catchment Models

This section offers advice on discharge scenarios that may benefit from the use of a Catchment Model such as SAGIS. In nearly all cases, however, good decisions can be made without a catchment model and their use should be reserved for situations which are either complex in nature (i.e. interaction of multiple discharges and management options) and/or significant in terms of the potential capital outlay or environmental risk. Catchment modelling requires considerable resource in terms of data, time and effort which may not always be justified. SEPA's Environmental and Spatial Informatics Unit can provide guidance on the use of catchment models.

Section 3 above discusses the data needed for a single discharge CD mass balance modelling exercise and provides guidance on the interpretation of results and the sensitivity of results to uncertainty in data. This advice applies equally to the use of Catchment Models. Essentially, the use of a catchment model is comparable to a repetition of the CD mass balance model at each discharge location and confluence, treating the incoming tributary as a discrete discharge. Where only two or three 'interacting' discharges require modelling, it is often feasible and sufficient to model the discharges in this way. However catchment models, which also take account of natural purification, are preferred for more complex catchments. That being said, the SAGIS models which are now available within SEPA may be an additional source of in-river data, especially when little or no monitoring data exists near the site of the discharge which is to be modelled.

8.1 Catchment Model Usage

Catchment models may be helpful and time-saving in situations where:

- A decision cannot be made on one discharge without taking decisions at upstream discharges
- Decisions cannot be made on a discharge without considering action to control diffuse pollution or, without taking account of natural purification
- The catchment is small relative to the discharges and there are complications such as diurnal variations in pollutant load
- There is a need to do many calculations for a catchment over a year or more. A model can save time in processing data, in doing calculations, keeping records and in preparing reports.

If catchment models are to be used they need to be capable of calculating the relationship between the summary statistics (i.e. means and percentiles) of discharge quality and river quality, which means that they must either:

- Be based on the technique of Monte Carlo Simulation (as in SAGIS); or
- Predict and summarise the daily time-series of values of water quality over at least two to three years, a more complex option.

Models which do no more than predict water quality over a few hours or days are not useful in determining numeric licence standards.

The models which are available within SEPA may have scenarios run upon them to see the change in a particular discharge filter throughout an entire catchment. At present the ESIU is responsible for running these scenarios though it may be a feature which becomes available through the suite of Spotfire tools in due course.

It is unlikely that many users of this manual will be required to undertake any catchment modelling exercises. If catchment modelling is being considered then advice should be sought from SEPA's Environmental and Spatial Informatics Unit.

9. Practical Example

9.1 Introduction

The following example is based on SEPA's 2008 WFD Classification scheme and standards. Other case studies can be found on the *ESIU webpage*. An example is presented here on determination of Licence standards for a proposed continuous discharge of treated landfill leachate to a small tributary just upstream of its confluence with a larger watercourse. The effluent performance standards of the passive treatment system being proposed (i.e. aerobic lagoons, reed beds and grass plots) is not stated in the application.

SEPA is required to protect both rivers from a downgrade in status. The current class in the larger watercourse (waterbody ID 3021) is Good for both Ammonia and BOD (see 9.2.1). The tributary is not classified, as it is a Small River Waterbody and these are not currently classified. Therefore we will have to assume that the class of the tributary is also Good for both Ammonia and BOD.

The water quality targets for the tributary receiving the discharge are to maintain Good quality with regard to Ammonia and BOD. *Spottfire DAVE Chemistry* and CD mass balance software is used to evaluate historical data and to derive licence standards which will allow these Water Quality Objectives to be met. Water Quality Objectives for the major watercourse are also to meet Good standards. If the tributary meets Good quality, then the discharge cannot jeopardise this objective. The relevant water quality targets for High, Good and Moderate Classes for BOD and ammonia are shown below in *Table 5*.

Table 1 A1/A2 Class Boundaries for BOD and Ammonia*

Determinand	A1	A2
Ammonia (mg/l) 90%ile	≤ 0.25	≤ 0.6
BOD (mg/l) 90%ile	≤ 2.5	≤ 4.0

*As defined in SEPA 2008 classification scheme.

9.2 Data Requirements and Methodology

The data requirements are more than normal for a single discharge scenario as the impacts both locally within the tributary and downstream in the main river need to be evaluated. Therefore, flow and quality data are required for both watercourses in addition to the discharge.

The approach required is to evaluate the downstream impact of the discharge on the receiving watercourse, then, assuming no 'natural purification' due to the short distance to the confluence, evaluate the impact in the main river. Therefore, the CD mass balance model is required to:

- Assess the impact of the proposed discharge on the tributary and calculate the discharge quality required to achieve the water quality objective for the receiving watercourse
- Assess the impact of the tributary on the quality of the main river, treating the tributary as the discharge

Only some of the analysis and modelling is presented here.

9.2.1 Data Collection

A range of sources of water quality information are available. In an ideal situation, you will find up-to-present monitoring data for your determinands of interest both upstream and downstream of the discharge site.

Use intranet GIS at a suitable scale for your area of interest, with the Monitoring theme added and the SEPA Historic River Monitoring Sites symbols displayed. Use the identify tool to find out information about sites that may be useful for your analysis. If you find any promising locations, note their location codes and use *Spotfire DAVE Chemistry* to see which parameters are available and what time period they cover.

