Protocols for the Optimal Measurement of Nutrient Loads

A Report to West Gippsland Catchment Management Authority

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1. Introduction

The accurate estimation of total loads of sediments and nutrients is a problem that is attracting considerable attention among natural resource managers, environmental protection agencies, governments, landowners, and the general community. The delivery of sediments from Queensland catchments has been identified as a threat to the ecosystem of the Great Barrier Reef, while point and diffuse sources of land-based nutrients are implicated in the increased frequency and severity of algal blooms in water bodies around the country, including the Gippsland Lakes. Accordingly, there has been a growing trend towards the expression of aspirational and compliance targets for nutrients and sediments in terms of either a relative or absolute reduction in total *load*. For example, a 20% nutrient reduction target has been imposed on Queensland catchments impacting the Great Barrier Reef while the Victorian EPA has required a 40% reduction in the total phosphorous load from the McAlister Irrigation District by 2005 and a commensurate 40% reduction in total nutrient loads to the Gippsland Lakes by 2022. A significant outcome from the Port Phillip Bay Environmental Study (Harris et al. 1996) was the detailed understanding of the Bay's ecosystem and the identification of threshold nutrient loadings for the bay. Management agencies have adopted the study's recommendation that the annual nitrogen load to Bay needs to be reduced by 1,000 tonnes per year and are now actively working toward achieving that target. We thus see that this single number – 'the load', has assumed a special significance in the management of water bodies and consequently much importance is placed on its quantification. Various tools exist to compute a load and these fall into two main categories. The *direct* approach is to use actual water quality data (flows and concentrations) to estimate the mass load. The *indirect* approach is to infer the mass load using a catchment model such as SEDNET or EMSS. While there are difficulties with both methods, we believe the model-based approaches require further development (for example in the representation of the distribution of concentrations and the assessment of uncertainty) before their outputs can be reliably used – particularly in the context of assessing change relative to a target. Given that two to ten-fold differences in load estimates produced from different models are not uncommon, it is easy to appreciate that this is a hopelessly inadequate way to determine if a 40% reduction, say, has been achieved over some prescribed period. We therefore need to address these ‘compliance’ type issues using direct estimation techniques. While there is broad guidance on the various calculations of load that can be used, it is commonly acknowledged that for any one catchment the most appropriate method will depend on (i) the hydrological features of the catchment, (ii) the accuracy in load estimation required and (iii) the quality of the available data. The work reported here extends these concepts and, importantly, we demonstrate that other factors such as ‘knowledge uncertainty’ are also important determinants of the accuracy and precision of load estimation.

Several important innovations to improve load estimation have been developed through research undertaken as part of this project:

1. The application of *mixture modelling* to identify underlying components of flow provides a basis on which to meaningfully stratify the annual flow regime and thereby provide greater certainty in (i) the detection of relationships between flow and concentration, (ii) the discrimination of changes in load over time that could be attributed to management interventions, and (iii) optimizing the allocation of sampling effort, either according to resource limitations or statistical considerations.

2. A new statistical algorithm and companion software tool have been developed to generate flow-biased probability samples from which unbiased estimates of annual load are computed.

3. A software tool known as GUMLEAF (Generator for Uncertainty Measures and Load Estimates using Alternative Formulae) (Tan et al. 2005a), has been developed to facilitate the computation of annual pollutant loads (incorporating sampling and method uncertainties) and visualisation of data and results, using 22 different computational methods.

4. Previous research (Littlewood, 1995) on transfer function modelling of concentration data has been extended and this has suggested an efficient composite sampling strategy for load estimation.

We believe this work has made a significant contribution to load sampling and estimation methodologies and has the potential to influence the way mass loads are computed in the future. Additional research is now required to:

- establish protocols to estimate the fate of sediment and nutrient loads passing through estuaries;
- develop methods for estimating load export from non-gauged catchments;
- run comparative studies to evaluate the performance of various sampling techniques;
- Undertake a detailed analysis of the relationships between TSS and turbidity considering also a number of covariates that might be important in describing the relations.

2. GLOSSARY OF TERMS

Accuracy	An *accurate* measurement or estimate is one that is (numerically) close to the true value.
Aliquot	A portion of a sample.
Bias	The degree to which an estimate deviates from the true (but unknown) value in the long run (*see also Error)*.
Discharge	The volume of water which passes a given point in a river or stream in a given period of time, a total quantity.
Efficient	In measurement, having relatively high accuracy and precision for a given amount of effort.
Error	The degree to which an individual estimate or measurement deviates from the true (but unknown) value
Flow	The rate at which water passes a given point in a river or stream at a given moment. The integral of flow over time is the discharge.
Flow-proportional sample:	A composite sample composed of aliquots taken in proportion to the flow rate.
Flow-weighted mean concentration (FWMC)	An average concentration whereby the *weight* assigned to an individual concentration is in direct proportion to the discharge (flow) observed at the time of sampling. In this scheme, concentrations measured during high flow events are given more importance than concentrations measured during low flow events.
Flux:	The rate at which a mass load passes a given point in a river or stream at a given moment. The integral of flux over time is the load. Estimated as the product of flow (volume) and concentration of constituents in the flowing water.
Load	The amount of material which passes a given point in a river or stream in a given period of time, a total quantity.
Mass Load	Sum of instantaneous flux occurring past a point on a river over a defined period of time (eg tonnes over a year)
Incertitude	Lack of knowledge about parameters or models, including parameter and model uncertainty.
Mean daily load	The average of the daily loads for a number of days.
Precision	Reciprocal of *variance*.
Random sampling	A probabilistic sampling strategy in which every member of the population has an equal chance of being included in the sample. In sampling over time, a useful technique for reducing bias due to unrecognized periodicities in the system being sampled.
Rating curve	In hydrology, a rating curve expresses the empirical relationship between stage, or height of the water, and flow. In load estimation, a rating curve is a relationship used to calculate daily loads or concentrations from flow and other independent variables, usually using some form of regression.
Residual	The difference between the observed or measured value and that which has been predicted from a statistical model.
Retransformation bias	The bias that arises from the fact that the mean (or 'expected value') of a function of some statistic is not the same as the function applied to the mean of the statistic.
Stratified sampling	A sampling strategy which apportions the total sampling effort among a number of strata (eg. seasons or flow regimes). Stratified sampling often leads to more efficient estimates of loads, particularly with ratio estimators.
Systematic sampling	Where a sample is taken at regular or fixed intervals. Systematic sampling can be more efficient than random sampling, but can produce biased results, particularly if periodicities in the data exist.
Time-proportional sample	A composite sample composed of aliquots taken without regard to flow. Equal volume aliquots are taken at equal intervals.
Total load	The load for an entire period of interest, usually a month or a year.
Water Quality Constituents	Includes any materials or chemicals transported by river (soluble and insoluble). Can range from sediment and nutrients to salts, pesticides and heavy metals
Variance	A statistical measure of variability. The (positive) square-root is called the *standard deviation*.

3. Setting and evaluating load-based targets

The measurement of the mass of materials carried by rivers to receiving waters such as wetlands, estuaries and oceans has been the subject of considerable measurement and research efforts. The primary intention of these efforts has been to provide reliable information for catchment and estuarine management (Littlewood, 1992). Constituents of water quality attracting most interest are commonly nutrients such as nitrogen (N) and phosphorus (P), and suspended sediments (TSS).

Regional Natural Resource Management is the ‘new’ business model for achieving environmental outcomes under the Commonwealth’s National Action Plan for Salinity and Water Quality (NAPSWQ) and the National Heritage (NHT2). Narrative and quantitative targets with differing timeframes — aspirational (10-50 y), resource condition (10-20 y) and management (1-5 y) — will be the performance benchmarks used to evaluate the success of regionally-developed Natural Resource Management Plans and Investment Strategies.

The setting, monitoring and auditing of load-based targets of a particular pollutant (e.g. suspended sediment, total nitrogen, total phosphorus) is a key feature of performance benchmarks with performance evaluation based on “reasonable assurance’ that specified load-based targets are being achieved. Other qualifiers such as *likelihood*, *estimated*, *variation*, *high degree of confidence* are often used in the context of load assessment. These are inherently statistical terms that impart a requirement to make explicit and manage the uncertainty associated with the targets. This is not a trivial task and requires complex statistical approaches to help ascertain whether compliance is being achieved with a specified level of confidence. Accurate load estimation requires comprehensive flow (often continuous) and concentration data (seldom more frequent than monthly), but as this is very seldom the case a variety of statistical time-averaging techniques (e.g. flow-weighted averaging, ratio, regression) and modelling approaches (e.g Sednet, EMSS, AQUALM) have been developed, that all broadly aim to interpolate a continuous data record in order to estimate a load.

3.1 Loads defined

The pollutant **load** is the mass or weight of pollutant, which passes a cross-section of the river in a specified time. The **loading rate**, or **flux**, is the instantaneous rate at which the load is passing a point of reference on a river, such as a sampling station, and has units such as grams/second or tonnes/day. This is the product of pollutant concentration and discharge rate. The **discharge rate**, or **flow,** is the instantaneous rate at which water is passing the reference point, and has units of volume/time such as cubic meters per second (cumecs).

The problem of accurately estimating the total mass load transported in a water body over some defined period of time is certainly not new and dates back to at least the 1940s (Campbell and Bauder 1940). In its simplest form, the aim is to approximate the integral

$$Load = \int_{t_0}^{t_1} F(t)\, dt \qquad (1)$$

where *F(t)* is the instantaneous *flux* (rate of mass transport) at time *t*. Replacing the integrand of equation 1 with the product of the instantaneous concentration and discharge at time *t* gives the more familiar version (equation 2).

$$Load = K\int_{t_0}^{t_1} C(t)\,Q(t)\, dt \qquad (2)$$

where *K* is a units conversion factor.

Although conceptually simple, the problem of obtaining 'representative' flow and concentration data in order to accurately and precisely estimate mass load is less straightforward. At its simplest level, the discrete analogue of equation 2 would suggest obtaining a sample of *n* pairs of measurements on flow and concentration $\{Q_i, C_i\}$, multiplying these together and summing *viz:*

$$Load = K\sum_{i=1}^{n} q_i\, c_i \qquad (3)$$

While the estimator given by equation (3) forms the basis of most load calculations, its statistical properties are critically dependent on the way in which the $\{Q_i, C_i\}$ data are collected.

The accuracy of the load estimate will depend on the proper application of the most appropriate method, little can be done to compensate for a data set which contains an insufficient number of observations collected using an inappropriate sampling design. Many load estimation programs choose monthly or quarterly sampling with no better rationale than that it's convenient. To avoid this, the sampling, which will be needed for load estimation, must be established in the initial planning process, based on quantitative statements of the precision required for the load estimate. If load estimates are to be made, determine the precision needed, based on the uses to which they will be put. For example, "I want the load estimates to be within 5% of the true loads in 90% of the years for which calculations will be made. The resources necessary to carry out the sampling program must be known, and budgeted for, from the beginning.

