GUMLEAF

Generator for Uncertainty Measures and Load Estimates using Alternative Formulae

User Guide and Reference Manual

Version 0.1 (alpha)

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Acknowledgements

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David - need help here!

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1 Introduction

1.1 The user guide/reference manual

1.1.1 Purpose

This user guide/reference manual is designed to provide all information required by GUMLEAF users, and references to technical reports and published literature where appropriate. In general, the accuracy and precision of annual load estimates will improve with good (both quantity and quality) input data as well as correct choice of estimation methods appropriate to the catchment being analysed. Users should make their own judgement in interpreting the model results. Experience and knowledge of pollutant generation and delivery processes and understanding of the advantages and limitations of various load estimation methods are valuable aids to interpreting results.

1.1.2 Structure

The user guide/reference manual comprises the following chapters:

- Chapter 1 introduces GUMLEAF and provides information on how to load the software.
- Chapter 2 presents the motivation and concept behind the development of GUMLEAF, and describes the load estimation methods used and the uncertainty measures implemented.
- Chapter 3 is a tutorial for using GUMLEAF, from starting a project, preparing input data and parameters, to running the modules/macros for estimating annual loads and uncertainties, simulating annual loads based on user-assigned prior probability for method selection, visualising outputs and interpreting results.
- Chapter 4 contains future research and development plan for an integrated modelling framework for assessing loads, uncertainties and optimum sampling protocol in rivers and waterways.
- Chapter 5 support this user guide and reference manual by listing references, providing associated technical reports and illustrating a sample data file format/worksheet template.

1.1.3 Overview

GUMLEAF is a Generator for Uncertainty Measures and Load Estimates using Alternative Formulae. It is a simple software for computation of annual pollutant loads (incorporating stochastic and knowledge uncertainties) and visualisation of input data and results. This version 0.1 (alpha) is coded in Microsoft® Excel VBA and is developed for in-house use only.

Basic input data required are the dates, daily flows (usually continuous) and sample concentrations (usually sparse, e.g. fortnightly), and some parameters/information about the site/data. A worksheet template "WORK" is provided. It is recommended that this template be copied/saved into a separate workbook for each site/pollutant, then input data/parameters and run modules/macros with the worksheet as the ACTIVE SHEET).

Main outputs are summary tables of annual load estimates and standard deviations, and visualisation (time series, box and whisker and histogram plots) for easy interpretation of results.

1.1.4 Features

GUMLEAF has the following functions/capabilities:

- Estimate annual loads and standard deviations (stochastic uncertainties) based on 22 load estimation methods, using daily flows (usually continuous) and sample concentrations (usually sparse, e.g. fortnightly) as inputs.

- Simulate annual loads (with uncertainties) based on the annual loads and stochastic uncertainties computed for all or part of the 22 methods. The users can assign different prior probability for each method based on their judgement (knowledge, experience, belief).

- Provide a simple table of summary statistics on the input flow and concentration data for each year.

- Produce a table of estimated loads, standard deviations and percentages of the coefficient of variation (i.e. standard deviation/mean) for each of the 22 methods for each year.

- Produce concurrent time series plots of the input daily flows and sampled concentrations.

- Produces scatter plots of ln(flow)–ln(concentration) relationship and TSS–turbidity relationship.

- Produce box and whisker plots of estimated annual loads (with standard deviations) by method.

- Produce annual time series of box and whisker plots of historical annual flows (with flow percentiles).

- Produce annual time series of box and whisker plots of the simulated annual loads (with load percentiles) based on the user-assigned prior probability for each method.

- Produces histogram plots of simulated annual loads for each year based on the user-assigned prior probability for each method.

- Produces histogram plots ln(flow) and ln(concentration).

1.1.5 Limitations

GUMLEAF is a prototype (alpha version) of an annual load estimation and visualisation tool. It is currently being applied and tested on limited number of rivers and waterways (e.g., rivers in Queensland coastal catchments, drains in the Shepparton Irrigation Region in the Goulburn-Murray catchment, and drains in the Macalister Irrigation District in West Gippsland). Further testing is required to ensure that the software is operating properly.

1.2 Data requirements

1.2.1 Input data

GUMLEAF allows any common text file data format that is compatible with (i.e., can be copied and pasted onto) Microsoft® Excel worksheet.

The input data should have the following format and sequence:

- Column 1 (or A) – dates formatted as 'DD/MM/YYYY' in daily time step. Dates must start on 01/01/YYYY for the starting year and must end on 31/12/YYYY for the ending year;

- Column 2 (or B) – daily flows in consistent units (e.g. Ml/day, m3/s). Zero flows are acceptable if legitimate, but gaps in daily flows should be left as empty cells;

- Column 3 (or C) – sampled concentration (e.g. TSS, TN or TP) in consistent units (e.g. mg/l) corresponding to the measurement date. Gaps in concentration data should be left as empty cells.

- Column 4 (or D) – Optional (used for investigating TSS-turbidity relationship). Measured turbidity in consistent units (e.g. NTU) corresponding to the measurement date. Gaps in turbidity data should be left as empty cells.

The basic time unit of GUMLEAF is daily, however it is anticipated that sub-daily data will be handled in the future (see Chapter 1).

Ideally, the input daily flow time series data are gap free, that is, there must be no empty cells if viewed in a worksheet. Users may decide to infill gaps in the input daily flow data using a third party software or other pre-processing tools (i.e. either by mathematical/interpolation technique, or hydrologic modelling). However, if flow gaps do exist, the pollutant loads within a duration (e.g., in a year, season or flow regime) will still be computed based on available daily flows within that duration, and the computed load will simply be scaled up by a time-based ratio (i.e., total number of days divided by number of non-gap days).

The input sampled concentration time series data is expected to contain gaps (and this is essentially the reason why various load estimation methods are assessed and the appropriate method(s) selected). In general the input concentration data comprise the measured instantaneous concentrations (assumed to be representative concentration for the day). If more than one measured instantaneous concentrations are available on a single day, an average concentration value may be used for that day.

GUMLEAF can handle any length of input data from 1 year (to be meaningful for annual load estimation) to 87 years (since Microsoft® Excel can only handle chart plotting of up to 32,000 points in a single time series).

1.2.2 Predicted or calculated data

Outputs from GUMLEAF are presented in both tables and charts (in Microsoft® Excel worksheet) for easy interpretation (see Section 1.1.4). The input and output can be saved as a single workbook for archiving and future reference.

1.3 Software components

GUMLEAFv0.1(alpha) contains the following five modules:

M1_LOAD – Computes annual loads and standard deviations (stochastic uncertainties) of annual loads.

M2_MCSimLOAD – Simulates annual loads via Monte-Carlo technique based on knowledge (method) uncertainty and stochastic (natural) uncertainty. User may assign different prior probability (weight) for each method based on their judgement (knowledge, experience, belief).

M3_XYPLOT – Generate time series plots of concurrent input daily flows and sampled concentration, and scatter plot of ln(flow)–ln(concentration). Scatter plot of TSS-turbidity is optional.

M4_BOXPLOT – Generate box and whisker plots of estimated annual loads by method (one plot for each year), and annual time series of box and whisker plots of simulated annual loads and historical annual flows (one plot each for loads and flows).

M5_HISTOPLOT – Generate histogram plots of simulated annual loads for each year based on the user-assigned prior probability for each method, and histogram plots of ln(flow) and ln(concentration).

1.4 References and training

GUMLEAF is an in-house tool developed by the Australian Centre for Environmentrics (ACE), University of Melbourne. GUMLEAF can be referenced as:

Tan, K. S., Etchells, T., and Fox, D. R. (2005). User Guide and Reference Manual for GUMLEAF v0.1alpha: Generator for Uncertainty Measures and Load Estimates using Alternative Formulae, Australian Centre for Environmentric, Univ. of Melbourne, June 2005.

Since this is an in-house tool developed to assist in data analysis, visualisation and interpretation for a number of research and consultancy projects undertaken by the ACE, there is no plan to conduct training workshop.

1.5 Installation

1.5.1 Technical specification

Table 1.1: Minimum system requirements

Processor	133 MHz Intel Pentium
Operating System	Windows XP, 2000, ME, 98, NT
Memory	128 MB RAM. 256 MB recommended
Hard Disk	10 MB of hard disk space required (depending on years of input data to be analysed)
Display	1024 x 768 or higher-resolution display with 256 colours
Input Device	Microsoft mouse or compatible pointing device
Other supporting software	Microsoft® Office Excel 2000 or 2003. 2003 recommended (adjust macro security level to medium or below) Microsoft® Visual Basic for Application (VBA) 6.0 or above Microsoft® Office Excel Add-Ins: Analysis ToolPak, Analysis ToolPak–VBA

1.5.2 Distribution

This GUMLEAF v0.1alpha is an in-house tool and is not to be distributed outside the ACE. However, stake holders and collaborators associated with ACE can request for a copy of the software for their evaluation only. Prior written permission and due reference are required if GUMLEAF were to be used in any project/studies not involving the ACE. The authors/ACE/University of Melbourne shall not be liable for all consequences arising from the direct and/or indirect use of GUMLEAF.

1.5.3 Starting and Closing GUMLEAF

It is recommended that user copy the Microsoft® Excel workbook/file GUMLEAF_Ver0_1.xls to the folder C:\GUMLEAF_Ver0_1\, and store all the workbooks for each project in appropriate sub-folders.

After copying the Microsoft® Excel workbook/file GUMLEAF_Ver0_1.xls to your PC/directory, double click the file (and 'Enable Macros' if asked) will open the workbook and upload the GUMLEAF 0.1 toolbar comprising five icons. Clicking on the icons will invoke the respective modules/macros embedded in the VBA codes. The GUMLEAF 0.1 toolbar will be made invisible upon closing the Microsoft® Excel workbook/file GUMLEAF_Ver0_1.xls.

The Microsoft® Excel workbook/file GUMLEAF_Ver0_1.xls contains the two worksheet: a front page worksheet 'GUMLEAF' (Figure 1.1) describing the software, and a template worksheet 'WORK' (Figure 1.2) to be copied and pasted into a new workbook and renamed accordingly for carrying out analysis for each pollutant-site.

To uninstall GUMLEAF, simply delete the file GUMLEAF_Ver0_1.xls from your PC/directory.