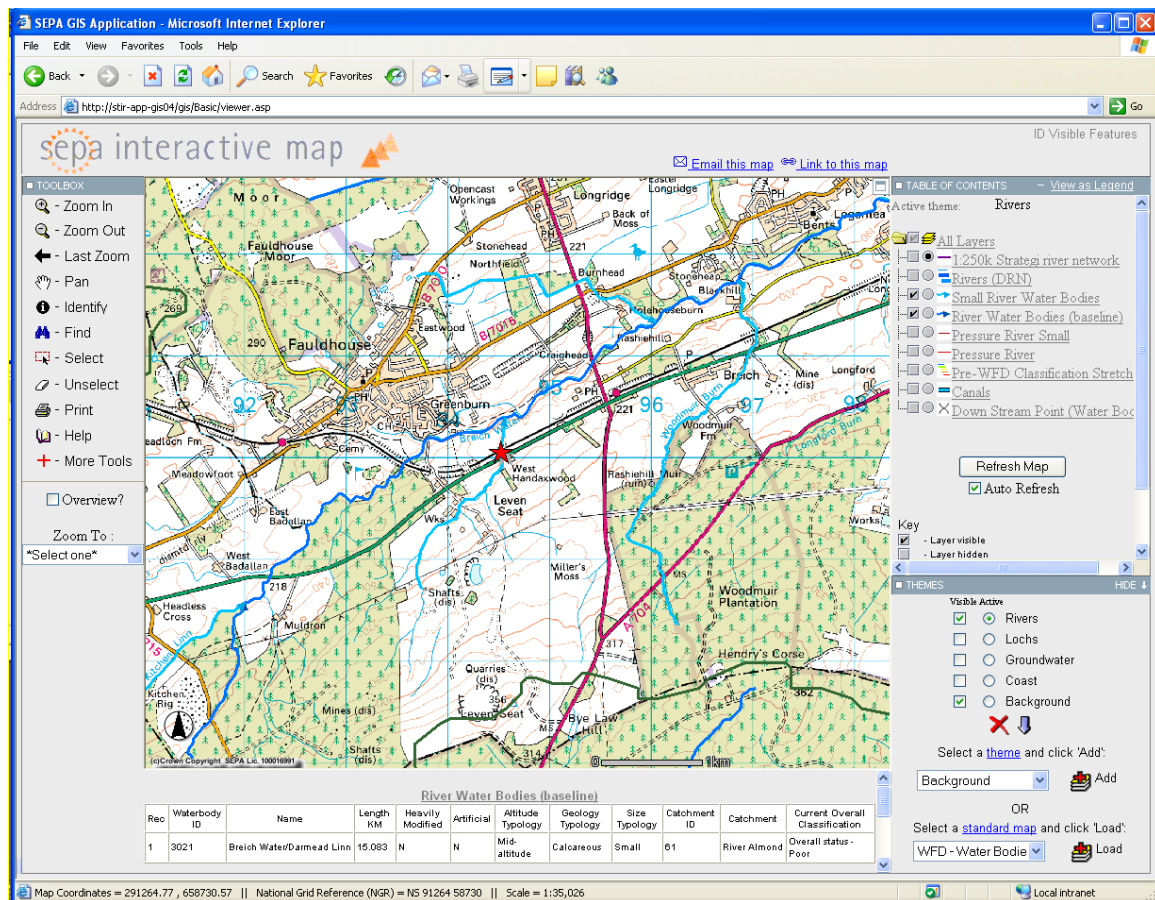
During the analysis, you will also need class information for each determinand (known as the face value class) in the receiving watercourse(s). The remainder of this section explains how to find this. As a minimum, you will need the class of the receiving watercourse in order to estimate its available capacity. In the situation where there is little or no monitoring data, you may need to use the class information to estimate the water quality of the upstream water – for example, if the class was Good you could assume that the ammonia 90%ile concentration was mid-class, in this case, 0.25 mg/l.

To find the face value class for each determinand for waterbodies, first the Waterbody ID needs to be identified, as follows:

Identify the Waterbody ID

Using intranet GIS, zoom to the location code or grid reference of the discharge. Add the standard map “WFD-Waterbodies”, and untick Lochs, Coastal and Groundwater so Rivers can be seen clearly. Use the identify tool to click on the baseline River Water Body that the discharge flows into. In this example, the discharge is on a Small River Water Body, the nearest baseline waterbody (ID 3021) has been highlighted (see Figure 23).

Figure 23 Find Waterbody ID of Receiving Baseline River Waterbody



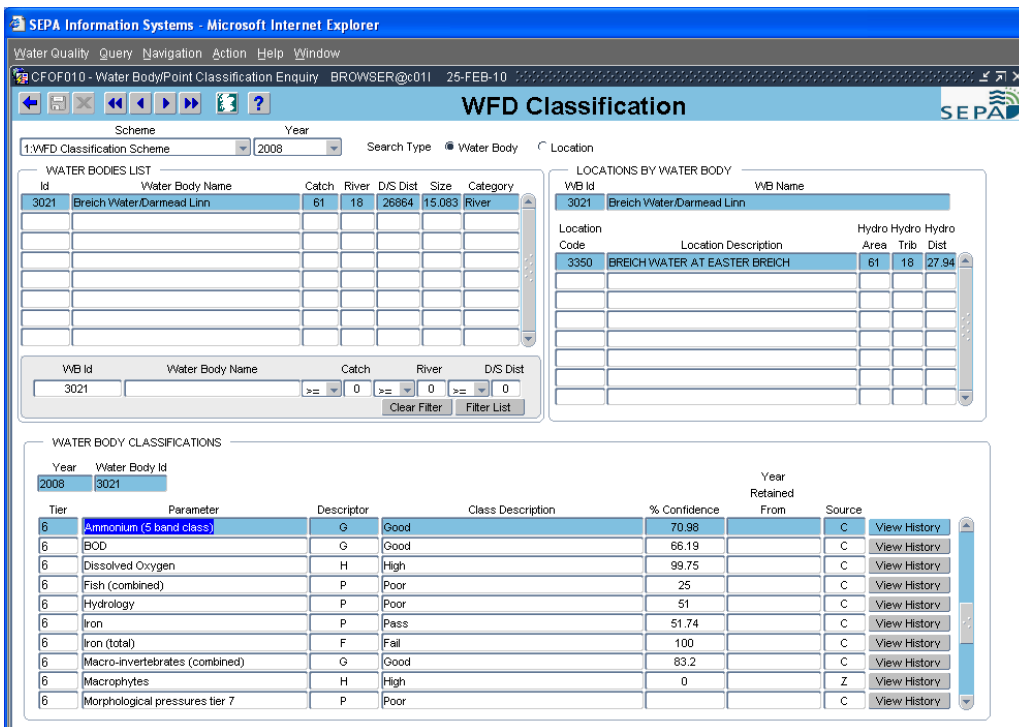
Determination of class for each determinand