Often detailed flow information is available whereas concentration observations are available less frequently than flow observations. This creates the basic problem of practical load estimation and we have following three choices of basic approach:

1. Abandon most of the flow data and calculate the load using the concentration data and just those flows, which were observed at the same time the samples were taken.
2. Find a way to estimate "missing" concentrations: i.e. concentrations to go with the flows observed at times when chemical samples were not taken.
3. Do something in between - find some way to use the more detailed knowledge of flow to adjust the load estimated from matched pairs of concentration and flow.

3.2 Error, Accuracy, Bias and Uncertainty

Precision and **accuracy** measure two related but different aspects of the behaviour of a measurement system. If repeated measurements are made of an object, the measurement process is called precise if the difference among measurements is small, and it is called accurate if the average measurement is close to the true value. **Bias** is the lack of accuracy; a measurement system which is unbiased is highly accurate. Load estimation approaches which produce low bias and high precision using relatively few samples are described as **efficient**. Generally we want an approach to load estimation which is as precise and accurate as possible for the number of samples taken, i.e. as efficient as possible. It is especially important to have *a priori* confidence in the lack of bias, since bias cannot be directly evaluated. However, when detecting a change in loads is more important than the actual level of the loads, we may choose a method which produces precise estimates, even if they are biased. Walling and Webb (1981) showed in a simulation study that the product of annual discharge and average concentration was strongly biased but quite precise, and pointed out that it might be useful for trend studies, in spite of the bias. Figure 1 provides examples of bias and precision.

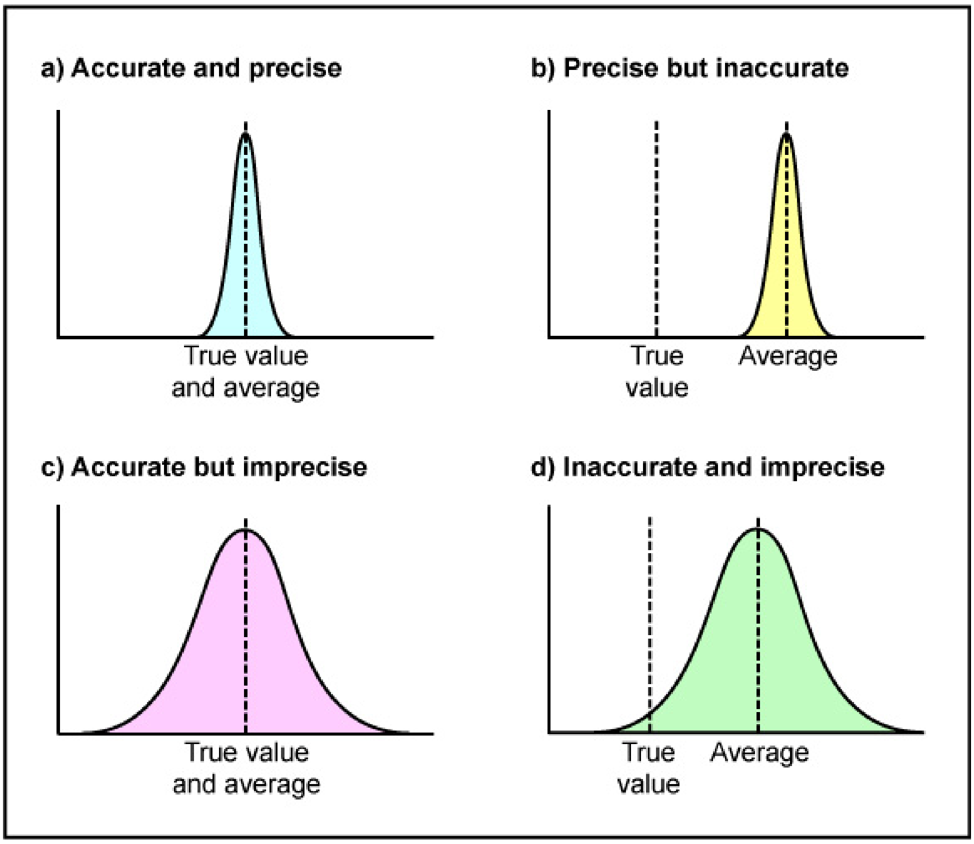


Figure 1 Illustration of accuracy and bias.

3.3 Types of Uncertainty

Uncertainty pervades the natural environment and obscures our view of it (Burgman 2004). To organize ideas about uncertainty, Burgman uses a taxonomy of uncertainty (Regan et al. 2002). At the highest level, it distinguishes between epistemic and linguistic uncertainty. Epistemic uncertainty exists because of the limitations of measurement devices, insufficient data, extrapolations and interpolations, and variability over time or space. In other words, we don't know what we don't know! Linguistic uncertainty, on the other hand, arises because natural language, including our scientific vocabulary, often is underspecific, ambiguous, vague, context dependent, or indeterminate. It is distinguished from epistemic uncertainty because it results from people using words differently or inexactly. Epistemic uncertainty reflects incomplete knowledge. It has six main types: measurement error, systematic error, natural variation, inherent randomness, model uncertainty; and subjective judgement. The terms 'variability' and 'incertitude' make a simple taxonomy of epistemic uncertainty worth describing because of its utility. **Variability** is naturally occurring, unpredictable change, differences in parameters attributable to 'true' heterogeneity or diversity in a population. **Incertitude** is lack of knowledge about parameters or models (including parameter and model uncertainty). Incertitude usually can be reduced by collecting more and better data. Variability is better understood and more reliably estimated, but is not reduced, by the collection of additional data. Model uncertainty occurs because models are simple abstractions of reality. Models may be based on language, diagrams, flow charts, logic trees, mathematics or computer simulations, among others. Model uncertainty arises in two main ways. Firstly, usually only variables and processes that are regarded as relevant and important for the purpose at hand are featured in the model. Secondly, the choice of a way to represent observed processes involves further abstractions. Uncertainty associated with model selection is a difficult area because there are no accepted methods for treating it and there are no general guidelines for measuring the adequacy of a model for its intended use. Mostly, individual scientists use a given model because it is convenient or they are familiar with it. The only way of determining how appropriate a model is for prediction is to validate it by comparing predictions with outcomes. It will be reliable if predictions are within an acceptable margin of error.

Table 1 Types of uncertainty affecting load estimation

Types of Uncertainty	Definition	Load Examples
Epistemic		
Measurement Error	Occurs because measuring equipment and observers are imperfect resulting in error.	
Systematic Error	occurs when measurements are biased.	Wrong instrument calibration
Natural Variation	environmental change with respect to time, space or other variables that is difficult to predict.	Variation in flow seasonality landforms
Model Uncertainty	occurs because models are simple abstractions of reality and sometimes significant factors causing variation are missed or factors are not properly represented or parameterised.	Wrong load algorithm Not accounting for estuaries or groundwater
Subjective judgment		Samples at wrong time or location resulting in unrepresentative sampling
Lingustic Uncertainty		
Vagueness	Arises because language permits borderline cases	“high” flow event
Context dependence	Arises from a failure to specify the context in which a proposition is to be understood	
Ambiguity	Arises when a word can have more than one meaning	Base load – is this the load by a ‘natural’ system or is this the load during ‘normal’ flows.
Theoretical indeterminacy	Arises from indeterminacies in our theoretical terms.	
Under-specificity	Arises when a statement doesn’t provide the degree of specificity require required	Accuracy, timeframe, place required for load estimation to occur

3.4 Sources of Uncertainty in Load Estimation

Overall, three sources of uncertainty contribute significantly to overall uncertainty in mass load estimation. Those three sources are knowledge uncertainty, stochastic uncertainty and measurement uncertainty (Figure 2).

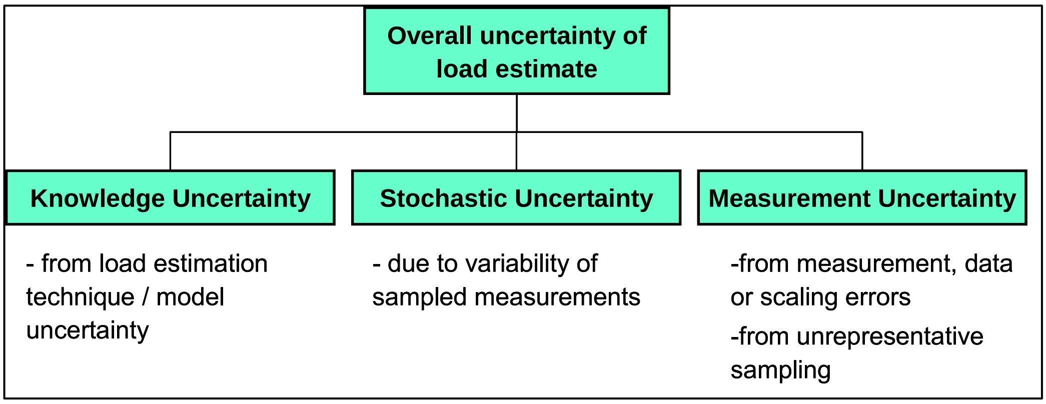


Figure 2 Sources of uncertainty in load estimation.

By way of example, figure 3 shows the variation in the total TP load in 2000 for Central Gippsland Main Drain #2 (CG02) arising from the application of 22 different load formulae. While the majority of estimates are around 12 tonnes, the lower estimates are 8 tonnes. Differences in the assessment of any load reduction will obviously arise depending on which technique has been used (for the same data). Thus, someone electing to use methods 2 or 9 (see table 3 for a description) could reasonably claim that the annual load was 67% lower. It is apparent that the assessment of the attainment of a nominal 40% load reduction target is potentially fraught with difficulties.

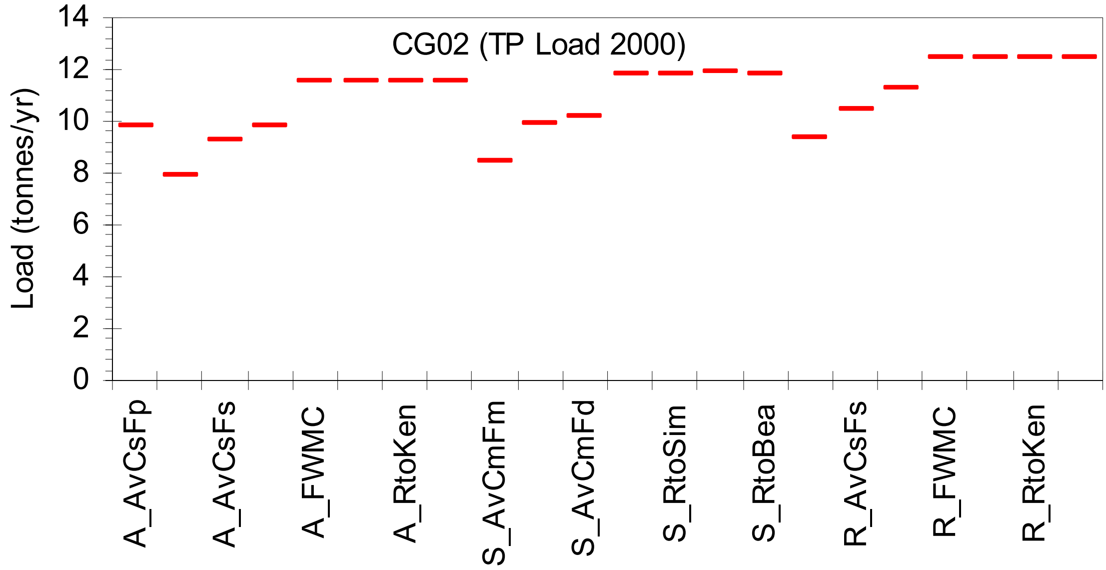


Figure 3 Differences in total 2002 TP load estimates for CG02.