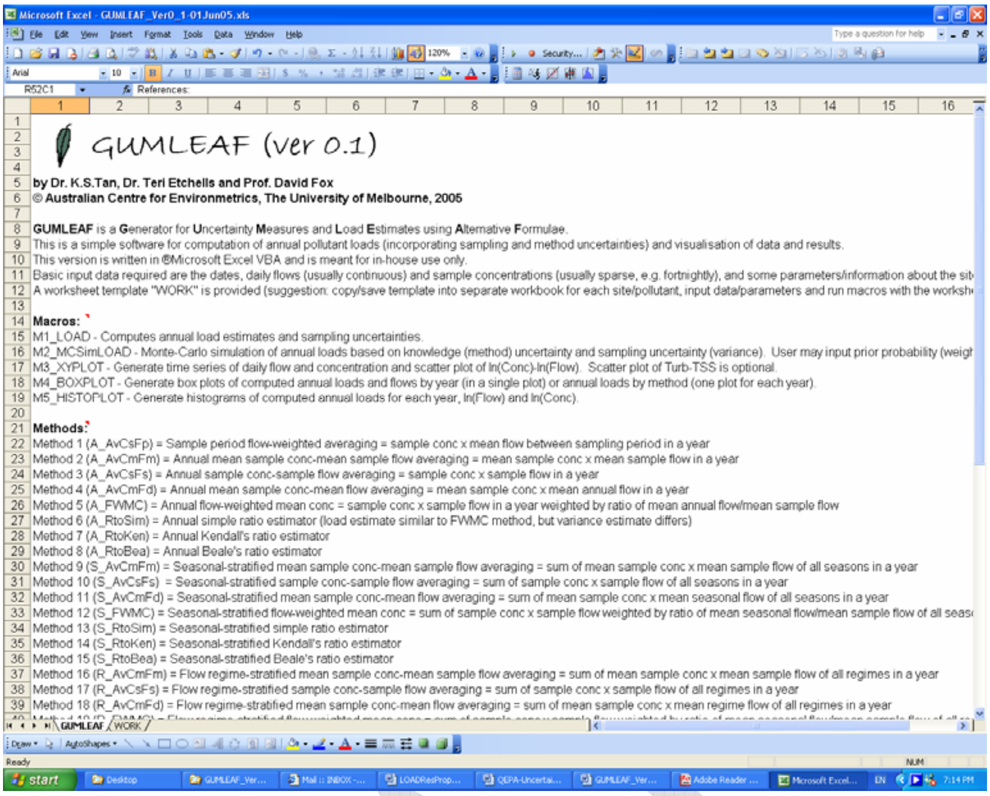

Figure 1.1: Example of GUMLEAF front page window

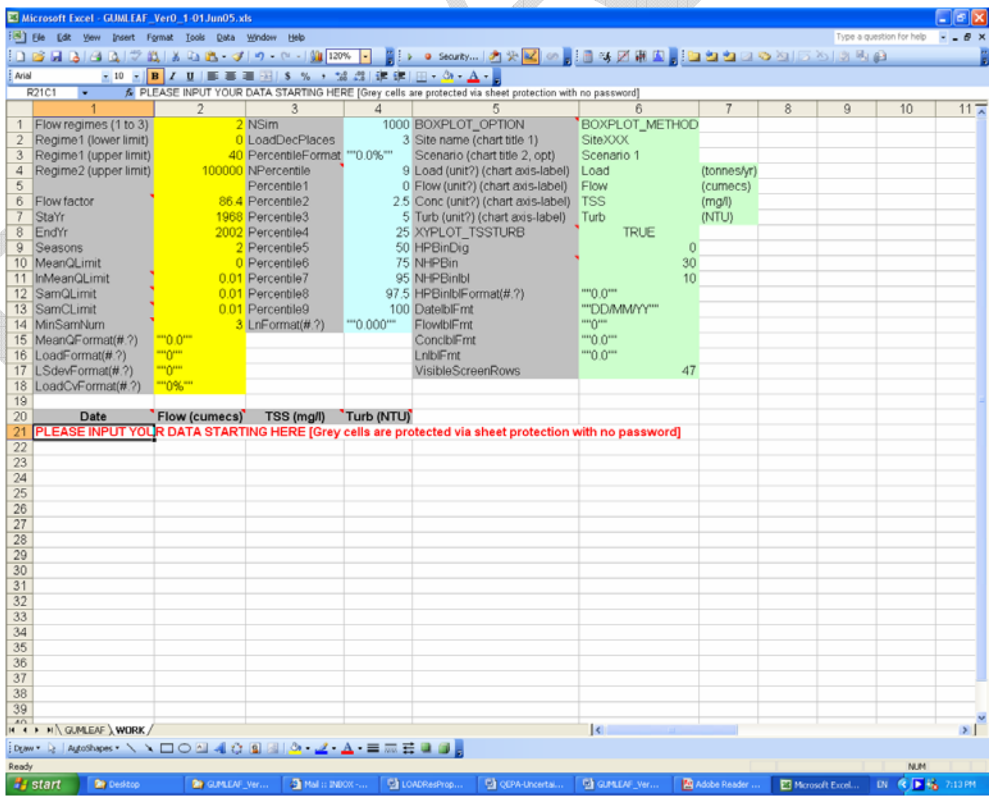

Figure 1.2: Example of GUMLEAF template worksheet

2 GUMLEAF Overview

2.1 Concepts and model structure

The estimation of pollutant loads, including sediments (e.g., total suspended sediment, TSS) and nutrients (e.g., total nitrogen, TN and total phosphorous, TP) from in rivers and waterways is an important aspect in natural resources management. Reliable estimation of pollutant loads is a challenging task since, hydrologically, river and irrigation systems operates (and flow data are measured) at daily or sub-daily time scale, but water quality (WQ) sampling data is relatively sparse (e.g. fortnightly or monthly). The sparse nature of the WQ data means the uncertainty in load estimates is potentially significant and should be considered in any analysis of pollutant loads.

Estimation of pollutant loads in rivers and waterways is predominantly based on daily flow data and sparse (typically monthly and sometimes fortnightly) WQ concentration data. Whilst fortnightly to monthly WQ sampling is not unusual (given the high cost of sampling), this relative scarcity of data creates significant uncertainties in load estimates and also presents major limitations in quantifying the error of load estimates.

There is a large body of research investigating load estimation techniques, however, little attention has been given to the quantum of uncertainty surrounding the estimated loads. Since the true load is not known. The selection of estimation technique is a key source of uncertainty (referred to as knowledge or method uncertainty). Additionally, significant variability is usually observed in the measured concentration and flow data (stochastic or natural uncertainty), and there can be random or systematic errors in the data collected (measurement or sampling uncertainty).

GUMLEAF presents a framework for quantifying the uncertainty in pollutant load estimates based on Monte-Carlo simulation, by considering the knowledge and stochastic uncertainties. However, since no information is available regarding measurement uncertainty, this source of uncertainty will not be considered in the load estimates.

The quantification of uncertainty presented in GUMLEAF is focussed on the use of historical data, and provides a range of load estimates which could have occurred. Future research will focus on the design of optimum sampling protocols to reduce the uncertainty present in load estimates, and the consideration of uncertainty in setting and assessing compliance with load-based targets (see Section 4.1 for more on future research).

The basic model structure/components of GUMLEAFv0.1alpha is already presented in Section 1.3.

2.2 Annual load estimation in rivers and waterways

2.2.1 Overview

As highlighted in Fox (2004), the problem of obtaining 'representative' load is difficult since WQ sampling data is sparse relative to the estimation of continuous flow-concentration flux. There are many potential approximation techniques with varying level of performance with regard to accuracy and precision. Three main types of estimation techniques: (i) interpolation techniques (ii) regression or rating curve techniques, and (iii) Averaging or ratio techniques, along with their relative advantages and limitations, are briefly discussed in Etchells et al. (2005) and Tan et al. (2005).

Many reviews of techniques for load estimation have been undertaken (e.g., Cohn et al., 1989; Degens and Donohue, 2002; Letcher et al., 2002; Littlewood, 1992; Mukhopadhyay and Smith, 2000; Preston et al., 1989). Unfortunately, these studies have usually concluded that there is no single method which provides universally accurate and precise estimates. However, these reviews have typically been limited to specific datasets and situations, and usually, presented no link between the characteristics of the sampling regime employed and the load estimation technique used. Consequently, no generalised framework has previously been developed linking the types of estimation technique results to the type of sampling regime.

Sampling and catchment behaviour should inform the choice of load estimation technique. In particular, the choice of technique should consider the regularity of sampling, the alignment of sampling effort with flow regime, and the variability of concentrations in relation to time or flow.

2.2.2 Flow regime and seasonal stratification

WQ sampling regimes in rivers and waterways are typically irregular and sparse, and have not been designed specifically to capture a 'proportionate' share of high-flow events (note that proportionality here refers to both the duration and variability of flows, see Fox, 2004 and Figure 2.1). These events have a very large impact on overall loads since the concentration during those events is multiplied by large volumes, and also, the variation in the high-flow concentration tends to be significantly higher than that in the low-flow periods.

In general, for sites with limited high flow samples, methods that do not account for flow stratification will be downwardly biased. Likewise, for sites with high seasonal concentration variation (e.g., irrigation areas), methods that do not account for time stratification will lead to imprecise and biased results.