Once the waterbody ID has been determined, there are two ways to find the class for each determinand of interest.

1. **Using SEPA Information Systems:** From the intranet homepage, open SEPA Information Systems; log in as browser, centralbrowser, c01l; select SEPA MENU | Water Quality | WFD Classification | Classification Enquiry | Enquiries | Waterbody/Point Classification Enquiry; Choose the most recent year; click water body button; enter the waterbody ID number into the WB Id box; click Filter List; in the table that appears, find the determinand of interest and note its class (this may be High, Good, Moderate, Poor or Bad, or it may just be Pass – this means Good or better). For Ammonia, refer to “Ammonium (5 band class)”, see Figure 24.

2. **Using intranet GIS:** Zoom to your waterbody ID. Add the theme “WFD Classification”, make it Active, select River Classification. Using the identify tool, click on the river of interest. A table of data appears that gives the overall class only. Click on the waterbody ID in column 2, which opens a new window showing the face value class confidence or certainty of class for various determinands (see Figure 25). Refer to the determinand of interest.

Figure 24 Find Face Value Classes of receiving Baseline River Waterbody using SEPA Information Systems



The screenshot shows the SEPA Information Systems interface in Microsoft Internet Explorer. The browser title is "SEPA Information Systems - Microsoft Internet Explorer". The address bar shows "CFOP010 - Water BodyPoint Classification Enquiry BROWSER@e011 25-FEB-10". The main content area is titled "WFD Classification".

At the top, there are filters for "Scheme" (1:WFD Classification Scheme) and "Year" (2008). Below this is a "WATER BODIES LIST" table:

Id	Water Body Name	Catch	River	D/S Dist	Size	Category
3021	Breich Water/Darried Linn	61	18	26864	15.083	River

Below the table is a filter section with fields for "WB Id" (3021), "Water Body Name", "Catch", "River", and "D/S Dist".

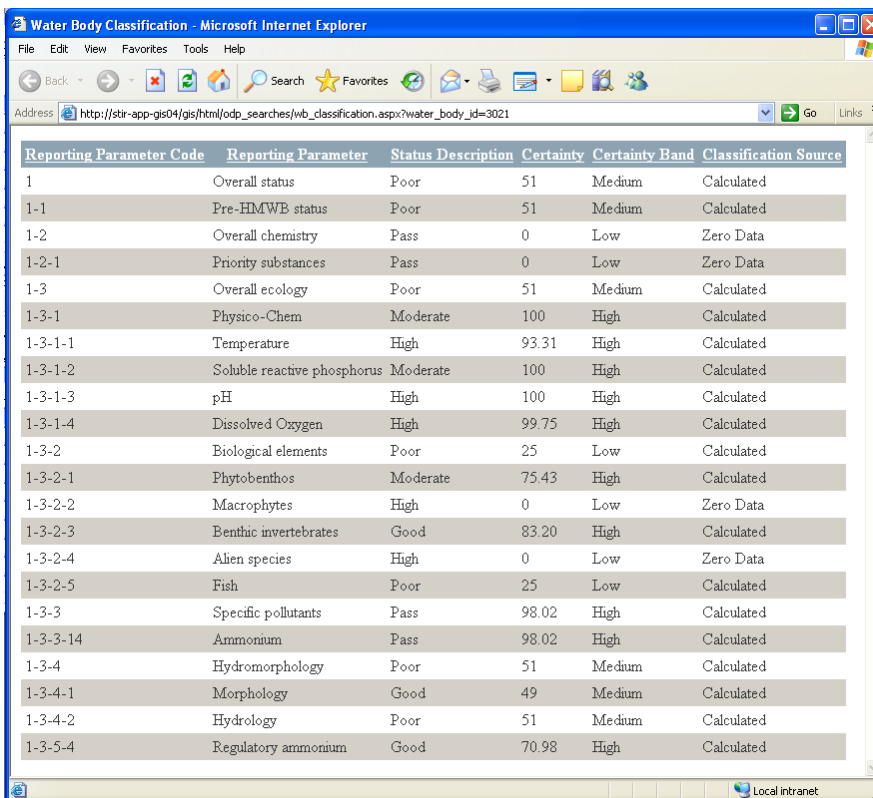
To the right, there is a "LOCATIONS BY WATER BODY" section with a table:

WB Id	WB Name	Location Code	Location Description	Area	Trib	Hydro Dist
3021	Breich Water/Darried Linn	3350	BREICH WATER AT EASTER BREICH	61	18	27.94

At the bottom, there is a "WATER BODY CLASSIFICATIONS" table for Year 2008 and Water Body Id 3021:

Tier	Parameter	Descriptor	Class Description	% Confidence	Year Retained From	Source
6	Ammonium (5 band class)	G	Good	70.98		C
6	BCD	G	Good	66.19		C
6	Dissolved Oxygen	H	High	99.75		C
6	Fish (combined)	P	Poor	25		C
6	Hydrology	P	Poor	51		C
6	Iron	P	Pass	51.74		C
6	Iron (total)	F	Fail	100		C
6	Macro-invertebrates (combined)	G	Good	83.2		C
6	Macrophytes	H	High	0		Z
6	Morphological pressures tier 7	P	Poor			C

Figure 25 Find Face Value Classes of receiving Baseline River Waterbody using Intranet GIS



The screenshot shows the "Water Body Classification" interface in Microsoft Internet Explorer. The browser title is "Water Body Classification - Microsoft Internet Explorer". The address bar shows "http://str-app-gis04/gis/html/odp_searches/wb_classification.aspx?water_body_id=3021".

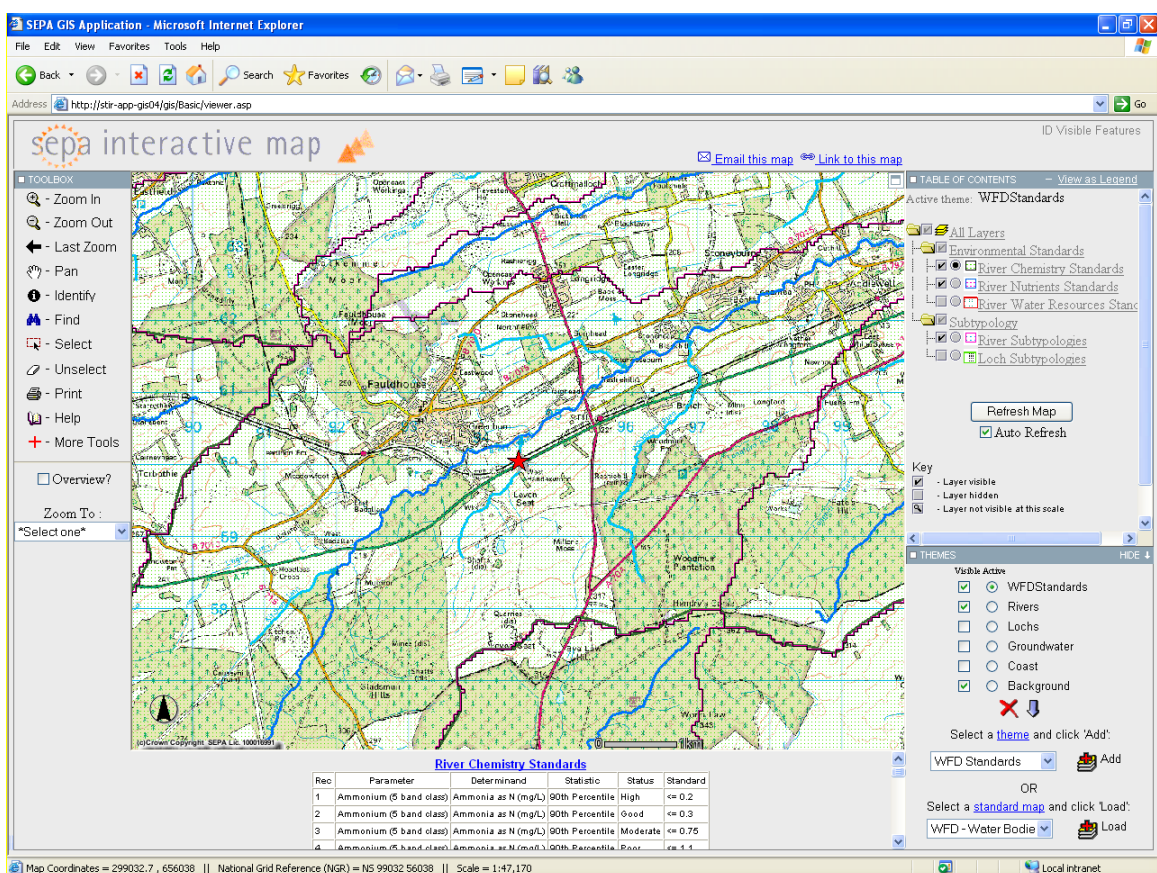
The main content area displays a table with the following columns: Reporting Parameter Code, Reporting Parameter, Status, Description, Certainty, Certainty Band, and Classification Source.