We have called the uncertainty in a load estimate arising from different computational approaches as ‘knowledge’ uncertainty. Knowledge uncertainty can be reduced through an increased understanding of the pollutant wash-off and transport processes which in turn helps inform the sampling and estimation procedures. In general, for sites with limited high flow samples, methods that do not account for flow stratification will tend to underestimate the ‘true’ load.

In addition to knowledge uncertainty, stochastic uncertainty also needs to be considered. Stochastic uncertainty is described by the deviation of water quality concentrations from any assumed value (e.g. a mean) and is measured as a variance.

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.

4. Sampling for load assessment

Much of ‘conventional’ statistical theory is built around the related concepts of unbiasedness and randomness. An unbiased estimator is one that theoretically neither consistently over-estimates nor under-estimates the true, but unknown parameter value. This property is generally regarded as overridingly important in the identification of candidate estimation methods. Simple random sampling (SRS) is a straightforward procedure that assigns equal probability of selection to all elements of the ‘population’. For example, a SRS of size n would be obtained by randomly generating (without replacement) n integers in the range 1 to 365. Concentration and flow measurements would then be obtained on the days corresponding to the n integers so obtained. While this procedure provides an unbiased estimate of annual load (since the random procedure neither favours nor handicaps the selection of any particular combination of flow and concentration), it will invariably be imprecise. This is due to this method’s lack of recognition of key features of flux patterns which if exploited, can potentially reduce the estimation variance. For example, it is a well known and often stated fact that most of an annual sediment or nutrient load is delivered during a small fraction of the year (corresponding to ‘peak’ flow events). Another sampling strategy that is easy to implement is systematic sampling (figure 4).

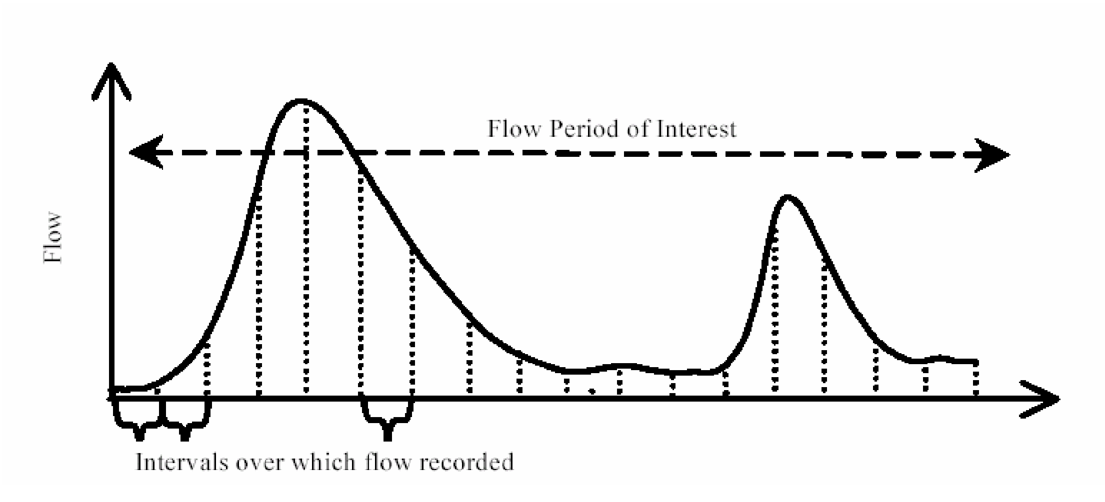


Figure 4 Illustration of systematic sampling (after Degens and Donohue, 2002)

Referring to figure 4, a concentration measurement would be obtained at regular time intervals (corresponding to the dashed lines). This would then be multiplied by the average flow during the interval to obtain a flux estimate for the interval. Summing over all the intervals in the period of interest (equation 3) gives an estimate of load for the period. While the systematic sampling strategy readily lends itself to automation using in-situ data loggers and is appealing from the perspective of representativeness, like the *SRS* strategy, it does not focus sampling effort where it is most important (eg. high flow events). Systematic sampling can give misleading results particularly in the presence of autocorrelation and periodicity. One approach that overcomes some of these difficulties is the *stratified sampling method*. This strategy assigns sampling effort in proportion to flux – periods of high flux are sampled more intensively than periods of low flux. One of the main advantages of stratified sampling is the potential reduction in estimation variance. It is well known that the variance of the stratified estimator (of a population mean or total) is less than that obtained from *SRS* when the 'between' stratum variation is high in comparison to the 'within' stratum variation (Cochran 1963). For load estimation this is likely to be the case and so substantial improvements in estimation efficiency can be expected from stratification. However, a number of studies have demonstrated that the most significant gains in precision and accuracy are obtained by relatively simple stratification strategies (eg. high-flow / low-flow dichotomy) (Littlewood 1992, Rekolainen et al. 1991, Richards and Holloway 1987, Thomas and Lewis 1995). Stratification is typically done with respect to time (Thomas and Lewis 1993) or flow (Thomas and Lewis 1995). Time-stratified sampling is achieved by firstly analyzing past hydrographs to identify appropriate time strata. Subsequent sampling is based on a random selection of a pre-determined number of samples within each time stratum. The approach to flow-based stratification is a little different in that regular updates of stage information are used to dynamically control strata allocation. A probabilistic calculation is performed to control the sampling within each stratum. A modification of this approach was provided by Burn (1990) whereby the sampling frequency is continuously updated in light of the sampling and flows that have already occurred. This added flexibility avoids under or over sampling and is suited to monitoring programs where financial &/or physical constraints limit the maximum number of samples that can be analysed (Degens and Donohue 2002).

4.1 Sampling frequency

The issue of an ‘appropriate’ sample size for load estimation has received considerable attention. Richards (1998) notes that monthly sampling for estimation of an annual load tends to seriously underestimate the true value. Shih at el. (1994) conclude that 8 time-integrated samples are required per runoff event to obtain a good load estimate while Yaksich and Verhoff (1983) suggest 12 samples per runoff hydrograph are required for satisfactory load estimation.

We have undertaken some preliminary research to investigate sample-size issues in two slightly different, but related contexts: (i) number of samples required to adequately describe the hydrograph; and (ii) number of samples required to estimate an annual load. Each of these is investigated in more detail in the following sections.

4.1.1 Sample size required to describe the hydrograph

We have undertaken a very preliminary analysis using the hydrograph shown in figure 5 as a test case.

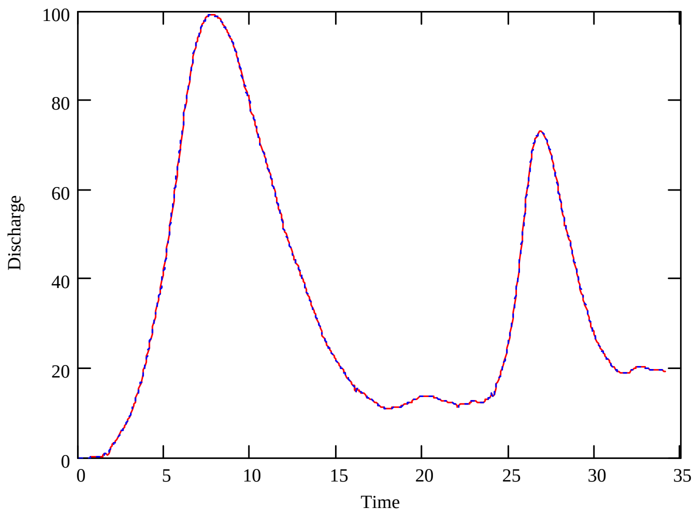


Figure 5 Typical flow hydrograph

One way of triggering sampling so that greater emphasis (monitoring effort) is applied to the rapidly rising or falling limbs of the hydrograph is to analyse a plot of the first derivative (figure 6). This can be approximated in real-time by examining successive differences in flow. The grey band in figure 3 denotes a region where the first derivative is not appreciably different from zero and so no sampling is undertaken at these times. How to determine the width of such a band is not considered here and would need to be the subject of more comprehensive research.

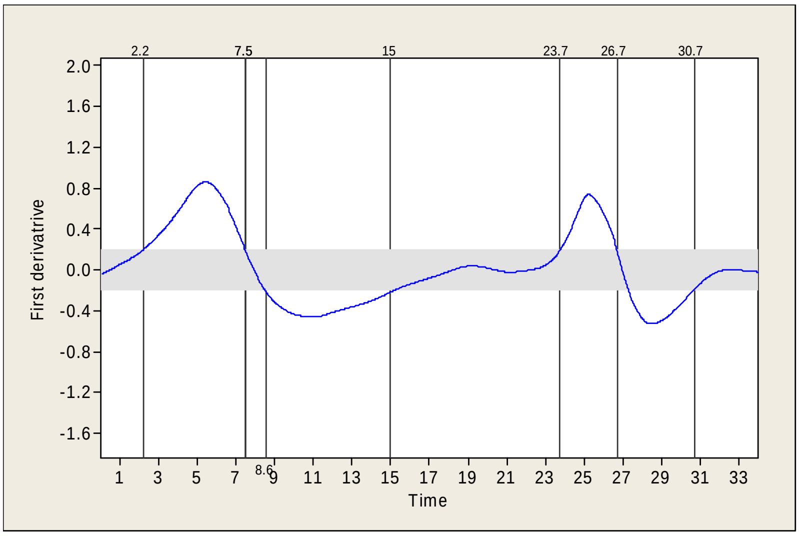
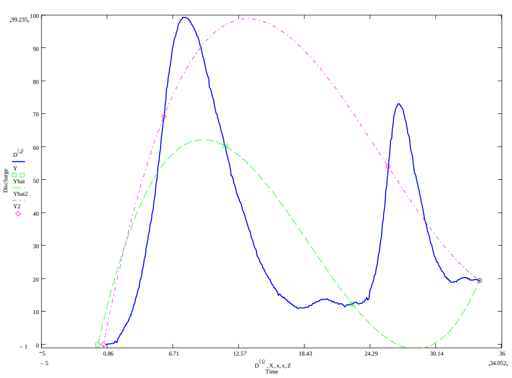
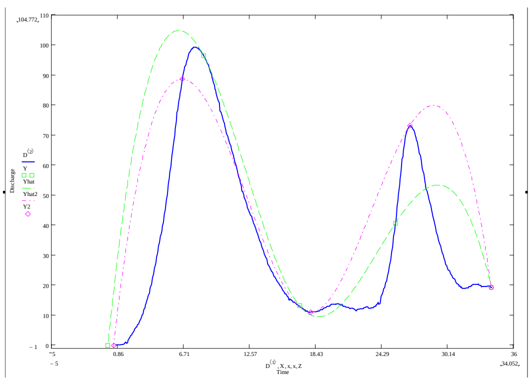


Figure 6 Plot of first derivative of hydrograph of figure 5.
Grey band is 'no sample' region. Vertical lines define sampling periods.