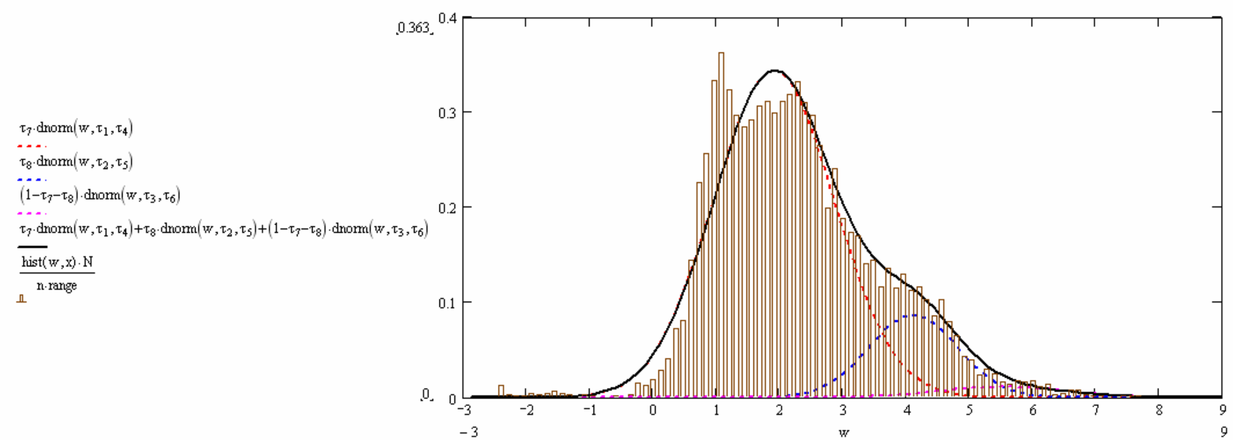

Figure 2.1: Example of flow regime comprising a mixture of log-normal distribution of base flow (red dotted), wet flow (blue dotted) and storm flow (pink dotted)

2.2.3 Typology of load estimation

Based on the above mentioned reviews and research, and overlaying the types of sampling regimes seen in practice, a simplified summary of appropriate (typology of) load estimation techniques is presented in Table 2.1. This matrix provides broad guidance on the categories of techniques to be considered, however, there are many specific variations of these techniques. Additionally, guidance on the sampling regime should be adjusted depending on the characteristics of the catchment and climate in question. The accuracy and precision in annual load estimates in rivers and waterways is an integrated process depending on the estimation techniques, sampling regimes, catchment characteristics and climate variability, and GUMLEAF is an analysis and visualisation tool that provides the first step towards the establishment of such an integrated framework based on the concept of load typology, which will ultimately lead to the establishment of optimum sampling protocols under different catchments and climate conditions.

Table 2.1: Typology of load estimation

Relationship between flow and concentration	Sampling Regime			
	Sparse sampling (monthly or less frequent)	Regular sampling (e.g. weekly, fortnightly)		Continuous sampling (e.g. daily, near daily)
		Limited event data	Representative event data	
No significant relationship present	Averaging or Ratio	Averaging or Ratio • Seasonal-stratified	Averaging or Ratio • Seasonal-stratified • Flow regime-stratified	Linear interpolation
Significant relationship present (and if time series of daily loads are needed as inputs to other models)	Regression	Regression or Averaging or Ratio • Seasonal-stratified	Averaging or Ratio • Seasonal-stratified • Flow regime-stratified	Linear interpolation

The typology presented in Table 2.1 has been constructed by excluding techniques that are not valid for particular sampling regimes and catchment characteristics, i.e., based on the principal of exclusion. Specifically, the typology reflects two premises: firstly, that regression techniques cannot be used unless a significant relationship can be demonstrated between water quality and some other variables such as flow (and if time series of daily loads are needed as inputs to other models such as bio-geochemical models), and secondly, that the interpolation techniques are not valid unless the water quality samples are almost continuous.

Based on these observations and in reference to Table 2.1, it is reasonable to focus on averaging or ratio methods to estimate annual loads. GUMLEAFv0.1alpha includes a variety of 22 annual load estimation methods (Table 2.2) and the associated stochastic uncertainties (see Section 2.3.2), comprising:

- Methods (1 to 8) that use annual data – eight basic averaging or ratio methods using annual data (which have been adapted from the references provided above);

- Methods (9 to 15) that use seasonal-stratified data – seven variations of the basic methods that use annual data (Methods 2 to 8) but consider seasonal stratification in each year; and

- Methods (16 to 22) that use flow regime-stratified data – seven variations of the basic methods that use annual data (Methods 2 to 8) but consider flow regime stratification in each year.

Note the duality between simple mean-based load (i.e. flow-weighted mean concentration) estimators (Method 5, 12, 19) and simple ratio estimators (Method 6, 13, 20), which has been pointed out in Fox (2005b), but some what confusingly considered as two different methods in most of the literature on load estimation. GUMLEAF has included both Method 5 and Method 6 (and also their variations for seasonal and flow regime stratification) because here, the variances in each of them are estimated based on different assumptions (see Section 2.3.2).

It is important to note that no sampling technique can overcome information deficiencies from a sampling regime where disproportionately few samples are taken in high flow events. There is an inherent assumption in the averaging or ratio methods, that sampling is representative of the general conditions. In practice, determining the pollutant concentration deriving from high flow events is particularly important since a large proportion of load is usually resulted from these events (due to the relatively large flow volume, and frequently, higher than average concentrations).

Table 2.2: Load estimation methods used

Group	Method	Short name	Description	Load equation	Reference	Variance equation	Reference
Annual	1	A_ AvCsFp	Sample period flow-weighted averaging	$k\sum_{i=1}^{n}\left(c_i \times \sum_{p=1}^{N_{Pi}} q_{Pi}\right) = k\sum_{i=1}^{n}\left(c_i \times Q_{Pi}\right)$	Walling & Webb (1981); Method 3 (Littlewood 1992); Method 5 (Letcher et al. 1999)	$\frac{(kN)^2\left(\sum_{i=1}^{n} Q_{Pi}{}^2\right)}{n\left(\sum_{i=1}^{n} Q_{Pi}\right)^2} Var[L]$	Derived based on Fox (2005b)[1]
	2	A_ AvCmFm	Annual mean sample conc-mean sample flow averaging	$kN\left(\sum_{i=1}^{n}\frac{c_i}{n} \times \sum_{i=1}^{n}\frac{q_i}{n}\right) = kN\bar{c}\bar{q}$	Walling & Webb (1981); Method 1 (Littlewood 1992); Method 1 (Letcher et al. 1999)	$\left(\frac{kN}{n}\right)^2 Var[L]$	Fox (2005b)[1]
	3	A_ AvCsFs	Annual sample conc-sample flow averaging	$kN\left(\sum_{i=1}^{n}\frac{c_i \times q_i}{n}\right) = kN\bar{l}$	Walling & Webb (1981); Method 2 (Littlewood 1992); Method 2 (Letcher et al. 1999)	$\frac{(kN)^2\left(\sum_{i=1}^{n} q_i{}^2\right)}{n\left(\sum_{i=1}^{n} q_i\right)^2} Var[L]$	Fox (2005b)[1]
	4	A_ AvCmFd	Annual mean sample conc-mean flow averaging	$k\left(\sum_{i=1}^{n}\frac{c_i}{n}\right)\left(\sum_{j=1}^{N} q_j\right) = k\bar{c}Q$	Walling & Webb (1981); Method 4 (Littlewood 1992); Method 3 (Letcher et al. 1999)	$\frac{kN}{n} Var[L]$	Derived based on Fox (2005b)[1]
	5	A_ FWMC	Annual flow-weighted mean conc	$k\left(\sum_{i=1}^{n}\left(c_i \times q_i\right)\right)\left(\frac{\sum_{j=1}^{N} q_j}{\sum_{i=1}^{n} q_i}\right) = k\bar{l}\frac{Q}{\bar{q}} = k\hat{R}Q$	Walling & Webb (1981); Method 5 (Littlewood 1992); Method 4 (Letcher et al. 1999)	$\frac{kN\left(\sum_{i=1}^{n} q_i{}^2\right)}{\left(\sum_{i=1}^{n} q_i\right)^2} Var[L]$	Fox (2005b)[1]
	6	A_ RtoSim	Annual simple ratio estimator (load estimate similar to FWMC method, but variance estimate differs)	$k\left(\frac{\sum_{i=1}^{n}\frac{c_i \times q_i}{n}}{\sum_{i=1}^{n}\frac{q_i}{n}}\right)\left(\sum_{j=1}^{N} q_j\right) = k\frac{\bar{l}}{\bar{q}}Q = k\hat{R}Q$	Cochran (1977); Eqn(5) Cooper & Watts (2002); Table 2 Method 1 (Preston 1989); Method 15 (Letcher et al. 1999)	$(kN)^2\left(\frac{1-\frac{n}{N}}{n(n-1)}\right)\left(\sum_{i=1}^{n}\left(l_i - \hat{R}q_i\right)^2\right)$	Eqn(6.9) Cochran (1977)

	7	A_ RtoKen	Annual Kendall's ratio estimator	$k\left[\left(\frac{N-1}{n-1}\right)\left(\bar{l}-\bar{c}\bar{q}\right)\right]\hat{R}Q$	Eqn(6, 7) Cooper & Watts (2002)	$\left(\frac{k\hat{R}Q}{n}\right)^2\left(\frac{Var[l]}{\bar{l}^2}+\frac{Var[q]}{\bar{q}^2}-\frac{2Cov[lq]}{\bar{l}\bar{q}}\right)$	Eqn(9) Cooper & Watts (2002)
	8	A_ RtoBea	Annual Beale's ratio estimator	$k\left[\frac{1+\left(\frac{1}{n}-\frac{1}{N}\right)\left(\frac{S_{lq}}{\bar{l}\bar{q}}\right)}{1+\left(\frac{1}{n}-\frac{1}{N}\right)\left(\frac{S_q^{\,2}}{\bar{q}^2}\right)}\right]\hat{R}Q$	Beale (1962); Eqn(10) Cooper & Watts (2002); Table 2 Method 5 (Preston 1989); Method 20 (Letcher et al. 1999), Eqn(4, 5) Mukhopadhyay & Smith (2000)[3]	$\left(k\hat{R}Q\right)^2 Var[\tau]$	Cooper & Watts (2002)[2]
Seasonal-stratified	9	S_ AvCmFm	Seasonal-stratified mean sample conc-mean sample flow averaging	$\sum_{S=1}^{T_S}\left[kN_S\left(\sum_{i=1}^{n_S}\frac{c_i}{n_S}\times\sum_{i=1}^{n_S}\frac{q_i}{n_S}\right)\right]$ $=\sum_{S=1}^{T_S}\left(kN_S\bar{c}_s\bar{q}_s\right)$	Dolan et al (1981); Table 1 Method 2 (Preston 1989); Method 10 (Letcher et al. 1999)	$\sum_{S=1}^{T_S}\left[\left(\frac{kN_s}{n_S}\right)^2 Var[L_S]\right]$	Fox (2005b)[1]
	10	S_ AvCsFs	Seasonal-stratified sample conc-sample flow averaging	$\sum_{S=1}^{T_S}\left(kN_S\bar{l}_S\right)$	Seasonal form of Verhoff et al. (1980); Table 1 Method 6 (Preston 1989); Method 14 (Letcher et al. 1999)	$\sum_{S=1}^{T_S}\left[\frac{(kN_s)^2\left(\sum_{i=1}^{n_S}q_i^{\,2}\right)}{n_S\left(\sum_{i=1}^{n_S}q_i\right)^2}Var[L_S]\right]$	Fox (2005b)[1]
	11	S_ AvCmFd	Seasonal-stratified mean sample conc-mean flow averaging	$\sum_{S=1}^{T_S}\left(k\bar{c}_SQ_S\right)$	Ferguson (1987); Table 1 Method 5 (Preston 1989); Method 13 (Letcher et al. 1999)	$\sum_{S=1}^{T_S}\left[\frac{kN_s}{n_S}Var[L_S]\right]$	Derived based on Fox (2005b)[1]
	12	S_ FWMC	Seasonal-stratified flow-weighted mean conc	$\sum_{S=1}^{T_S}\left(k\hat{R}_SQ_S\right)$	Seasonal form of Walling & Webb (1981); Method 5 (Littlewood 1992); Method 4 (Letcher et al. 1999)	$\sum_{S=1}^{T_S}\left[\frac{kN_S\left(\sum_{i=1}^{n_S}q_i^{\,2}\right)}{\left(\sum_{i=1}^{n_S}q_i\right)^2}Var[L_S]\right]$	Fox (2005b)[1]