Reporting Parameter Code	Reporting Parameter	Status	Description	Certainty	Certainty Band	Classification Source
1	Overall status	Poor		51	Medium	Calculated
1-1	Pre-HMWB status	Poor		51	Medium	Calculated
1-2	Overall chemistry	Pass		0	Low	Zero Data
1-2-1	Priority substances	Pass		0	Low	Zero Data
1-3	Overall ecology	Poor		51	Medium	Calculated
1-3-1	Physico-Chem	Moderate		100	High	Calculated
1-3-1-1	Temperature	High		93.31	High	Calculated
1-3-1-2	Soluble reactive phosphorus	Moderate		100	High	Calculated
1-3-1-3	pH	High		100	High	Calculated
1-3-1-4	Dissolved Oxygen	High		99.75	High	Calculated
1-3-2	Biological elements	Poor		25	Low	Calculated
1-3-2-1	Phytobenthos	Moderate		75.43	High	Calculated
1-3-2-2	Macrophytes	High		0	Low	Zero Data
1-3-2-3	Benthic invertebrates	Good		83.20	High	Calculated
1-3-2-4	Alien species	High		0	Low	Zero Data
1-3-2-5	Fish	Poor		25	Low	Calculated
1-3-3	Specific pollutants	Pass		98.02	High	Calculated
1-3-3-14	Ammonium	Pass		98.02	High	Calculated
1-3-4	Hydromorphology	Poor		51	Medium	Calculated
1-3-4-1	Morphology	Good		49	Medium	Calculated
1-3-4-2	Hydrology	Poor		51	Medium	Calculated
1-3-5-4	Regulatory ammonium	Good		70.98	High	Calculated

Determination of class boundaries

The class boundary limits vary depending on your location (i.e. to reflect different catchment typologies). To find the class boundaries relevant to your discharge: Use intranet GIS to zoom to the location code or grid reference of your discharge. Add the theme “WFD Standards” and make it active. Click on River Chemistry Standards, River Nutrient Standards and River Subtypologies. Then use the identify tool and click on the receiving waterbody. At the bottom of the screen, tables of the class boundaries appear, along with details of the sub-typologies of waterbody (see Figure 26).

Figure 26 Find Class Boundary Limits of Receiving Baseline River Waterbody Using Intranet GIS



Class boundary limits (EQSs) for other parameters (e.g. metals) can be found in WAT-SG-53 Environmental Standards for Surface Waters.

To determine flow data

The Hydrology department was asked to source data/information on flows in both the tributary and main river. The minimum requirement is an estimate of the mean and Q95 (5%ile exceedance flow). In this case, theoretical calculation was used to estimate the figures. However, subsequent modelling showed that the Licence conditions were sensitive to both river and discharge flow regimes, so Hydrology were asked to carry out some field measurement of flows.

If sensitivity analysis shows that decisions regarding Licence limits are sensitive to one or more input parameters and these inputs are 'uncertain', further data collection will be required to minimise uncertainty where environmental risk and/or investment costs are significant, as described in Sensitivity Analysis.

Table 6 Flows For Input To CD Mass Balance Model

	Mean flow (l/s)	Q95 flow (l/s)
Discharge	0.5 l/s	
Tributary	84	5.5
Main River	1019	81

Data for the proposed treated leachate discharge is limited. An average daily flow figure was agreed, but flow variability was unknown. However, discharge flow was likely to be positively correlated with rainfall and could be controlled by a weir structure, if required. A maximum permitted discharge flow rate would be required by Licence, with perhaps storage/recirculation of excess flows. With this sort of arrangement in place flow variability would be limited.

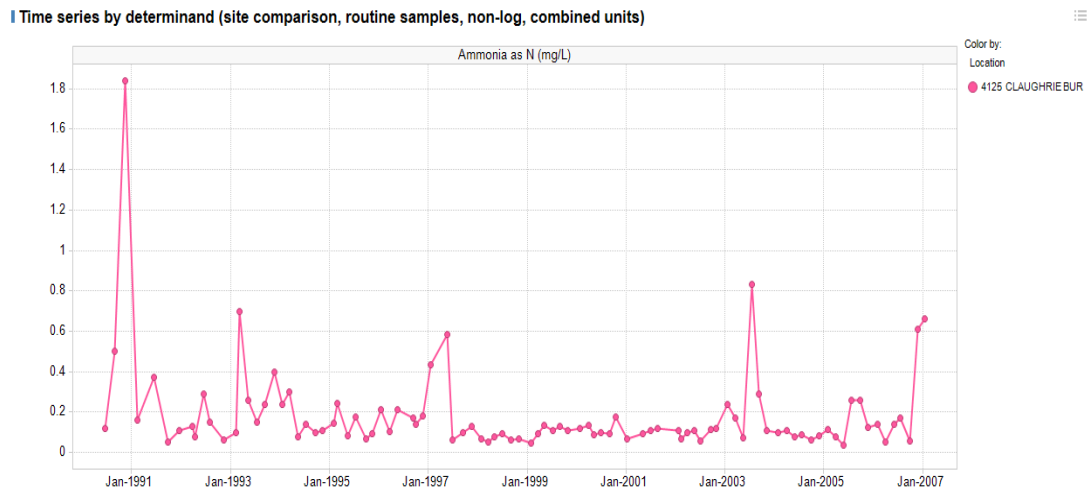
Treated leachate quality was also unknown. Data for untreated leachate quality supplied by the applicant from a similar site was used to examine a 'worst case scenario' as this particular site was known to provide poor treatment. In order to calculate the discharge quality required to meet the Water Quality Targets, the relative variability of the discharge quality had to be estimated. For the purposes of this exercise a Coefficient of Variation of 1 was assumed, representing a fairly variable effluent quality. However, sensitivity analysis should always be undertaken to assess the effect of any assumptions. In this case, the results were not sensitive. If available, comparable data from elsewhere should be used to estimate likely variability of quality.

9.2.2 Data Analysis Using Spotfire DAVE Chemistry

River quality data was analysed using *Spotfire DAVE Chemistry* to produce summary statistics representative of current water quality. Some relevant plots are reproduced below with a brief description of the decision making process.

Figure 27 is the full ammonia dataset. One outlier of nearly ~2 mg/l was later removed from the dataset after confirmation that this was a high value sampled during 'unusual conditions'.