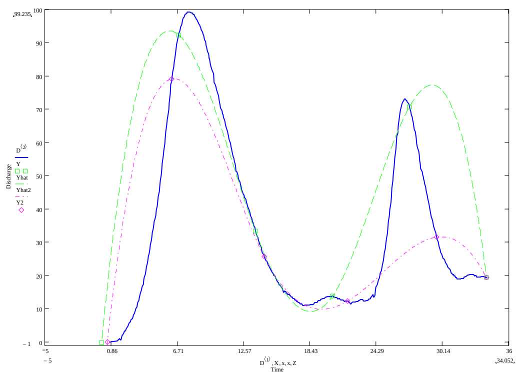
Determination of the sample size n is a trade-off between accurate representation of the flow-duration curve (implying large n) and resource efficiency (implying small n). A common mathematical approach to curve-fitting is via the use of interpolatory splines. The panels of figure 7 shows the resulting spline fits as a result of varying the sample size from four to twenty-one. One spline is fit to the flow measured at equi-spaced times and a separate spline is fit to the flow measured at optimized time intervals. The criterion used in the optimization is minimum root mean square error between the fitted spline and the true curve.



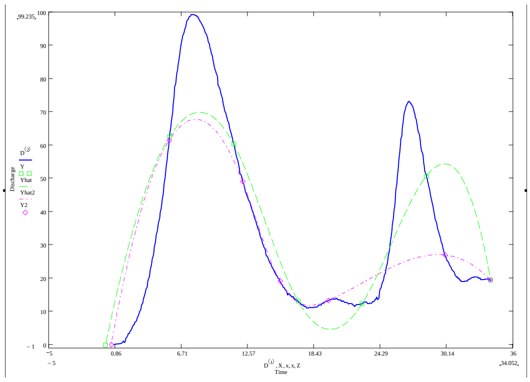
n = 4



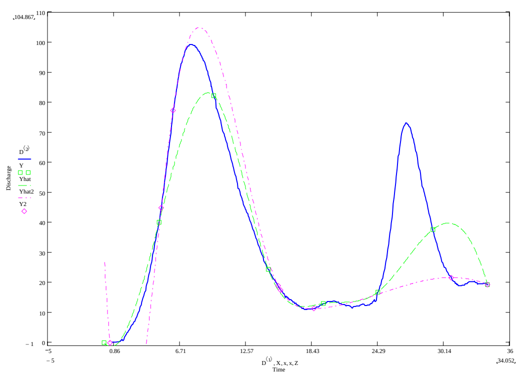
n = 5



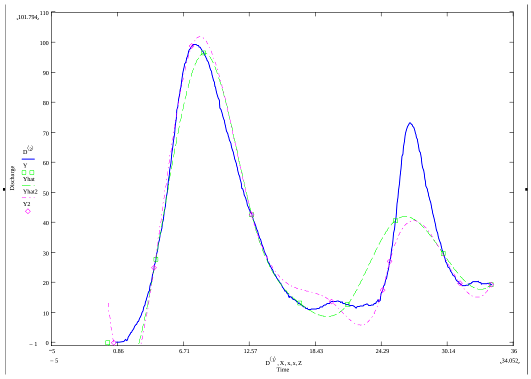
n = 6



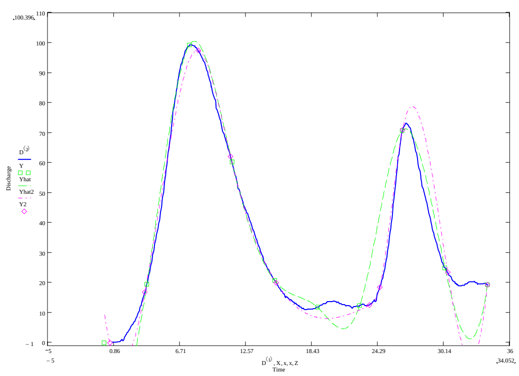
n = 7



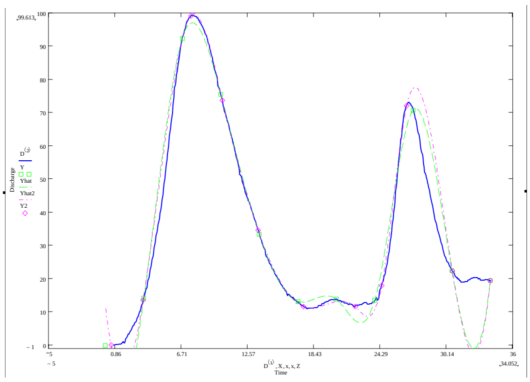
n = 8



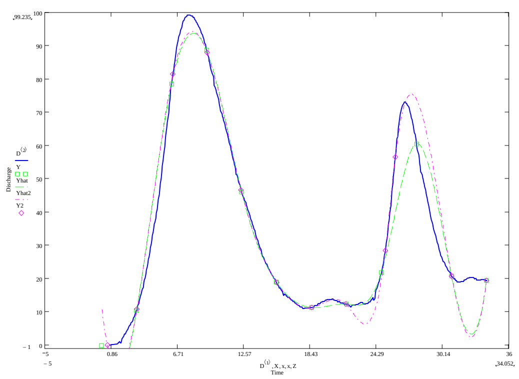
n = 9



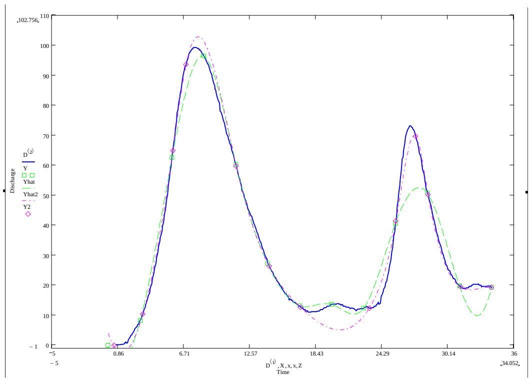
n = 10



n = 11



n = 12



n = 13

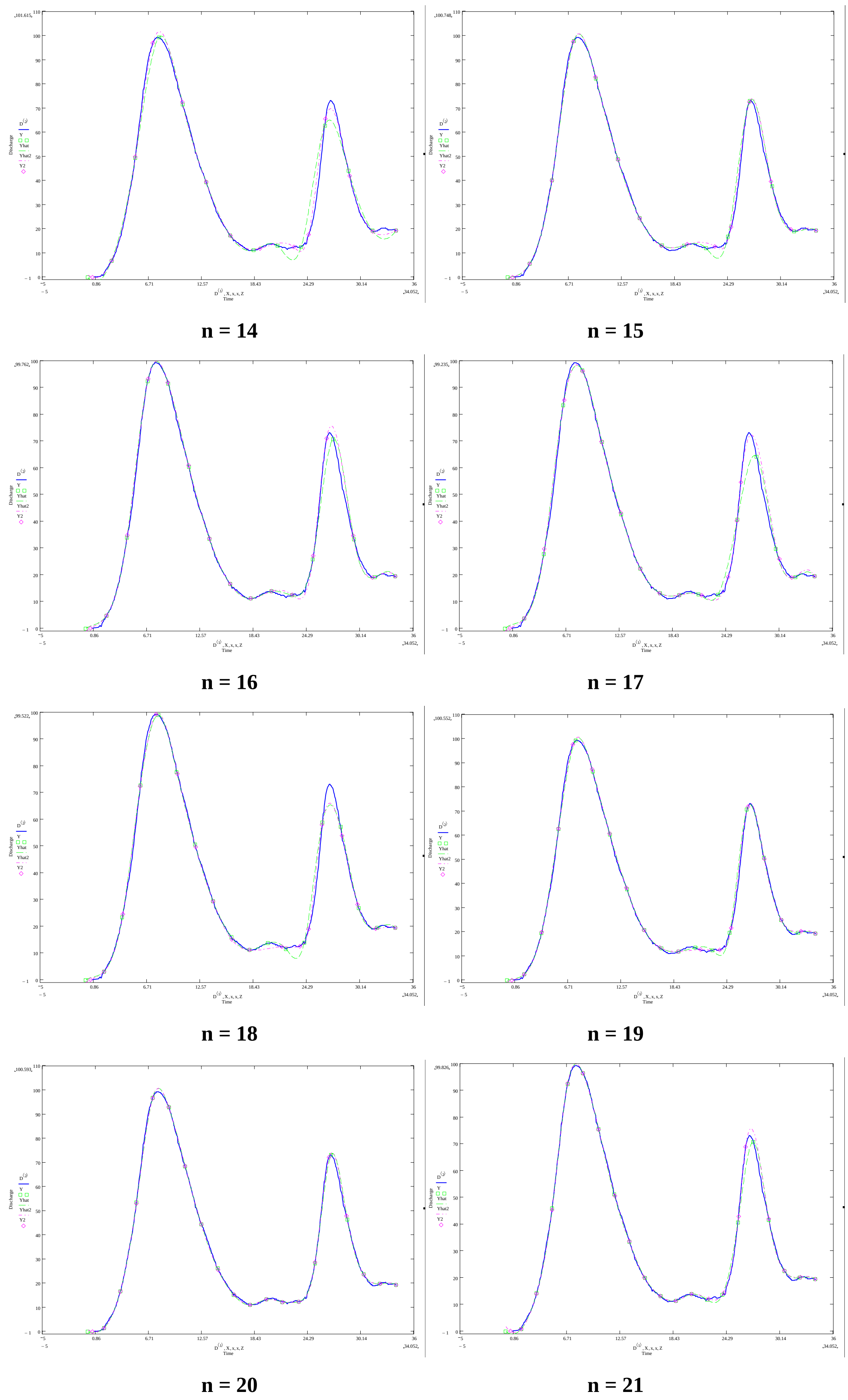


Figure 7 Cubic spline representation of hydrograph of figure 5 as a function of sample size. Blue curve is true flow duration; green curve corresponds to equi-spaced monitoring times; maroon curve is optimised sampling times to give best fit.