	13	S_ RtoSim	Seasonal-stratified simple ratio estimator	$\sum_{S=1}^{T_S}\left(k\hat{R}_S Q_S\right)$	Seasonal form of Cochran (1977); Table 2 Method 1 (Preston 1989); Method 15 (Letcher et al. 1999)	$\sum_{S=1}^{T_S}\left[(kN_s)^2\left(\frac{1-\frac{n_s}{N_s}}{n_s(n_s-1)}\right)\left(\sum_{i=1}^{n_s}\left(l_i-\hat{R}_s q_i\right)^2\right)\right]$	Cooper & Watts (2002)
	14	S_ RtoKen	Seasonal-stratified Kendall's ratio estimator	$\sum_{S=1}^{T_S}\left(k\left[\left(\frac{N_S-1}{n_S-1}\right)\left(\bar{l}_S-\bar{c}_S\bar{q}_S\right)\right]\hat{R}_S Q_S\right)$	Seasonal form of (Kendall et al., 1983)	$\sum_{S=1}^{T_S}\left[\left(\frac{k\hat{R}_S Q_S}{n_S}\right)^2\left(\frac{Var[l_S]}{\bar{l}_S^{\,2}}+\frac{Var[q_S]}{\bar{q}_S^{\,2}}-\frac{2Cov[lq]_S}{\bar{l}_S\bar{q}_S}\right)\right]$	Cooper & Watts (2002)
	15	S_ RtoBea	Seasonal-stratified Beale's ratio estimator	$\sum_{S=1}^{T_S}\left(k\left[\frac{1+\left(\frac{1}{n_S}-\frac{1}{N_S}\right)\left(\frac{[S_{lq}]_S}{\bar{l}_S\bar{q}_S}\right)}{1+\left(\frac{1}{n_S}-\frac{1}{N_S}\right)\left(\frac{[S_q]_S^{\,2}}{\bar{q}_S^{\,2}}\right)}\right]\hat{R}_S Q_S\right)$	Seasonal form of Beale (1962); Table 2 Method 5 (Preston 1989); Method 20 (Letcher et al. 1999)	$\sum_{S=1}^{T_S}\left[\left(k\hat{R}_s Q_s\right)^2 Var[\tau_s]\right]$	Cooper & Watts (2002)
Flow regime-stratified	16	R_ AvCmFm	Flow regime-stratified mean sample conc-mean sample flow averaging	$k\sum_{R=1}^{T_R}\left[N_R\left(\sum_{i=1}^{n_R}\frac{c_i}{n_R}\times\sum_{i=1}^{n_R}\frac{q_i}{n_R}\right)\right]$ $=k\sum_{R=1}^{T_R}\left(N_R\bar{c}_R\bar{q}_R\right)$	Flow regime form of Dolan et al (1981); Table 1 Method 2 (Preston 1989); Method 10 (Letcher et al. 1999)	$k^2\sum_{R=1}^{T_R}\left[\left(\frac{N_R}{n_R}\right)^2 Var[L_R]\right]$	Fox (2005b)[1]
	17	R_ AvCsFs	Flow regime-stratified sample conc-sample flow averaging	$k\sum_{R=1}^{T_R}\left(N_R\bar{l}_R\right)$	Verhoff et al. (1980); Table 1 Method 6 (Preston 1989); Method 14 (Letcher et al. 1999)	$k^2\sum_{R=1}^{T_R}\left[\frac{N_R^{\,2}\left(\sum_{i=1}^{n_R}q_i^{\,2}\right)}{n_R\left(\sum_{i=1}^{n_R}q_i\right)^2}Var[L_R]\right]$	Fox (2005b)[1]
	18	R_ AvCmFd	Flow regime-stratified mean sample conc-mean flow averaging	$k\sum_{R=1}^{T_R}\left(\bar{c}_R Q_R\right)$	Flow regime form of Ferguson (1987); Table 1 Method 5 (Preston 1989); Method 13 (Letcher et al. 1999)	$k\sum_{R=1}^{T_R}\left[\frac{N_R}{n_R}Var[L_R]\right]$	Derived based on Fox (2005b)[1]

	19	R_ FWMC	Flow regime-stratified flow-weighted mean conc	$k\sum_{R=1}^{T_R}\left(\hat{R}_R Q_R\right)$	Flow regime form of Walling & Webb (1981); Method 5 (Littlewood 1992); Method 4 (Letcher et al. 1999)	$k\sum_{R=1}^{T_R}\left[\frac{N_R\left(\sum_{i=1}^{n_R} q_i^2\right)}{\left(\sum_{i=1}^{n_R} q_i\right)^2} Var\left[L_R\right]\right]$	Fox (2005b)[1]
	20	R_ RtoSim	Flow regime-stratified simple ratio estimator	$k\sum_{R=1}^{T_R}\left(\hat{R}_R Q_R\right)$	Flow regime form of Cochran (1977); Table 2 Method 1 (Preston 1989); Method 15 (Letcher et al. 1999)	$k^2\sum_{R=1}^{T_R}\left[N_R^2\left(\frac{1-\frac{n_R}{N_R}}{n_R\left(n_R-1\right)}\right)\left(\sum_{i=1}^{n_R}\left(l_i-\hat{R}_R q_i\right)^2\right)\right]$	Cooper & Watts (2002)
	21	R_ RtoKen	Flow regime-stratified Kendall's ratio estimator	$k\sum_{R=1}^{T_R}\left(\left[\left(\frac{N_R-1}{n_R-1}\right)\left(\bar{l}_R-\bar{c}_R\bar{q}_R\right)\right]\hat{R}_R Q_R\right)$	Flow regime form of (Kendall et al., 1983)	$k^2\sum_{R=1}^{T_R}\left[\left(\frac{\hat{R}_R Q_R}{n_R}\right)^2\left(\frac{Var\left[l_R\right]}{\bar{l}_R^{2}}+\frac{Var\left[q_R\right]}{\bar{q}_R^{2}}-\frac{2Cov\left[lq\right]_R}{\bar{l}_R\bar{q}_R}\right)\right]$	Cooper & Watts (2002)
	22	R_ RtoBea	Flow regime-stratified Beale's ratio estimator	$k\sum_{S=1}^{T_S}\left(\left[\frac{1+\left(\frac{1}{n_R}-\frac{1}{N_R}\right)\left(\frac{\left[S_{lq}\right]_R}{\bar{l}_R\bar{q}_R}\right)}{1+\left(\frac{1}{n_R}-\frac{1}{N_R}\right)\left(\frac{\left[S_q\right]_R^2}{\bar{q}_R^{2}}\right)}\right]\hat{R}_R Q_R\right)$	Beale (1962); Table 2 Method 5 (Preston 1989); Method 20 (Letcher et al. 1999)	$k^2\sum_{R=1}^{T_R}\left[\left(\hat{R}_R Q_R\right)^2 Var\left[\tau_R\right]\right]$	Cooper & Watts (2002)

Notations:

n, n_S, n_R = number of sampled concentration days over a duration (year, season, flow regime)

N_{Pi} = number of measured flow days over period between mid of consecutive samples *i*

N, N_S, N_R = number of measured flow days over a duration (year, season, flow regime)

T_S, T_R = total number of strata (seasons, flow regimes) in a year

k = scaling factor to account for days in a duration (year or season or flow regime) with flow gaps (if any) by simple proportion

Q_{Pi} = total measured flow over period between mid of consecutive samples *i*

Q, Q_S, Q_R = total measured flow over a duration (year, season, flow regime)

c_i = sampled concentration

$\bar{c}, \bar{c}_S, \bar{c}_R$ = average sampled concentration over a duration (year, season, flow regime)

q_i = sampled flow

q_{Pi} = sampled flow over period between mid of consecutive samples *i*

$\bar{q}, \bar{q}_S, \bar{q}_R$ = average sampled flow over a duration (year, season, flow regime)

$\bar{l}, \bar{l}_S, \bar{l}_R$ = average load over a duration (year, season, flow regime)

$\hat{R} = \frac{\bar{l}}{\bar{q}}, \hat{R}_S = \frac{\bar{l}_S}{\bar{q}_S}, \hat{R}_R = \frac{\bar{l}_R}{\bar{q}_R}$ = load-flow ratio over a duration (year, season, flow regime)

Abbreviations:
Av = Averaging method, Rto = Ratio method,
Cs = Sample concentration, Cm = Mean sample concentration
Fs = Sample flow, Fm = Mean sample flow, Fp = Flow over period between mid of consecutive samples, Fd = Flow over specific duration (e.g., annual, season, flow regime)
FWMC = Flow-weighted mean concentration
Sim = Simple, Ken = Kendall, Bea = Beale

Notes:
[1] Variances for all averaging methods are based on bi-variate log-normal distribution of concentration and flow,
where $Var[L] = E[L^2] - (E[L])^2$, see Fox (2005b) for theoretical expressions of $E[L]$ and $E[L^2]$.