Figure 27 Time Series Plot on the Tributary

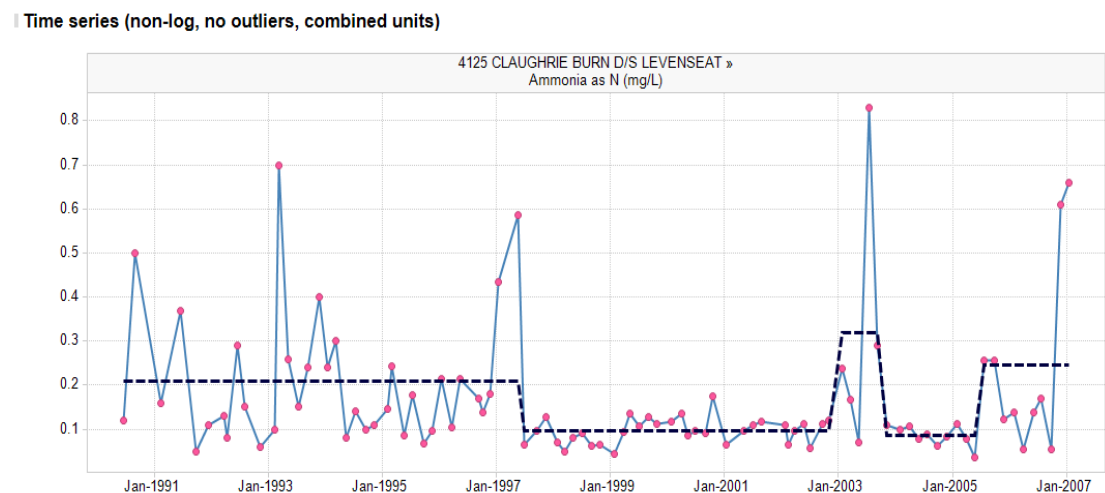


NB Each plot is saved to a Word or Powerpoint document, along with key comments and decisions, to keep an auditable trail of how standards were derived

The type of distribution of each dataset was determined. If there was found to be a 'not poor' goodness of fit against a lognormal distribution, then the mean and standard deviation of the distribution was used to input this dataset to the CD model.

Figure 28 is CUSUM analysis of the Ammonia data (with an outlier removed) which suggests an improvement in river quality since mid 1997.

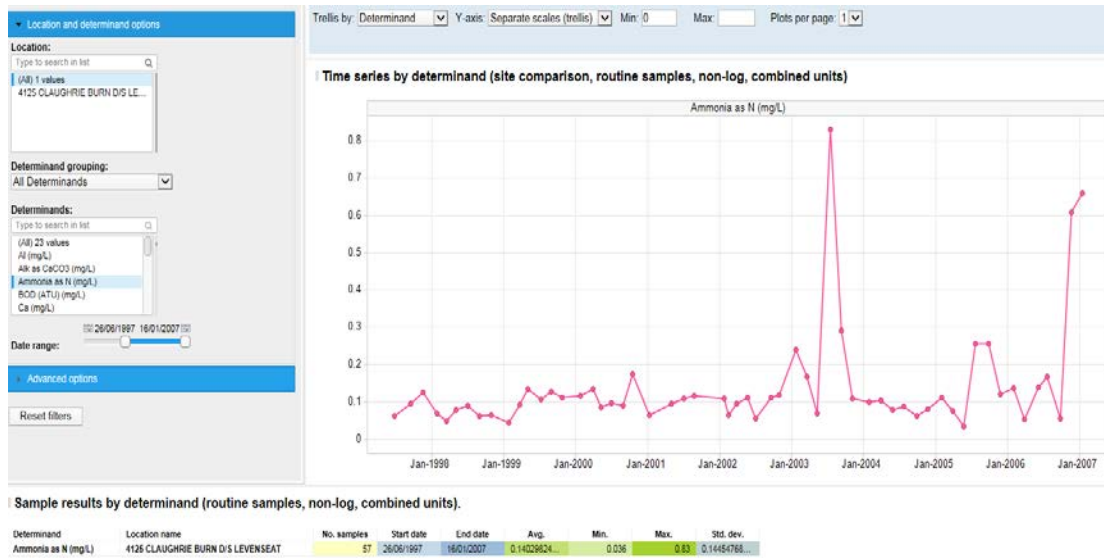
Figure 28 CUSUM Restricted Data



Summary statistics were produced for both the complete period 1990-present and mid 1997-present. Both sets were used in CD modelling to assess the significance of the apparent improvement in upstream quality.

Figure 29 shows summary statistics for Ammonia (restricted by Date) for period Mid 1997-present.