It can be seen from the panels of figure 7 that a reasonable representation (using spline fits) of the true flow duration curve is not achieved with samples less than about $n = 10$. For $n \geq 15$ the spline fit using either equi-space monitoring times or optimized monitoring times is exceptionally good. An objective appraisal of the adequacy of the fitted splines is provided by plotting the root mean square error (rmse) as a function of *n* (figure 8).

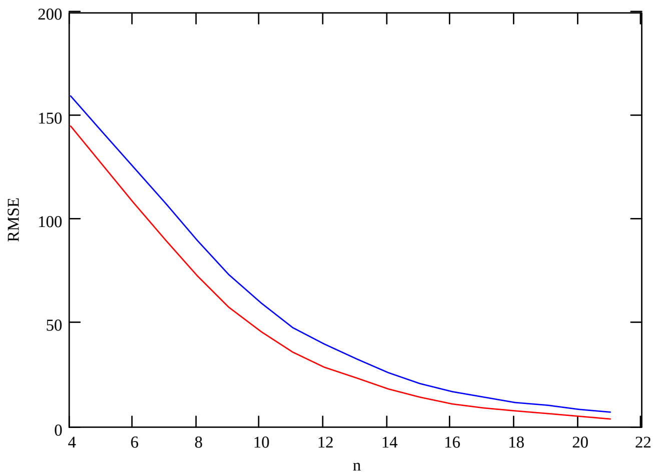


Figure 8 Plot of root mean square error of spline fit as a function of number of data points. Blue curve corresponds to equi-spaced samples; red curve is optimised sampling times.

The preceding analyses (figure 7) were performed over a nominal 34 hour time period. With $n = 15$ sampling occasions this implies a 2-3 hour monitoring interval. By restricting the spline fitting to the first 24 hour period we see that in this case very good representations are obtained with either $n=8$ (figure 9) as suggested by Shih at el. (1994) or n=12 (figure 10) as suggested by Yaksich and Verhoff (1983).

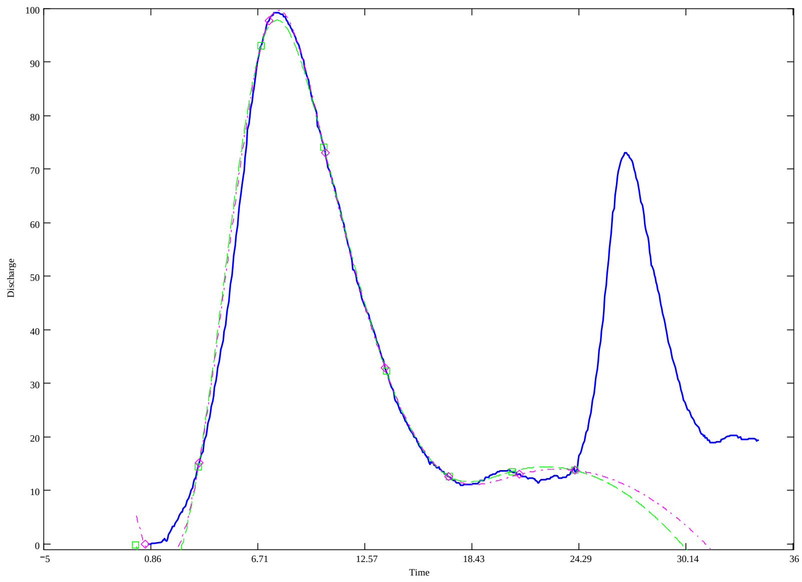


Figure 9 Splines fitted to first 24 hours only. Green curve is equi-spaced samples; maroon curve corresponds to optimised sampling times. N=8 in both cases.

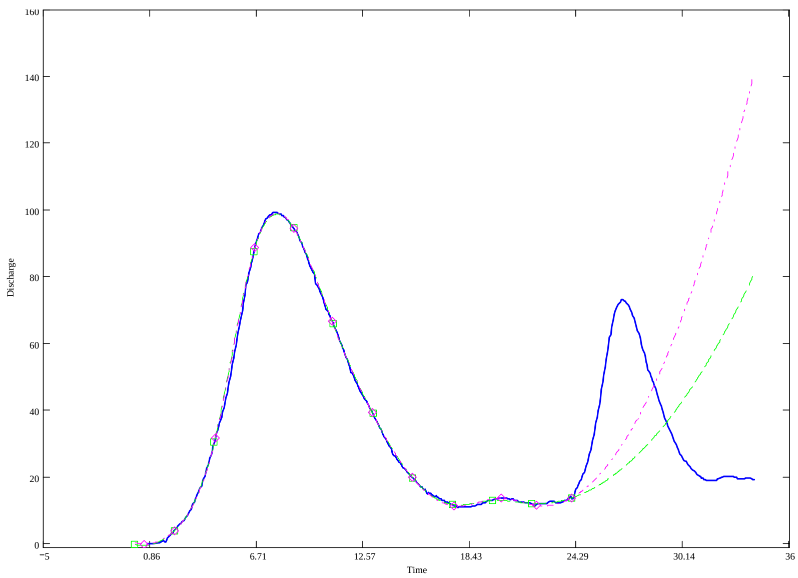


Figure 10 Splines fitted to first 24 hours only. Green curve is equi-spaced samples; maroon curve corresponds to optimised sampling times. N=12 in both cases.

4.1.2 Sample size required to estimate an annual load

The determination of an appropriate sample size required to estimate an annual load with some prescribed level of accuracy and precision is non-trivial and will depend on many factors – not least of which is the hydrology of the system under investigation.

The sample size question is also an inherently statistical issue and can only be addressed in the context of the *sampling strategy* employed. For example, one may choose to use a *systematic sample* whereby data on both flow and concentration are collected at fixed time intervals or *purposive sampling strategies* may employed where the sampling intensity is a function of the hydrograph (eg. more sampling effort is devoted to the rising and falling limbs of the hydrograph, figure 11).

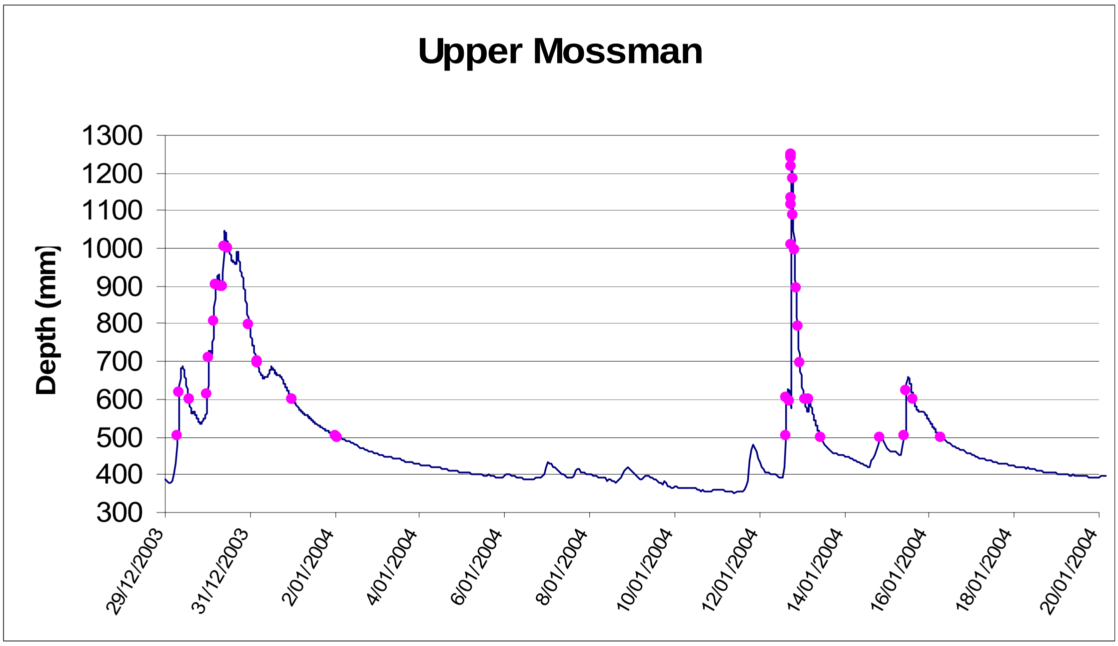


Figure 11 Record of depth data (-) and automatic sampling points (•) during the period 29/12/2003 to 20/01/2004 for the Upper Mossman station. (From McJannet et al. 2005).

We have seen in the previous section that the hydrograph is well described by sampling at intervals of 2-3 hours. While this is entirely feasible for *flow* it is unrealistic to expect that concentration data will be acquired at such a high sampling intensity since this would be prohibitively expensive. As will be seen in section 5, the relationship between flow and concentration is not stable and varies over a wide range of temporal scales. This makes it difficult to estimate a concentration from flow data alone. As part of our research we have investigated two fundamental sampling strategies for (annual) load estimation. The first is a probabilistic, *biased* sampling strategy that concentrates sampling effort on high flow events and is more suited to load estimation for 'flashy' catchments (ie. those showing high variability in flow regime). The second development represents an extension of the model-based approach suggested by Littlewood (1995) and uses a mathematical model (a transfer function model) to impute concentration data on a daily time-step from sparsely sampled data (typically monthly). We have trialled this second method on Southern Rural Water’s drain monitoring data with promising results, suggesting that nutrient monitoring in the drains of the MID could potentially be reduced from daily to monthly sampling without significantly impacting the quality of the annual load estimates.

In concluding this section, we believe that it is difficult to provide a generic statement about the sample size required for annual load estimation. It has been our experience that this is more a question of cost and logistics than of statistical precision. The *daily* nutrient monitoring for total phosphorous in the MID drains undertaken by Southern Rural Water is unique in Australia and while this has provided us with a very rich data set (enabling highly accurate load estimates to be obtained), it is not a viable option in most cases. Based on the current research and work we have undertaken elsewhere in Australia, it would appear that at best, fortnightly monitoring of nutrients can be contemplated, although monthly monitoring is more common. With this in mind, we suggest that our software tool for performing size-biased sampling (Figure 12 and Appendix J) with a sample size of 20 to 30 be used for ‘flashy’ catchments and monthly composite sampling be used in conjunction with our transfer function modelling approach (Appendix K) be used for drains and streams having more consistent flow patterns.