[2] Variance for Beale's ratio method is based on bi-variate normal distribution of load and flow,
see Appendix: Variance of the Beale Estimator in Cooper & Watts (2002) for theoretical expression of $Var[\tau]$.
[3] Modified variance and covariance for Beale's ratio method are based on bi-variate normal distribution of load and flow,
see Eqn(4, 5) Mukhopadhyay & Smith (2000) for theoretical expressions of S_{lq} and $S_q{}^2$.

2.3 Uncertainty measures

Figure 2.2 presents the three sources of uncertainties in load estimates.

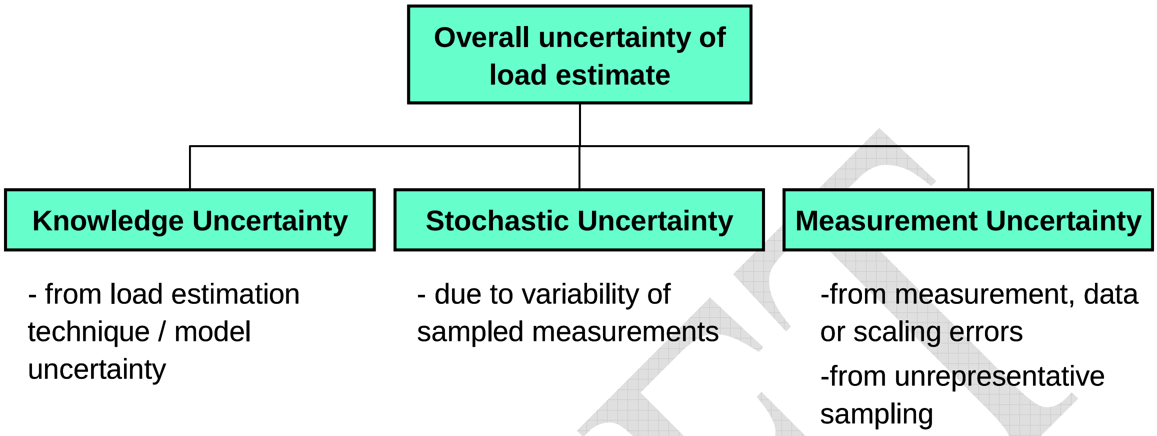

Figure 2.2: Sources of uncertainty in load estimates

2.3.1 Knowledge (method) uncertainty

The estimated annual loads in the example plot given in Figure 3.3 show significant variation for different estimation techniques. Unless other overriding factors are considered to be relevant, all of these are equally legitimate as estimates of the 'true' load. However, the 'true' load is not known, and therefore, the selection of estimation technique is one source of uncertainty in load estimation. This source of uncertainty can be called 'knowledge' uncertainty, since it is not known which method (if any) could result in the 'true' load.

Knowledge uncertainty can be reduced through an increased understanding of the pollutant wash-off and transport processes. In general, for sites with limited high flow samples, methods that do not account for flow stratification will be downwardly biased. Likewise, for sites with high seasonal concentration variation (e.g., irrigation areas), methods that do not account for time stratification will lead to imprecise and biased results. Such knowledge uncertainty can be incorporated by the specification of user-assigned prior probabilities (weights) reflecting the user's judgement (knowledge/experience/belief) in each of the methods.

2.3.2 Stochastic (natural) uncertainty

In addition to knowledge uncertainty, stochastic uncertainty also needs to be considered. There is considerable inherent variability in the data used to estimate loads and the standard deviation of loads estimates provides a measure of stochastic uncertainty. Furthermore, the variance of sampled concentrations can become significantly greater when they are adjusted to correspond to population variances. The standard deviations used in the analysis are presented in Figure 3.3. The standard deviations (and variances) of the averaging methods (Methods 1 to 5) and their seasonal-stratified (Methods 9 to 12) and flow regime-stratified (Methods 16 to 19) variations are based on the assumption of bi-variate log-normal (BVLN) distribution in flow and concentration data (see Fox, 2005b), while those of the ratio methods (Methods 6 to 8) and their seasonal-stratified (Methods 13 to 15) and flow regime-stratified (Methods 20 to 22) variations are based on the assumption of bi-variate normal (BVN) distribution in load and flow (see Cooper and Watts, 2002). Figure 3.5 shows the example histogram plots of ln(flow) and ln(concentration), suggesting BVLN distribution in flow and concentration data. The visualisation will assist user in ensuring that these assumptions are consistently valid.

2.3.3 Measurement (sampling) uncertainty

Finally, a third source of uncertainty needs to be considered arising from errors in the measurement, scaling or application of data. Errors could potentially arise from drift or mis-calibration in equipment, infilling missing data, poor sampling techniques or inaccurate scaling assumptions. Additionally, data and sampling uncertainty will arise from unrepresentative sampling, for instance, where few high-flow samples are available. However, since no information is known about the magnitude of these errors, they will not be considered for the purposes of this analysis.

2.4 Monte-Carlo simulation of loads

The procedure used to quantify uncertainty is based on a Monte Carlo simulation (e.g. 1000 repetitions) where the knowledge uncertainty and stochastic uncertainty are considered.

For each load estimate in the simulation, the knowledge uncertainty is first reflected in which one method (from the 22 possible methods) is randomly selected (each method is given an equal probability of being selected, or user-assigned prior probabilities (weights) reflecting the user's judgement (knowledge/experience/belief) in each method, hence providing a particular mean and variance of that method for consideration. Next, stochastic uncertainty is considered by assuming the load is normally distributed around the mean, and a load estimate is simulated by generating a random normal variate with the mean and variance of the selected method.

The steps for simulating annual load estimates (incorporating knowledge and stochastic uncertainties) for each year and each pollutant-site are:

1. Generate a uniform random number between 0 and 1. If it is less than or equal to the normalised cumulative weight of a particular method of load estimation, that method will be selected.

2. Generate another uniform random number between 0 and 1, and simulate an annual load by assuming normal distribution using the mean (μ) and standard deviation (σ) of the load of the method selected in (1) above.

3. Repeat the process for the number of simulation desired by the user (e.g., 1000 repetitions).

3 Using GUMLEAF

3.1 Getting started

Double click on the Microsoft® Excel workbook/file GUMLEAF_Ver0_1.xls in your PC/directory and click on 'Enable Macros'. The workbook GUMLEAF is now opened and the GUMLEAF 0.1 toolbar uploaded.

3.2 Preparing a project/scenario

3.2.1 Starting a new project/scenario

Before running the modules/macros in GUMLEAF, the user must first prepare separate worksheet for each pollutant-site. User may also choose to store worksheets for different pollutants (e.g. TSS, TN and TP) of the same site in the same workbook.

On the opened Microsoft® Excel workbook/file GUMLEAF_Ver0_1.xls, right click on the tab of the template worksheet named 'WORK' (Figure 1.2), select 'Move or Copy', then click on the drop down menu 'Move selected sheets' 'To book' and select '(new book)'. Click on the check box 'Create a copy' and then click 'OK'. A new workbook with worksheet named 'WORK' is now created. Save this new workbook using an appropriate file name. The new workbook is now ready for inputing data and specifying parameters for analysing the pollutant-site of interest.

3.2.2 Assigning inputs

Input the time series data (date, flow and concentration) in the format and sequence as described in Section 1.2.1.

3.2.3 Specifying information/parameters

Specify the basic information and parameters about the pollutant-site being analysed. In general, the parameters in worksheet column 2 (or B, yellow cells) are related to module/macro M1_LOAD, column 4 (or D, blue cells) are related to module/macro M2_MCSimLOAD, and column 6 (or F, green cells) are related to module/macro M3_XYPLOT, M4_BOXPLOT and M5_HISTOPLOT, although some of these information/parameters may also be used across different modules/macros.

These information/parameters can be classified into two types, those required for computation, and those required for labelling and formatting output tables and charts. Description and guidance for some of the parameters required for computation are given in the comment boxes. The comment box will appear when the mouse pointer is placed over those cells with little red triangle on the top right corner. Not all parameter cells have comment boxes and those without are usually self-explanatory. Contents in the grey cells are protected. To unprotect the template worksheet 'WORK' (if necessary), select 'Tools' from the Microsoft Excel drop down menu, click on 'Protection' and 'Unprotect Sheet'. To protect the template worksheet 'WORK', select 'Tools' from the Microsoft Excel drop down menu again, click on 'Protection', 'Protect Sheet' and 'OK' (without password).

3.3 User interface/macro icons

Once the input data and parameters are prepared and checked, analysis may begin. The worksheet name 'WORK' must always be the ACTIVE SHEET, and GUMLEAF must be run sequentially (M1 to M5) using the five modules/macros in order to work properly. For example, to run the module/macro M1_LOAD, click on the first icon on the GUMLEAF 0.1 toolbar on top of the Microsoft® Excel window. The other icons are for M2_MCSimLOAD, for M3_XYPLOT, for M4_BOXPLOT, and for M5_HISTOPLOT.

Several simple error trapping routines are embedded in some of the modules/macros and user may be prompted from time to time while running the modules/macros. Depending on the PC capacity and input data file size, each macro usually takes a few seconds to a minute to run. A pop up message box will appear notifying that a module/macro is completed.

3.4 Running a project/scenario

3.4.1 Load Estimation Module (M1_LOAD)

M1_LOAD – Computes annual loads and standard deviations (stochastic uncertainties) of annual loads. Upon completion of this module/macro, four summary tables will be generated: across the worksheet from left to right: starting with a table of input data statistics, a table of estimated annual load, a table of estimated standard deviations of annual load, and a table of coefficient of variation (%) of annual load for each year (row) and each method (column).

3.4.2 Monte-Carlo Simulation Module (M2_MCSimLOAD)

M2_MCSimLOAD – Simulates annual loads via Monte-Carlo technique based on knowledge (method) uncertainty and stochastic (natural) uncertainty. User may assign different prior probability (weight) for each method based on their judgement (knowledge, experience, belief). Normally, probabilities (weights) ranging from 0 to 1.0 may be used, but other range are also acceptable, since these are these values are in fact 'relative' weights, and zero weight means a method is rendered inoperative. The weight corresponding to each estimation method is input in the blue coloured cells (Row 2) above the output summary table of estimated annual loads after running M1_LOAD.