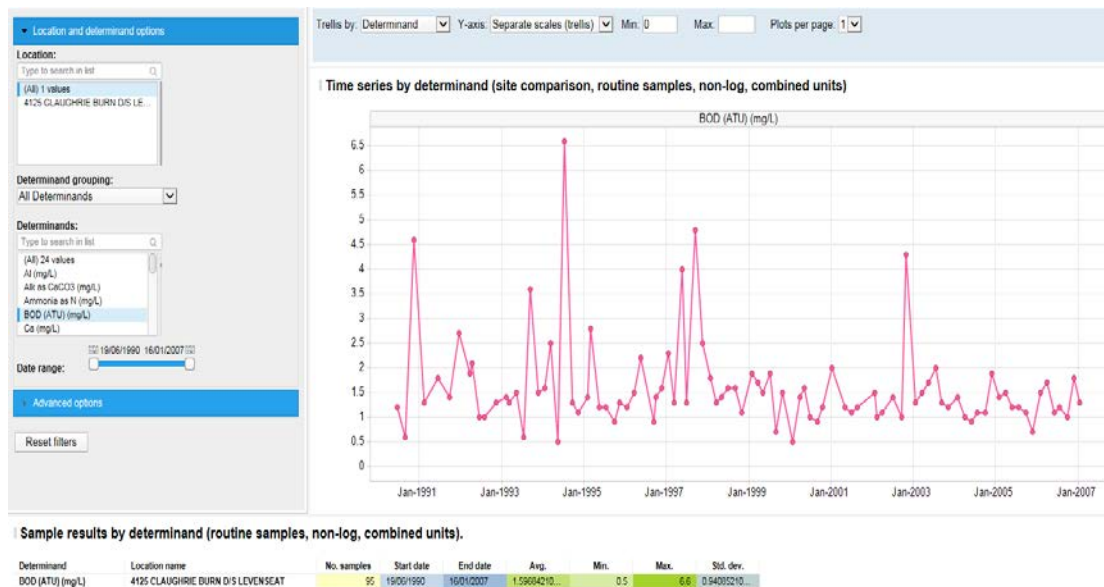
Figure 29 Determinand Summary



The mean and standard deviation were entered in the CD mass balance software.

Figure 30, BOD data for the tributary shows no outliers or temporal trends. The complete 1990-present data set is used to produce summary statistics for the CD mass balance model.

Figure 30 BOD data for the tributary



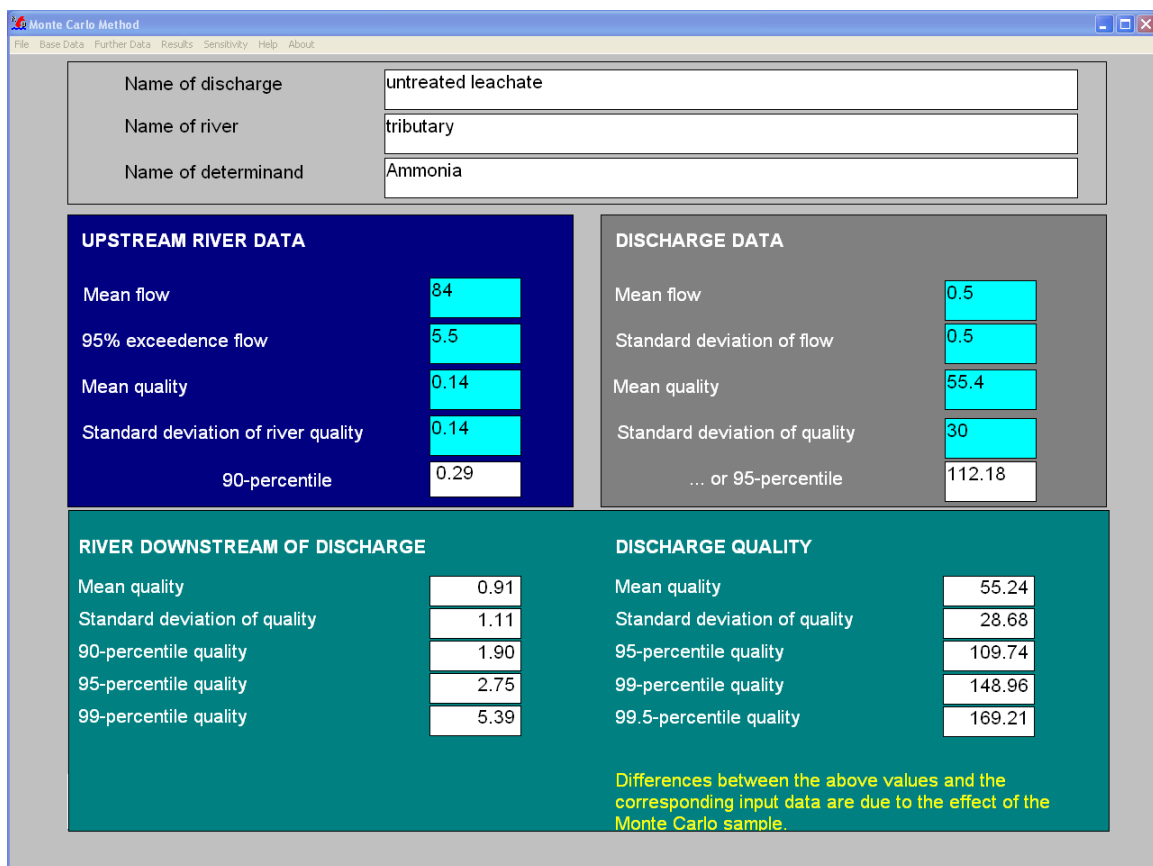
9.2.3 CD Mass Balance Modelling

The summary statistics produced using *Spotfire DAVE Chemistry* are used, together with estimates of river flow, discharge flow and variability of discharge quality, are input to the CD mass balance modelling software to calculate the required discharge quality. Information on untreated effluent quality is also used to evaluate the ‘worst case’ impact of a poorly performing treatment system.

Monte-Carlo simulation is used for evaluating 95%ile limits (Lower Tier Limits) (e.g. for ammonia, BOD and soluble reactive phosphorus) or mean discharge limits (e.g. iron).