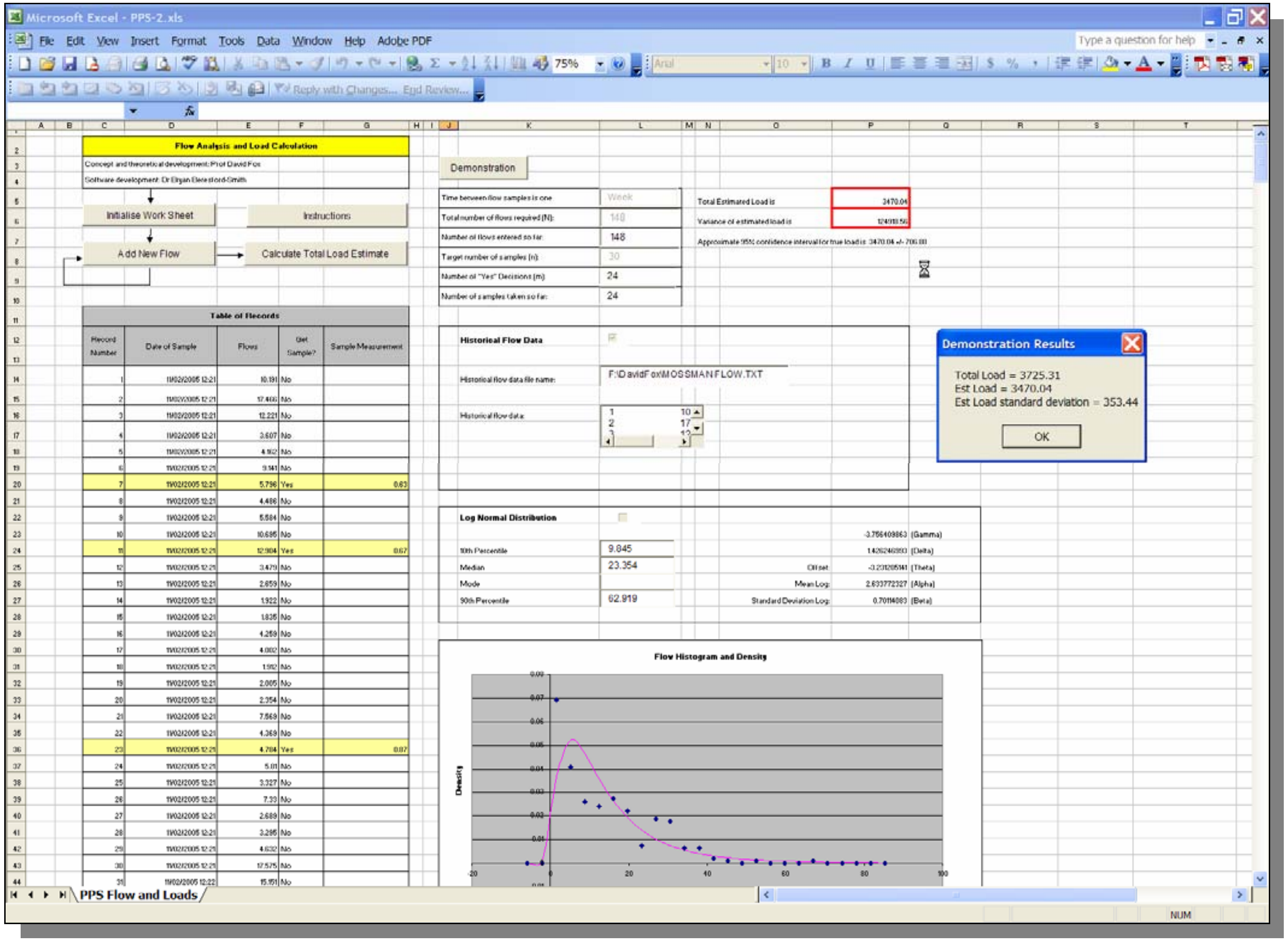


Figure 12 Screen capture from the FSS software tool for selecting flow-biased samples.

5. Estimating Loads from Sparse Water Quality Data

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

Due to the relatively sparse nature of concentration data, some estimation technique must be applied, based on some assumptions about the behaviour of pollutant concentrations in-stream in the times when water quality was not sampled. Three main types of data imputation techniques can be used:

1. **Interpolation Techniques:** where assumptions are made about how concentrations vary in time between samples. Typical interpolation techniques are to linearly interpolate between concentrations or apply cubic splines to a time series of concentrations. These techniques require that concentrations from individual samples are assumed to represent the average daily concentration for the sampled day, and then the average daily concentration on non-sampled days is determined by linearly interpolating between fortnightly sampled concentrations.

Regression or Rating Curve Techniques: where a relationship is assumed to hold between flow and concentration of a particular time period, say daily, and the concentration of non-sampled periods is inferred from the flow data. These techniques can also be extended to include relationships with other variables such as lagged concentrations, lagged flows, seasons of a year and long-term trend. These techniques can only be used where a relationship between variables is established and that relationship can reasonably be expected to hold in non-sampled periods. One of the difficulties with the rating curve method for deriving concentration estimates is the well know problem of different functional relationships between *Q* and *C* over different portions of the hydrograph (Preston et al. 1989). This has been attributed to differences in system hydrology and constituent behaviour as depicted in figure 13 (Richards and Holloway 1987; Johnson 1979).

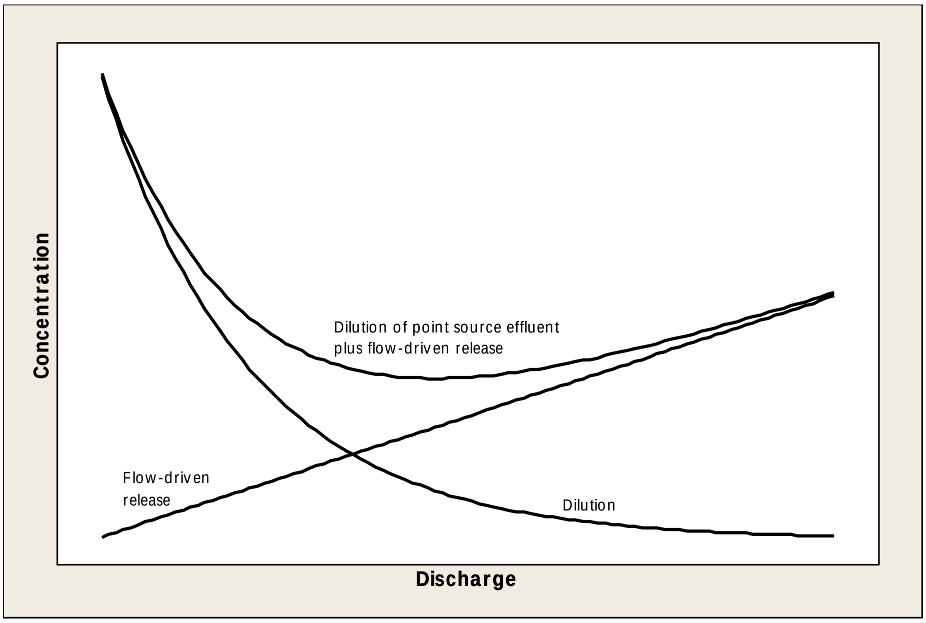


Figure 13 Indicative relationship between concentration and discharge (adapted from Preston et al. 1989).

Because of this anomaly, fitted linear regression lines to *Q*-*C* data over the entire range of discharge tend to perform poorly. If the situation was as straightforward as indicated in figure 13, then clearly a better representation would be afforded by fitting a more complex model. However, it is often the case that strong *Q*-C relationships are either non-existent or masked by high levels of ‘noise’. One way of potentially improving the estimation of *C* is to partition or stratify the discharge regime and develop separate regression relationships in each stratum. It is also important to note that the fundamental *Q*-*C* relationship changes during the year. This is evidenced by the monthly sequence of bivariate probability distributions for CG03 shown in figure 14.

2. **Averaging or Ratio Techniques:** where statistics derived from the available concentration samples and flow time series are used to estimate loads of longer time spans. For example, the annual load could be calculated as the average concentration of samples multiplied by the total annual measured flow. There are several different Averaging or Ratio Techniques and a comparison is given.

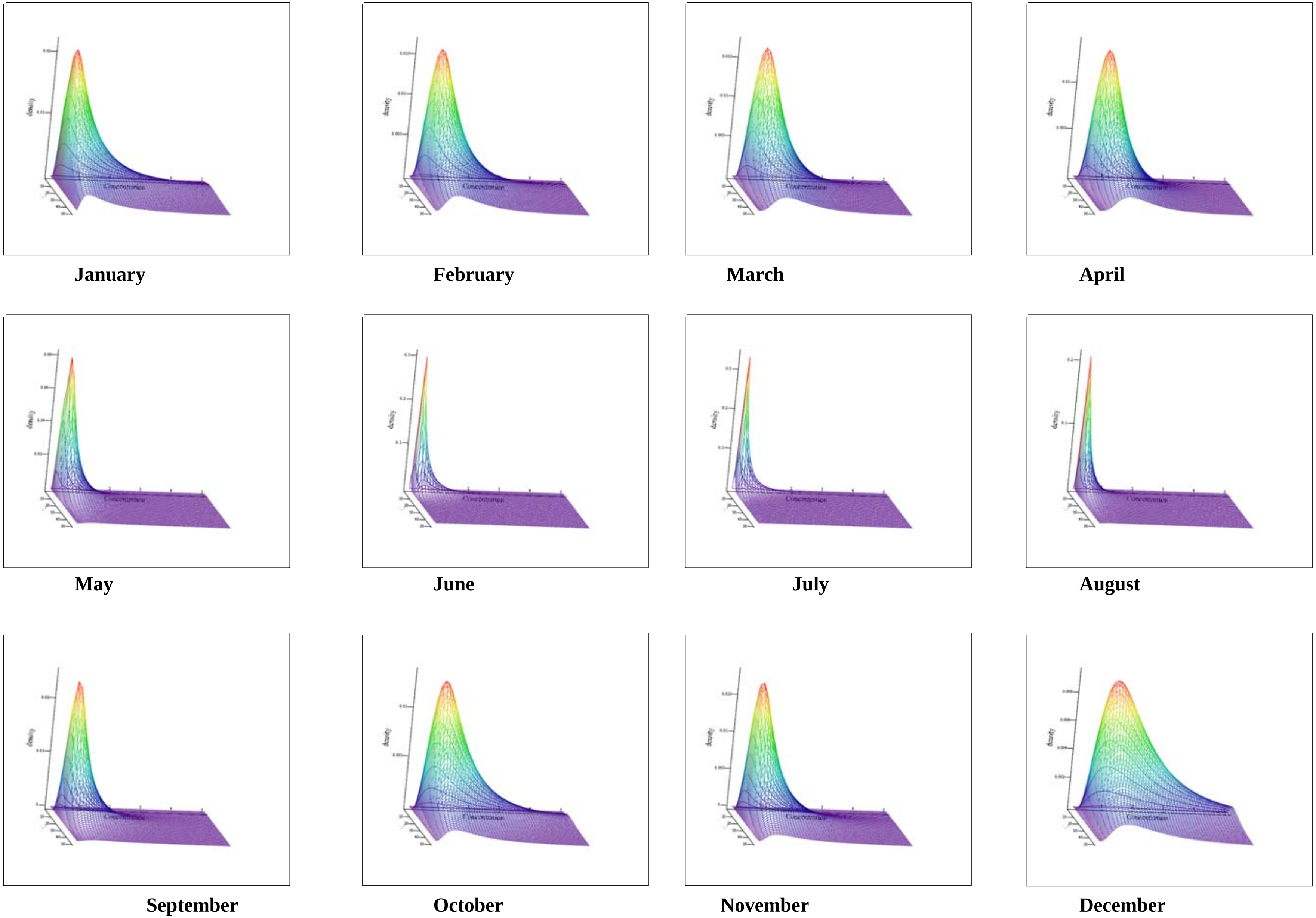


Figure 14. Monthly bivariate lognormal probability distributions for monthly flow and concentration data for CG03

5.1 Statistical characterisation of discharge

Analysis of discharges in the main drains of the McAlister irrigation district in Central Gippsland, Victoria uncovered interesting phenomena in the distributions of *log*-transformed flow data (Fox 2003) and these have been used as the basis of flow stratification (figure 15).