3.5 Visualising inputs and outputs

Visualisation is one of the important features of GUMLEAF. A few simple plots can be very useful and informative for viewing and checking the data being analysed, as well as for easy interpretation of the results.

GUMLEAF provides the median as the measure of central tendency for the estimated annual load and historical annual flows, while the measures of variation around these are the standard deviations and coefficient of variation (CV) which is the standard deviation/mean, and the uncertainty/variability of load (L) and flow (Q) defined by percentiles (e.g. $L_{2.5}$, L_{5}, L_{10}, L_{25}, L_{50}, L_{75}, L_{90}, L_{95}, and $L_{97.5}$).

3.5.1 Time series and scatter plotting module (M3_XYPLOT)

M3_XYPLOT – Generate time series plots of concurrent input daily flows and sampled concentration (Figure 3.1), and scatter plot of ln(flow)–ln(concentration) (Figure 3.2). Scatter plot of TSS-turbidity is optional (Figure 3.2).

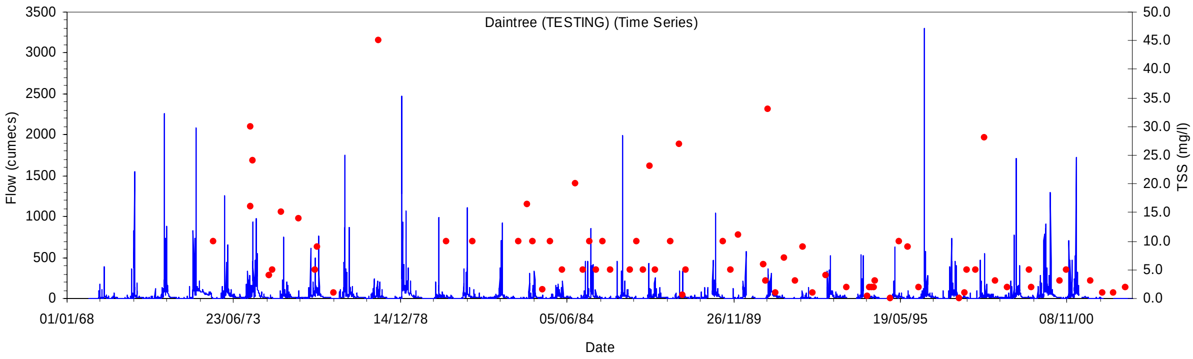

Figure 3.1: Example of time series of plots of concurrent input daily flows and sampled concentration generated by module/macro M3_XYPLOT

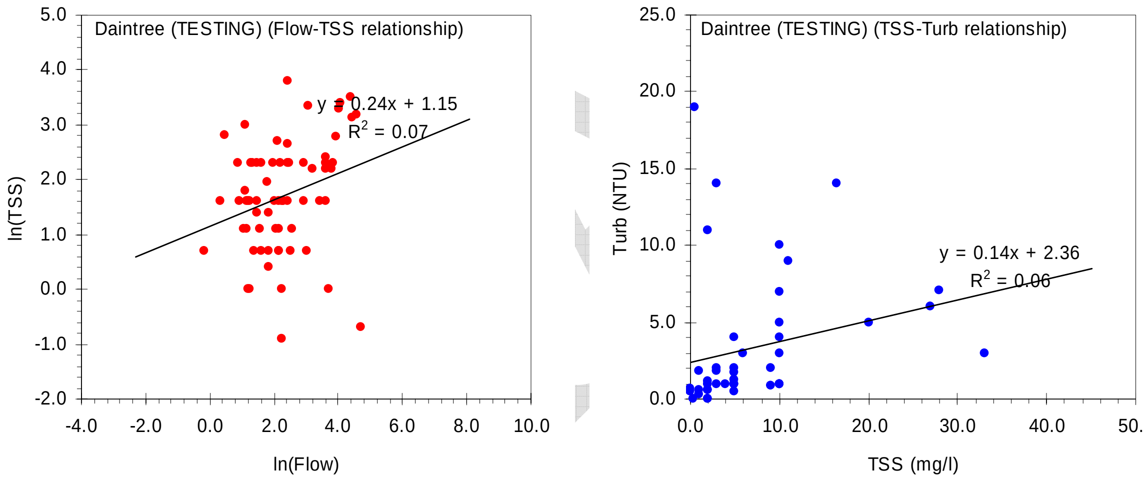

Figure 3.2: Example of scatter plots of ln(flow)–ln(TSS) and TSS-turbidity relationships generated by module/macro M3_XYPLOT

3.5.2 Box and whisker plotting module (M4_BOXPLOT)

M4_BOXPLOT – Generate box and whisker plots of estimated annual loads. There are two options (BOXPLOT_OPTION, to be specified in cell (1,6) of worksheet) in this module/macro:

BOXPLOT_METHOD – Generate box and whisker plots of estimated annual loads by method (one plot for each year) (Figure 3.3)

BOXPLOT_YEAR – Generate annual time series of box and whisker plots of simulated annual loads and historical annual flows (one plot each for loads and flows) (Figure 3.4).

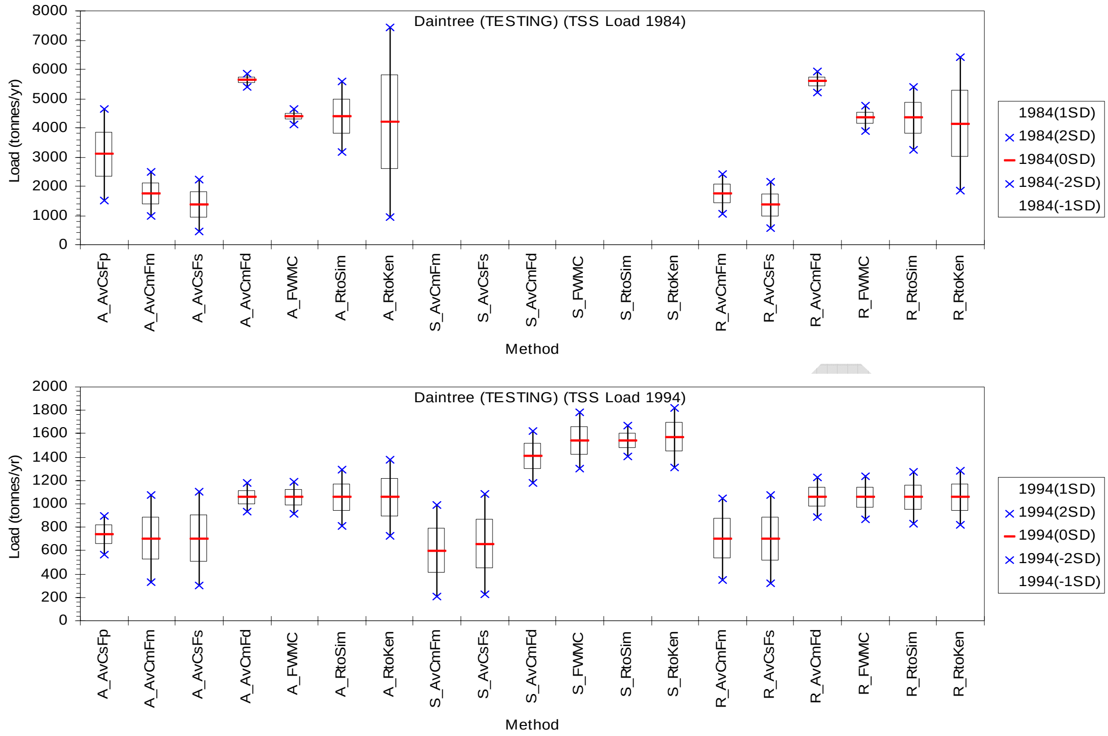

Figure 3.3: Example of box and whisker plots of estimated annual TSS loads (with uncertainties expressed in standard deviations) by method for two years generated by module/macro M4_BOXPLOT (BOXPLOT_METHOD)

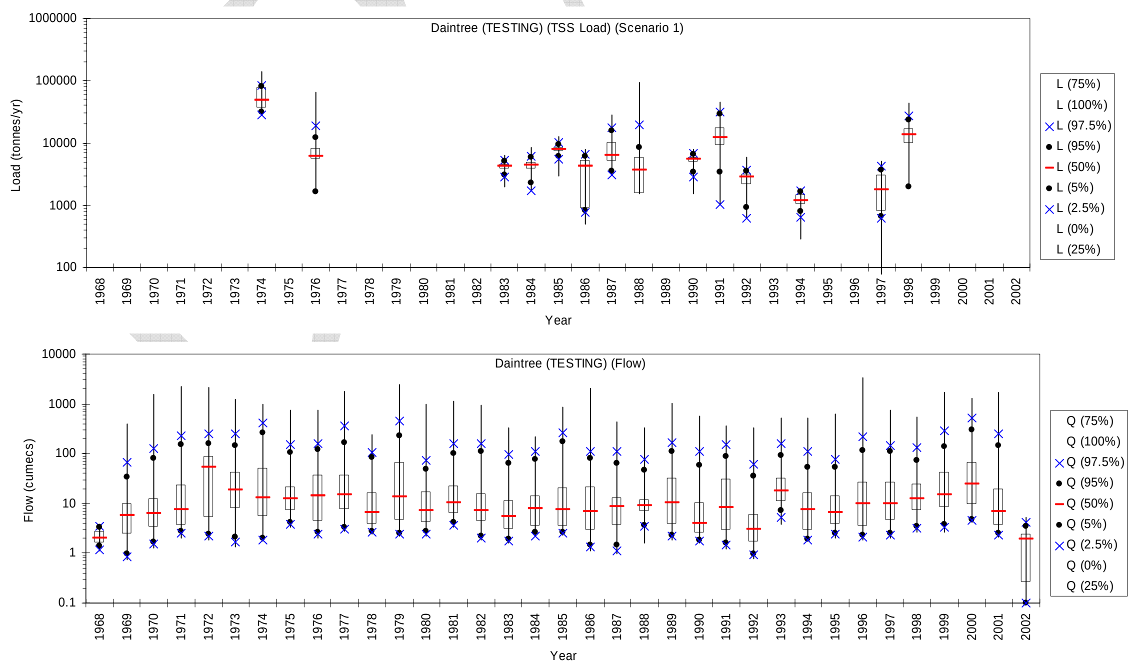

Figure 3.4: Example of box and whisker plots of simulated annual TSS loads and annual flows (with uncertainties expressed in percentiles) generated by module/macro M4_BOXPLOT (BOXPLOT_YEAR)

3.5.3 Histogram plotting module (M5_HISTOPLOT)

M5_HISTOPLOT – Generate histogram plots of simulated annual loads for each year based on the user-assigned prior probability for each method (Figure 3.5), and histogram plots of ln(flow) and ln(concentration) (Figure 3.6). The histograms are plotted on an automatically created worksheet with suffix '(HP)'.