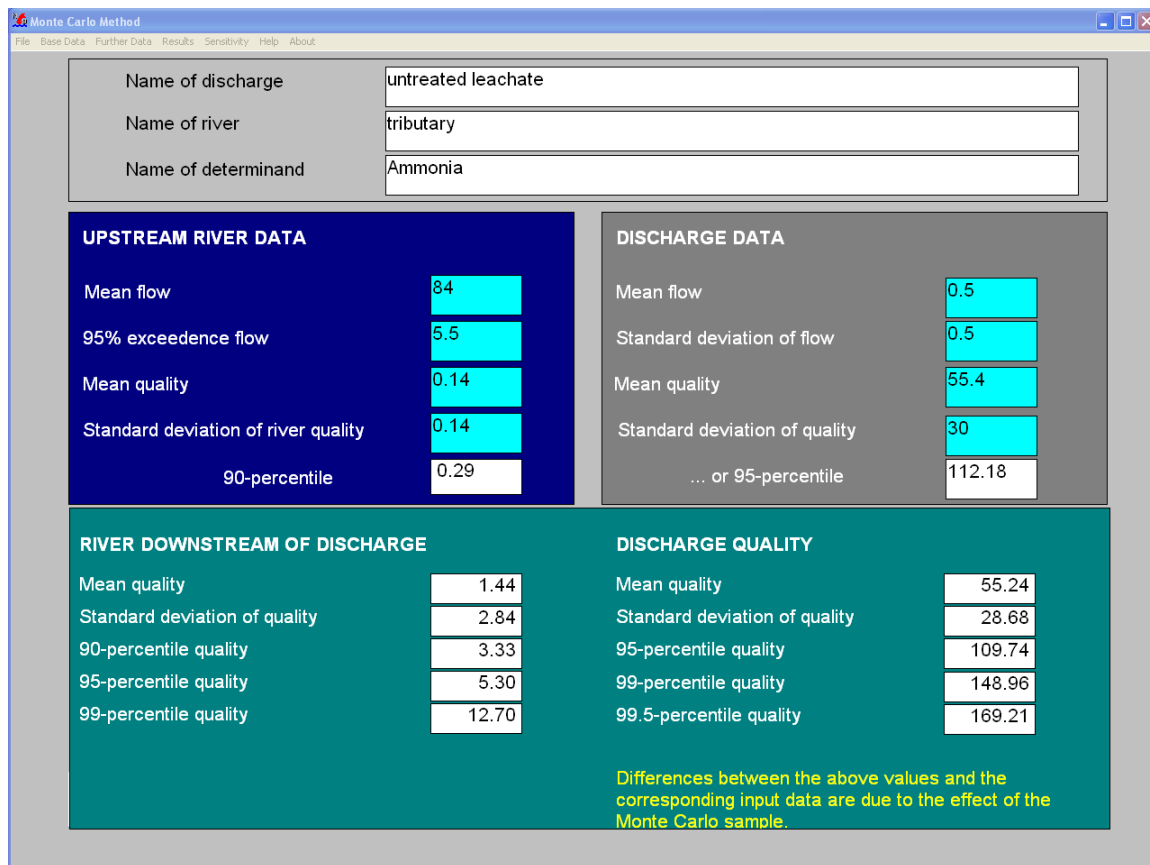
Figure 31 shows the potential impact of ‘untreated’ leachate on the tributary. Mean ammonia levels increase by a factor of 6, from 0.14 mg/l to 0.91 mg/l. This assumes the software’s default correlation of 0.6 between river flow and discharge flow.

Figure 31 Monte Carlo Result Screen



9.2.4 Correlation Coefficient

If the correlation coefficient for discharge and river flow is set to zero the downstream quality deteriorates further to a mean of 1.44 mg/l, 90%ile of 3.33mg/l, see Figure 32.

Figure 32 Correlation Coefficient set to Zero

9.2.5 Calculation of Discharge Quality required to meet specified downstream Water Quality target

Refer to *WAT-RM-21: Allocation of Capacity and Protection of the Water Environment*.

For this example the upstream 90%ile quality for ammonia is 0.29mg/l:

Assuming the High/Good boundaries are 0.2 and 0.3mg/l, this means the existing upstream quality is in amber, i.e. between 20% and 3% of the class boundary. WAT-RM-21 says that in this case, we should model to determine if BAT discharge standards maintain the amber status.

A forward calculation can also be made to determine the impact of a discharge with BAT standard of 1mg/l as a 95%ile.

To keep a clear audit trail, the various spreadsheet output files should be saved to a folder.

Assuming this discharge quality is implemented with a resultant downstream quality on the tributary, further modelling can be undertaken to determine the impact on the main river by treating the tributary as a discharge.

Key References

Regulatory Methods & Supporting Guidance

- [WAT-FORM-19: CAR Licence Decision Record](#)
- [WAT-RM-03 Sewage Discharges to Surface Waters](#)
- [WAT-RM-21: No Deterioration and Allocation of Capacity](#)
- [WAT-SG-02: Modelling Continuous Discharges to Rivers](#)
- [WAT-SG-13: Municipal Sewage Treatment Works \(STW\)](#)
- [WAT-SG-53: Environmental Quality Standards and Standards for Discharges to Surface Waters](#)

Tools

- [Environmental and Spatial Informatics Unit](#) (SEPA Intranet page)
- RQP (River Quality Planning) Monte Carlo software (contact IS to have this available)
- [Spotfire DAVE Chemistry](#)
- [Spotfire Source Apportionment GIS](#) SAGIS, (SEPA Intranet page)
- [Two-tier Multiplier Tables](#) (ex-WAT-SG-77) (SEPA Intranet page)

- End of Document -