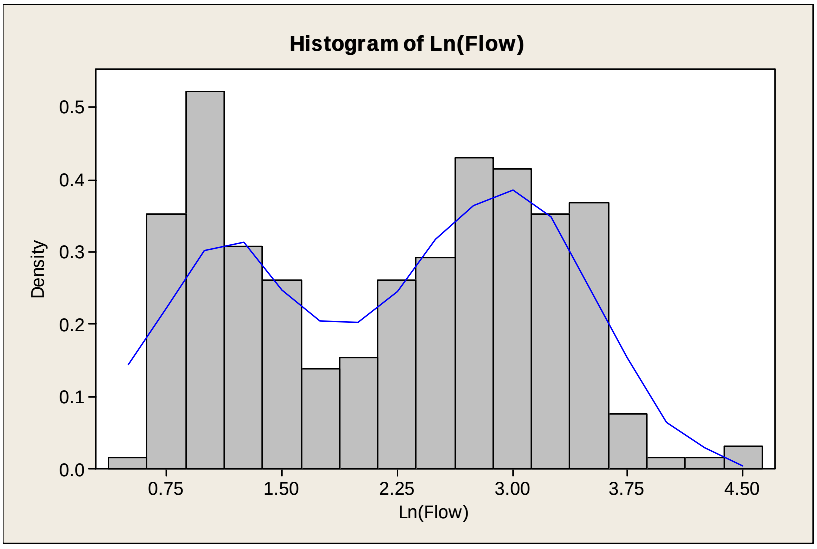


Figure 15 Smoothed empirical histogram of log-transformed 1998 flow data for Gippsland Central Drain No. 3

A obvious feature of figure 15 is the bimodality of the empirical distribution. This phenomenon has been extensively investigated by Fox (2004) and has been attributed to base-flow and peak-flow components of the overall flow distribution. Following Fox (2004) we find that the overall empirical distribution (log-scale) is well described by a mixture of two normal distributions (figure 16).

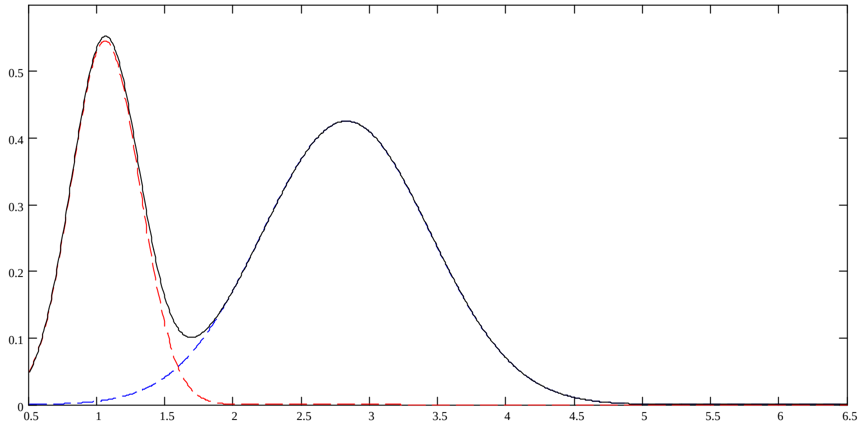


Figure 16 Mixture of fitted normal distributions for log-transformed 1998 flow data for Gippsland Central Drain No. 3

The parameters of the normal distributions and the mixing parameter are given in table 2 and a comparison of the resulting fit is shown in figure 17.

Table 2 Parameters of fitted normal distributions for *log*-transformed 1998 flow data for CG03 (ϕ is referred to as the 'mixing' parameter).

Flow regime (*i*)	μ_i	σ_i	ϕ
'Base flow'	1.057817	0.2513603	0.34391
'Peak flow'	2.825229	0.6155076	0.65609

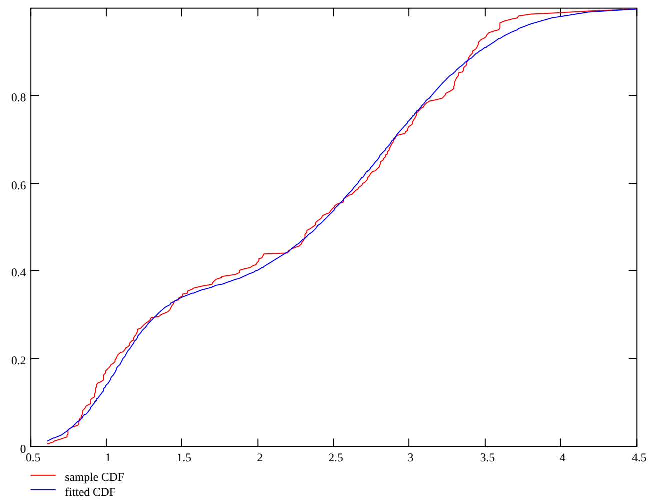


Figure 17 Comparison of fitted distribution (blue line) and observed sample distribution (red line) for log-transformed 1998 flow data for Gippsland Central Drain No. 3

Note, the 'Peak' flow mixing parameter of 66% in table 2 is in line with the proportion of time corresponding to the irrigation season (68%). Thus a more apt description of the flow regimes might be 'Non-irrigation' and 'Irrigation'.

As described in Fox (2004), the theoretical mixture distributions permit the identification of an 'optimal' classification rule for any flow. In this case the rule is:

$$Flow = \begin{cases} \text{'non-irrigation'} & \text{if } \log(flow) \le 1.5919 \\ \text{'irrigation'} & \text{if } \log(flow) > 1.5919 \end{cases}$$

A graphical representation of this classification scheme is depicted in figure 18.

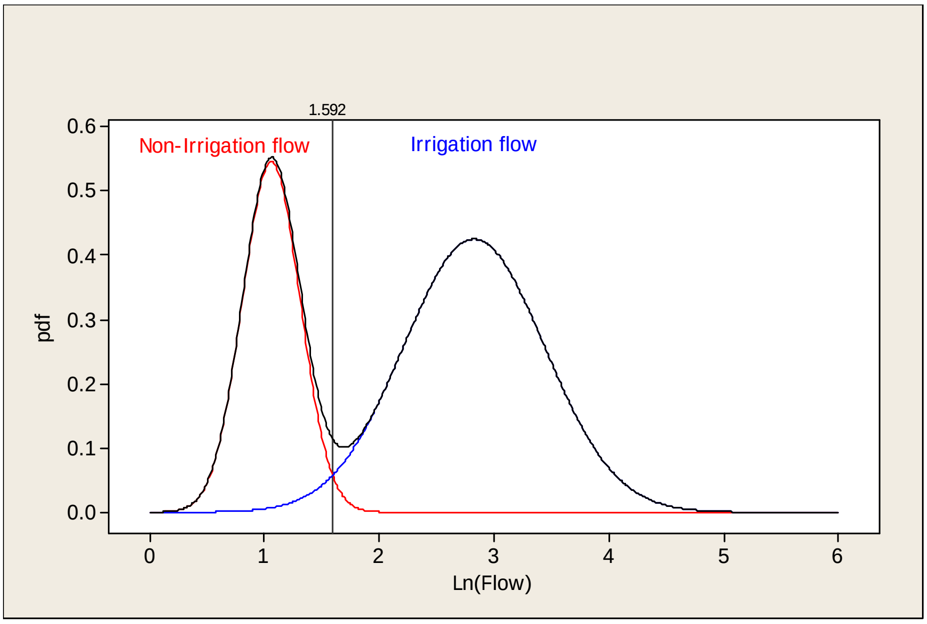


Figure 18. Optimal classification of G3 log-flows.

The performance characteristics of the optimal classification scheme have been summarised by the matrix of conditional probabilities (Table 3).

Table 3 Conditional probabilities for optimal flow classification rule.

Classified Flow	True Flow: Non-Irrigation Flow	True Flow: Irrigation Flow
Non-Irrigation Flow	0.9832	0.0225
Irrigation Flow	0.0168	0.9775
Prior probability	0.34391	0.65609

The overall 'success' rate for this classification scheme is (0.34391)(0.9832) + (0.65609)(0.9775) = 0.979. In other words, an unknown flow will be correctly classified 98% of the time. This technique of flow stratification enables more precise (ie. smaller variance) annual load estimates to be computed since the flow and concentration characteristics are likely to be very different in the two flow regimes.

5.2 Load estimation techniques

Once data is available, the analyst is confronted with a seemingly long list of alternative computational formulae for load estimation. Letcher et al. (1999) provide a list of no fewer than twenty load formulae although many of these are variants of a common approach (eg. estimation based on a weighted average with different assignment of weights). Degens and Donohue (2002) have also documented and compared the main load estimation procedures and cite numerous other similar studies. In some cases the computational approach will be dictated by the sampling protocol. For example, the use of a stratified estimator is clearly linked to a stratified sampling plan. All analytical methods fall into one of two main categories: weighted averages (which includes simple averaging and stratified methods) and ratio / regression estimators (these are combined since the ratio estimator can be thought of as a special case of regression estimation). Cohn (1995) also discusses the use of rating curves for load estimation. This is a (regression) model-based approach for 'infilling' concentration data when only flow has been measured and is thus a regression procedure.

Many reviews of techniques for load estimation have been previously undertaken (Preston et al. (1989), Cohn et al. (1989), Littlewood (1992), Letcher et al. (2002), Degens and Donohue (2002), Mukhopadhyay and Smith (2000)). These studies have usually concluded that there is no single method which provides universally precise and unbiased 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. Based on the available research (listed above) and overlaying the types of sampling regimes seen in practice, a simplified summary of appropriate load estimation techniques has been prepared (Table 4). This matrix provides broad guidance on the categories of techniques to be considered, however, there are many specific variations of these techniques.