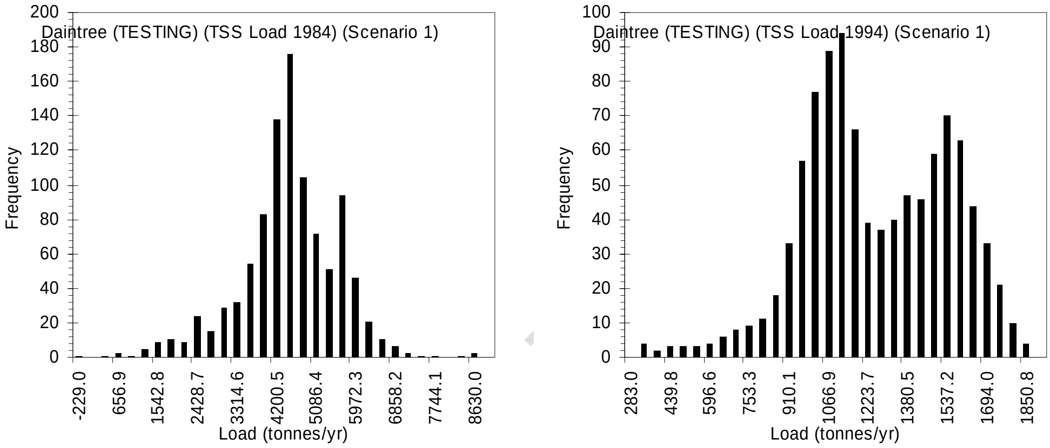

Figure 3.5: Example of histogram plot of simulated annual loads for two years based on the user-assigned prior probability for each method generated by module/macro M5_HISTOPLOT

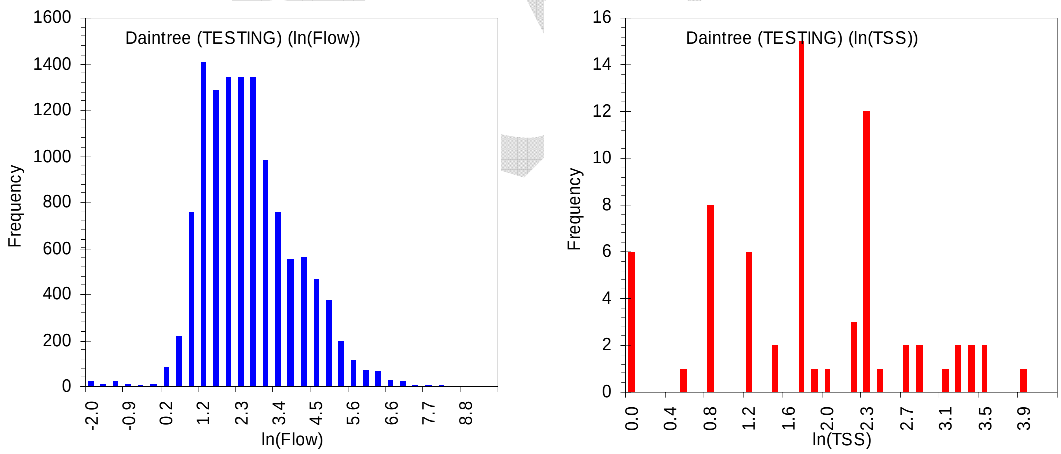

Figure 3.6: Example of histogram plot of ln(flow) and ln(concentration) generated by module/macro M5_HISTOPLOT

3.6 Saving projects/scenarios

Once all the five modules/macros have been executed, and the results (tables and plots) generated, the workbook can be saved for future interpretation and reference. The tables and plots can also be exported for reporting purposes.

3.7 Interpreting results – Annual load estimates and uncertainty measures

Using the examples above, 22 separate estimates of annual load were calculated for the years when WQ and flow data are available.

Figure 3.1 is useful for checking the concurrent input daily flows and sampled concentration data, allowing the user to detect anomalies in the data (e.g. data gaps, outliers, proportion of sampling during high flows, etc.). The scatter plot of ln(flow)–ln(concentration) and TSS-turbidity (optional) (Figure 3.2) illustrate whether the correlations are significant.

The TSS load estimates (with uncertainties expressed in standard deviations) presented in Figure 3.3 show considerable differences in the annual TSS load estimates using different methods, and demonstrate that the 'true' load is subject to high uncertainty (i.e., both knowledge uncertainty and stochastic uncertainty). Unless some other information or analysis is presented to limit the validity of particular estimation methods, it is reasonable to assume that each of these estimates could be equally likely to be the 'true' load.

Figure 3.4 shows box and whisker plots of simulated annual TSS loads and annual flows (with uncertainties expressed in percentiles) and presents another perspective in estimating and interpreting the annual loads using the 22 load estimation methods. Model averaging (i.e., Monte-Carlo simulation with 1000 repetitions) is possible by the specification of user-assigned weights reflecting the user's judgement (knowledge/experience/belief) in each of the methods.

Clearly, base on Figure 3.1 and Figure 3.4, the annual flow variability, as well as the WQ sampling regime (i.e., frequency and timing with flows) are related to the accuracy and precision of each of the 22 methods under consideration, hence it is important to visualise and interpret the load estimation results in conjunction with this information. There is an obvious Bayesian extension to this and this is something that will be pursued in future research.

The histogram plots of the simulated loads for each year (Figure 3.5) allow user to visualise the resulting range of load estimates (based on a user-assigned prior probability scenario). Note that the x-axis varies from year to year to cover the range of simulated annual loads. These simulated annual load histograms show that whilst some estimates are relatively precise, and therefore reliable, other estimates are much less certain (e.g., bi-modal). While the histogram plots of ln(flow) and ln(concentration) (Figure 3.6) allow the user to visualise if the assumption of bi-variate log-normal distribution of flow and concentration is valid.

From the management perspective, it is desirable that these annual load estimates (with uncertainties) can be used for setting and assessing load based targets in sediment and nutrient reduction plan. The annual time series plot of simulated annual loads (Figure 3.4) can be used to investigate the trend (reduction) in the annual pollutant loads.

Generally, the more frequent (and representative) the samples are collected, the more accurate and precise the annual load estimates will be. GUMLEAF allow user to specify the minimum number of samples (absolute minimum is three) within a year (for annual methods) or a season/flow regime (for stratified methods) for estimating annual load in that year or strata. Besides, strictly speaking, such an assessment should be informed by the magnitude of flow in those years (since dry years will necessarily have lower flows and therefore relatively lower loads), of which a framework for such quantification will be pursued in future research.

Overall, there are significant sources of uncertainty in the estimation of pollutant loads, arising from the choice of estimation technique (knowledge uncertainty), fluctuations in flow and concentration (stochastic uncertainty) and measurement uncertainty. By applying a variety of 22 valid load estimation techniques, it can be seen that there is a wide range of possible results, particularly for years which are relatively wet.

The choice of estimation technique has been shown to have a large impact on the final estimate and therefore, it is recommended that more emphasis be given to the selection and documentation of load estimation techniques in future. In particular, it is recommended that the framework provided in Table 2.1 (or similar logic) is applied to select appropriate techniques for each pollutant-site in question. Furthermore, any estimation of loads should be accompanied by clear documentation of the techniques used (which is often missing in practice) and a justification of the technique selected. Additionally, when assessing changes in loads over time at each site, it is essential that the same estimation technique is applied to determine all annual estimates for comparative purposes (i.e. apples to apples comparison).

The accuracy and precision in annual load estimates in rivers and waterways is an integrated process depending on the estimation techniques, sampling regimes, catchment characteristics and climate variability, and GUMLEAF is an analysis and visualisation tool that provides the first step towards the establishment of such an integrated framework based on the concept of load typology, which will ultimately lead also to the establishment of optimum sampling protocols under different catchments and climate conditions.

4 Future Research and Development Plan

4.1 An integrated framework for estimating loads, quantifying uncertainties, designing optimum sampling protocols and assessing compliance with load-based targets in rivers and waterways

A document outlining the potential future research direction is provided in Appendix C – Research proposal for an integrated framework for estimating loads, quantifying uncertainties, designing optimum sampling protocols and assessing compliance with load-based targets in rivers and waterways.

4.2 Integration of GUMLEAF into the e-Water CRC toolkit WaQ-AT

Natural resources managers are faced with the problems of estimating loads, quantifying uncertainties, designing optimum sampling protocols and assessing compliance with load-based targets in rivers and waterways. Surprisingly, there is hardly any integrated framework or guideline for doing these.

The basic framework for estimating loads, quantifying uncertainties and establishing load typology embedded in GUMLEAF, and the integrated framework for estimating loads, quantifying uncertainties, designing optimum sampling protocols and assessing compliance with load-based targets in rivers and waterways put forward in Section 4.1 have showcased the potential for a very important and challenging research area, which will lead to a new methodology, knowledge and tool to assist natural resources managers in informed decision-making.

It is recommended that no further development of GUMLEAF shall be undertaken. Instead, the basic concept and structure of GUMLEAF should be transferred into the e-Water CRC toolkit WaQ-AT which is currently at the initial stage of development. An e-Water CRC interim project (July-December 2005) on this has been put forward by the ACE/University of Melbourne (which is a partner organisation in the e-Water CRC) to jointly develop and enhance WaQ-AT with other partner organisation (e.g., Queensland EPA, Goulburn-Murray Water, Southern Rural Water, etc.). Further development and expansion of WaQ-AT beyond the e-Water CRC interim project may be carried out following research on the integrated framework put forward in Section 4.1.

5 Appendices

5.1 Appendix A – References to load estimation techniques and uncertainty measures

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5.2 Appendix B – ACE Technical Reports

B1 – Fox, D.R. (2004), Statistical Considerations for the Modelling and Analysis of Flows and Loads - Components of Load. Tech. Rep. 02/04, Australian Centre for Environmetrics, Jun 2004, 60pp.

B2 – Fox, D.R. (2005), Protocols for the Optimum Measurements and Estimation of Nutrient Loads - Error Approximations, Tech. Rep. 03/05, Australian Centre for Environmetrics, Apr 2005, 8pp.

5.3 Appendix C – Research proposal for an integrated framework for estimating loads, quantifying uncertainties, designing optimum sampling protocols and assessing compliance with load-based targets in rivers and waterways

5.3.1 Research aims

The research aims at developing an integrated framework for estimating loads, quantifying uncertainties, designing optimum sampling protocols and assessing compliance with load-based targets in rivers and waterways. Specifically, this includes:

1. Estimating annual load estimates using existing flow (typically continuous daily) and WQ sampling (typically sparse instantaneous, e.g. fortnightly or monthly) records
2. Quantifying uncertainty in load estimates (knowledge and stochastic uncertainties)
3. Designing optimum sampling protocol
4. Investigating appropriate time scale in load estimation
5. Deriving typology of load estimation
6. Inferring loads derived from ungauged and tidally-affected catchments
7. Investigating potential for continuous turbidity measurement as surrogate/supplement for TSS sampling
8. Setting and assessing compliance with load-based targets

In addition, the research will also resulted in:

9. Development of an integrated software tool having capabilities (incorporating all the above research outcomes) in estimating loads, quantifying uncertainties, designing optimum sampling protocols and assessing compliance with load-based targets in rivers and waterways
10. Provision of information for parameterising and/or calibrating other process-based water quality models (e.g., SedNet, CMSS)
11. Compilation of a water quality database

5.3.2 Annual load estimates

Estimating annual load estimates using existing flow (typically continuous daily) and WQ sampling (typically sparse instantaneous, e.g. fortnightly or monthly) records, considering seasonal and flow regime stratifications.

Assume historical record of continuous daily flow is available, or flow gap can be infilled/estimated via other pre-processing tools in the CRC Toolkit (e.g., either by mathematical functions or hydrologic techniques).

Apart from the averaging and ratio approach, to include other approaches (e.g, linear/spline interpolation, regression/transfer function).

Some techniques have the advantage of providing concentration/load at fine time step (corresponding to flow time step), which is potentially useful as inputs for other work (e.g., bio-geochemical/WQ modelling of lakes, estuaries and coastal seas).

One example is multi-variate linear regression that include flows and other explanatory variables (e.g., seasonality, flow regime/baseflow index, storm timing/hysterisys (climbing/falling limb), antecedent condition (pollutant wahsoff-buildup/auto-correlation)).

5.3.3 Uncertainty in load estimates

Currently considers knowledge (method) and stochastic (natural) uncertainties. Measurement (sampling) uncertainty cannot be quantified and is ignored.

For knowledge uncertainty, prior probability based on user's judgement (knowledge/experience/ belief). Can be easily extended to include Bayesian approach?

For stochastic uncertainty, need to test the validity and adequacy of bi-variate (log-)normal distribution of flow and concentration using more datasets.

5.3.4 Optimum sampling protocol

Ideally, there will be continuous/near-continuous daily flow and concentration data (at least 1 year, ideally 3 years covering wet and dry years) from different types of catchments (catchment size, flow regime/climate, landuse/geology, etc.) available to test optimum sampling protocol. Currently very limited datasets of this kind is available (e.g., Drain CG2 in MID by SRW?) or forth-coming (e.g., Tambo River in East Gippsland by VicEPA?).

Assume true annual load = sum of (daily flow x daily concentration)

Resample from test dataset by mimicking different sampling strategies (e.g., weekly/fortnightly/monthly regular sampling, weekly/fortnightly/monthly composite sampling, deterministic/probabilistic storm sampling, and their combinations). For example, a transfer function sampling protocol using monthly composite samples has been proposed by Fox (2005a).

Also test different load estimation techniques against true annual load with regard to the accuracy/bias and precision/uncertainty under different types of catchment characteristics and climate conditions. This will eventually lead to the derivation of a typology of load estimation.

5.3.5 Appropriate time scale in load estimation

The load estimation approach described above assumes that annual loads can be estimated using daily flow and instantaneous concentration. There are two (or indeed only one) scaling mis-match issues here. Firstly, the instantaneous concentration is assumed to be the representative average concentration for the day the sample is taken. Secondly, flow variability within the day (i.e., sub-daily) is ignored, which may be acceptable for large and catchments, but not acceptable for small or flashy systems. Future research should investigate the scale issues in sampling and load estimation, and determine the appropriate time scale in load estimation under different catchment and climate conditions. This will also eventually lead to the derivation of a typology of load estimation.

5.3.6 Typology of load estimation

A simple matrix on typology of load estimation is presented in Table 2.1. The concept of load typology can be extended and refined using more dataset. This will greatly assist natural resources managers to make informed decision-making in an integrated framework considering the estimation techniques, sampling regimes, catchment characteristics and climate variability

5.3.7 Loads from ungauged and tidally-affected catchments

As far as annual load estimation is concerned, there are two types of ungauged catchments.

Firstly, those ungauged areas downstream of a gauging site in the same river system where loads are estimated using one of the above load estimation techniques. Annual load can be estimated using simple area ratio method, but weighted/scaled by the relative proportion of landuse/geology and pollutant generation rate (from literature or experimental catchments in the same region) between the gauged and ungauged areas.

Secondly, for those ungauged catchments, regionalisation/correlation approach (similar to that used in flood assessment) based on basic hydrologic characteristics (e.g. catchment size/slope-length/time of concentration, mean annual flow/flow variability, climate, landuse/geology, etc.) can potentially be adopted to estimate the annual load.

For coastal catchments, most of the flow gauging and water quality sampling stations are located upstream from the river mouths, but annual pollutant loads generated in the catchment and delivered to the river mouths are needed for assessing the environmental impacts (e.g., the impacts of sediment and nutrient loads from Queensland coastal catchments on the GBRMPA). More often than not, the flow from these ungauged areas downstream of the gauging/sampling stations are urban or cultivated lands, hence they contribute substantially to the loads.

Conventional flow gauging stations measure stage heights and convert to flows using appropriate stage-discharge relationship derived for the river section at the gauging station. This gauging stations are hence located upstream from the river mouth away from backwater and tidal influence. Similarly WQ sampling stations are usually located at or near the flow gauging stations to avoid the effects of tidal sloshing on pollutants (and that the measured flow from the gauging station can be directly used to estimate loads).

It is difficult to measure the net in-coming flows (or expensive using ADCP) and pollutant concentration deriving from these ungauged downstream catchments. However, loads from these ungauged areas can be estimated by using the simple area ratio method, or by deriving the net in-coming flows from rainfall (with appropriate empirical runoff coefficients) in conjunction with the pollutant generation rate (for that landuse/geology from literature or experimental catchments) and assuming 100% delivery ratio into the waterways.

The other consideration is the effects of diffused sources versus point sources on load estimated at near downstream section of a river system. It may be difficult to distinguish the proportion of loads arising from point/diffused sources at the downstream monitoring site (even if the total load from point sources within the catchment is measured at source), since the pollutant delivery ratio is not known. However, information on point sources can be used in conjunction with the estimated loads at gauging sites, to parameterised/calibrate processed-based/distributed WQ model (e.g. SedNet) for catchment/waterway planning and management.

5.3.8 Potential use of continuous turbidity measurement

Turbidity can be inexpensively monitored on a continuous basis using turbidity sensor/logger, whereas TSS must be sampled and analysed individually. Many studies have shown that turbidity measurements can be potentially attractive as surrogate of or supplement for TSS concentration measurements. This will allow more accurate/precise long-term (annual) TSS load to be aggregated from short-time scale (e.g. daily or sub-daily) estimates. Since some pollutants (e.g. TP) is associated with TSS, the approach can also improve their estimates. However, the relationship between TSS and turbidity is not always significant or well-understood.

Future research can be targeted to establish the TSS-turbidity relationship using more comprehensive datasets (are these currently available/sufficient for testing?), and to relate the unexplained variances of the relationship using other basic hydrologic characteristics (e.g. catchment size/slope-length/time of concentration, mean annual flow/flow variability, climate, landuse/geology, etc.).

5.3.9 Setting and assessing compliance with load-based targets

The difficulty with setting and assessing water quality load-based targets (e.g. 40% nutrient reduction based on the annual load of a selected reference year) is that it is not known what should constitute the reference load, and having set the reference load, what is the objective method for assessing the achievement (or non-achievement) of the load-based target. For example, even if the landuse and farming practices (irrigation flow and fertilizer application) in a particular catchment is unchanged for consecutive years, the daily flows and concentrations generated (hence the annual loads) may be very different due to the effect of flow variability (i.e. whether it is a wet or dry year, and the flow variability within a year, even if both years have similar annual total flows) due to both climate and man-induced factors.

This is because annual pollutant loads in a river system is the aggregation of loads generated and delivered at the effective process time scale (e.g. daily or sub-daily), which in turn is a non-linear function of flow and concentration at that time scale. The challenge is thus about understanding and establishing the pollutant generation and delivery at the process time scale, and relating this to the pollutant load at the space and time scale of interest (annual loads at the catchment outlet).

A statistical method for assessing compliance with nutrient reduction targets was proposed by Fox (2002). The statistical method, in its present form, does not include the effect of non-linearity in load generation and delivery due to the variability in streamflow, and it is proposed that this method be extended to include the effect of flow variability.

5.3.10 Potential Research Funding

The funding for whole or part of the above research may be obtained from e-Water CRC, industry partners (DEH, Vic EPA, Qld EPA, DSE, CMAs, regional water authorities (e.g. GMW, SRW)), or thru competitive grant bidding (e.g. ARC, L&W) although this may be more difficult as it involved a larger component of applied/translational research.

In any case, the emphasis of the research should focus on establishing an integrated framework (and new methodology in some of the research components?) and developing solutions to the problems, rather than implementing existing knowledge and developing tools for the industry.

However, tools will still be developed and tested to realise the full potential of the research and to deliver capacity to the industry, and this can be done thru the Toolkit development team of the e-Water CRC.