Table 4 Typology of annual nutrient load estimation methods

<table>
<tr><th></th><th colspan="4">Sampling Regime for Pollutant Concentration</th></tr>
<tr><th></th><th rowspan="2">Sparse sampling
(> monthly)</th><th colspan="2">Regular sampling (e.g. weekly, fortnightly, monthly)</th><th rowspan="2">Continuous sampling
(e.g. daily, near daily)</th></tr>
<tr><th></th><th>Limited event data</th><th>Representative event data</th></tr>
<tr><td>No significant[1] relationship present (between flow and nutrients)</td><td>Averaging or Ratio</td><td>Averaging or Ratio
• Seasonally stratified</td><td>Averaging or Ratio
• Seasonally stratified
• Flow- weighted stratified</td><td>Linear interpolation</td></tr>
<tr><td>Significant relationship present</td><td>Regression</td><td>Regression or Averaging or Ratio
• Seasonally stratified</td><td>Regression or Averaging or Ratio
• Seasonally stratified
• Flow- weighted stratified</td><td>Linear interpolation</td></tr>
</table>

Additionally, guidance on the sampling regime should be adjusted depending on the characteristics of the catchment in question and this issue will be investigated in future research. The typology presented in Table 4 has been constructed by excluding techniques that are not valid for particular sampling regimes and catchment characteristics. 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 secondly, that the interpolation techniques cannot be assumed to be valid unless the water quality samples are almost continuous. The issue of regression techniques was addressed by Peel and McMahon (2001) in their study of the power of nutrient load estimates where they assessed the significance of relationships between instantaneous flow and Total Nitrogen (TN), and instantaneous flow and TP. They concluded that the variance in TN and TP explained by instantaneous flow was too low to justify use for infilling unknown values of TN or TP concentrations. Therefore, unless a significant relationship is established for a particular site, regression techniques are of limited use (and are therefore not included in the following analyses).

Figure 19 highlights the many decisions to be made in load estimation and also highlights how the same seven methods can be applied in three different ways: using

[1] The significance of a regression relationship can be tested using statistical hypothesis testing techniques.

the data as a whole, on a seasonal basis and using flow stratification (where calculations are made for high and low flows). Further details of the methods are given in Table 5 below and Appendix A.

Table 5 Load estimation methods used in this report

Method 1 (A_AvCsFp) = Sample period flow-weighted averaging = sample conc x mean flow between sampling period in a year
Method 2 (A_AvCmFm) = Annual mean sample conc-mean sample flow averaging = mean sample conc x mean sample flow in a year
Method 3 (A_AvCsFs) = Annual sample conc-sample flow averaging = sample conc x sample flow in a year
Method 4 (A_AvCmFd) = Annual mean sample conc-mean flow averaging = mean sample conc x mean annual flow in a year
Method 5 (A_FWMC) = Annual flow-weighted mean conc = sample conc x sample flow in a year weighted by ratio of mean annual flow/mean sample flow
Method 6 (A_RtoSim) = Annual simple ratio estimator (load estimate similar to FWMC method, but variance estimate differs)
Method 7 (A_RtoKen) = Annual Kendall's ratio estimator
Method 8 (A_RtoBea) = Annual Beale's ratio estimator
Method 9 (S_AvCmFm) = Seasonal-stratified mean sample conc-mean sample flow averaging = sum of mean sample conc x mean sample flow of all seasons in a year
Method 10 (S_AvCsFs) = Seasonal-stratified sample conc-sample flow averaging = sum of sample conc x sample flow of all seasons in a year
Method 11 (S_AvCmFd) = Seasonal-stratified mean sample conc-mean flow averaging = sum of mean sample conc x mean seasonal flow of all seasons in a year
Method 12 (S_FWMC) = Seasonal-stratified flow-weighted mean conc = sum of sample conc x sample flow weighted by ratio of mean seasonal flow/mean sample flow of all seasons in a year
Method 13 (S_RtoSim) = Seasonal-stratified simple ratio estimator
Method 14 (S_RtoKen) = Seasonal-stratified Kendall's ratio estimator
Method 15 (S_RtoBea) = Seasonal-stratified Beale's ratio estimator
Method 16 (R_AvCmFm) = Flow regime-stratified mean sample conc-mean sample flow averaging = sum of mean sample conc x mean sample flow of all regimes in a year
Method 17 (R_AvCsFs) = Flow regime-stratified sample conc-sample flow averaging = sum of sample conc x sample flow of all regimes in a year
Method 18 (R_AvCmFd) = Flow regime-stratified mean sample conc-mean flow averaging = sum of mean sample conc x mean regime flow of all regimes in a year
Method 19 (R_FWMC) = Flow regime-stratified flow-weighted mean conc = sum of sample conc x sample flow weighted by ratio of mean seasonal flow/mean sample flow of all regimes in a year
Method 20 (R_RtoSim) = Flow regime-stratified simple ratio estimator
Method 21 (R_RtoKen) = Flow regime-stratified Kendall's ratio estimator
Method 22 (R_RtoBea) = Flow regime-stratified Beale's ratio estimator

(Source: Refer to Appendix A)

A review of the load estimation literature suggests that there are different approaches and needs for load estimation exercises in urban and rural settings. Load estimation in the urban environment usually done using models and rural settings with intensive agriculture will also fall into this category. This is mainly due to the fact that fluxes have different sources of variation other than the flow rate. It is also important to note that models generally do not work reliably at the watershed scale however relative estimates are useful for comparison or evaluating management scenarios.

Method	Flow data from all days used	Only flow data from sample days	Naïve daily load used	Bias correction factor applied	No stratification	Seasonally Stratified	Flow Stratified
1	√				√		
2		√			√		
3		√	√		√		
4	√				√		
5	√		√		√		
6	√		√		√		
7	√		√	√	√		
8	√		√	√	√		
9		√				√	
10		√	√			√	
11	√					√	
12	√		√			√	
13	√		√			√	
14	√		√	√		√	
15	√		√	√		√	
16		√					√
17		√	√				√
18	√						√
19	√		√				√
20	√		√				√
21	√		√	√			√
22	√		√	√			√

Figure 19 **Key characteristics of twenty two load estimation methods**

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.

There are many candidate methods for estimating the quantity of sediment and nutrients discharged from a stream. In the first instance, Fox (2004) distinguishes *direct* estimation methods (using measured concentration and flow data) from *indirect* methods (using simulated loads from catchment models), and further identifies statistical design (i.e. the spatial and temporal scales of data collection) and analytical methodology as key issues for any direct estimation method. This report focuses on issues associated with the analytical methodology of direct estimation, while future reports will address issues of statistical design.

As highlighted in Fox (2004), the problem of obtaining ‘representative’ load is difficult since WQ data is sparse relative to the estimation of continuous flow-concentration flux. There is a plethora of algorithms which can be simplified to the following categories.

5.2.1 Numerical integration

The simplest approach is direct numeric integration, and the total load is given by

$$\text{Load} = \sum_{i=1}^{n} c_i q_i t_i$$

where

c_i is the concentration in the i^{th} sample
q_i is the corresponding flow
t_i is the time interval represented by the i^{th} sample.

Numerical integration is only satisfactory if the sampling frequency is high – often on the order of 100 samples per year or more, and sufficiently frequent that all major runoff events are well sampled. This method, and particularly the sampling strategy, assumes that flows are highly variable and that concentrations increase with flow. The sampling strategy is based on the assumption that most of the load occurs in a short period of time during storm runoff events, and that accurate loads can be obtained by sampling primarily during that period of time. If a pattern can be identified which will allow sampling to be allocated more efficiently by concentrating sampling at certain times, the schedule can be adjusted. For the period-weighted approach, measured concentrations were linearly interpolated through time between samples.

As a numeric integration method, averaging approaches use some form of average in the calculation of the loads. The simplest approach involves multiplying the average concentration for some period of time by the mean daily flow for each day in the time period to obtain a succession of estimated daily (unit) loads. Generally, averaging approaches tend to be biased if concentration is correlated with flow: the calculated load is too low if the correlation is positive and too high if the correlation is negative.

The flow interval technique (Yaksich and Verhoff, 1983) is a semi-graphical technique, which begins with a plot of the year’s observed instantaneous fluxes as a function of instantaneous flows at the time the samples were taken. The plot is divided into several intervals of uniform size covering the range of mean daily flows for all days of the year. For each interval, the average flux is calculated and the number of days with mean daily flows in the interval is determined. The interval load is calculated as the product of the average flux, the number of days in the interval, and the appropriate units conversion factor. The annual load is calculated by summing the interval loads.

5.2.2 Regression

Regression approaches develop a relationship between concentration and flow based on the samples taken. These data are used to establish a regression relationship of the form

$$c_i = \beta_0 + \beta_1 q_i$$

where c_i is a measured concentration corresponding to flow q_i.

The parameters, β_0 and β_1 are estimated using ordinary least squares (OLS) regression and the estimated model then used to estimate concentrations for days not sampled. In many applications, both concentration (and flux) and flow are log-transformed to improve the model fit. Regression relationships between log-transformed concentration or flux and flow are often called **rating curves**.

Simple regression approaches assume that the relationships between concentration and the independent variables (eg. flow, lagged-flow, season etc.), are all linear. A more sophisticated (non-linear) regression model is the USGS Seven-parameter Model:

$$\ln(c_i) = \beta_0 + \beta_1 \ln(q_i) + \beta_2 (\ln q_i)^2 + \beta_3 t_i + \beta_4 t_i^2 + \beta_5 \sin(2\pi t_i) + \beta_6 \cos(2\pi t_i) + \varepsilon_i$$

where q is discharge (flow) and t is time.

5.2.3 Ratio estimators

In this method, the daily load is calculated as the product of concentration and flow on days on which samples are taken, and the mean of these loads is also calculated. The mean daily load is then adjusted by multiplying it by a flow ratio, which is derived by dividing the average flow for the year as a whole by the average flow for the days on which chemical samples were taken. The adjusted mean daily load is multiplied by

365 to obtain the annual load. A bias correction factor can be included in the calculation, to compensate for the effects of correlation between discharge and load.

The basis of ratio estimators is the assumption that the ratio of total load to total flow *for the entire year* should be approximately the same as the ratio of total load to total flow *for the sample*. Thus, assuming a sample size of *n* and a period of interest, *N* (eg. *N=365*), the ratio estimator is obtained by equating

$$\frac{\sum_{i=1}^{n} L_i}{\sum_{i=1}^{n} Q_i} = \frac{\sum_{i=1}^{N} L_i}{\sum_{i=1}^{N} Q_i}$$

which gives

$$\sum_{i=1}^{N} L_i = \left(\frac{\sum_{i=1}^{N} Q_i}{\sum_{i=1}^{n} q_i} \right) \sum_{i=1}^{n} L_i$$

Note, that the ratio estimator requires knowledge of the *total discharge* for the period of interest (the numerator inside the bracket above).

Ratio estimators assume that there is a positive linear relationship between concentration and flow. In most applications of ratio estimators to pollutant load estimation, the calculations and sometimes the sampling program have been stratified, usually by flow and/or season.

5.2.4 Composite methods

The composite method is a new approach to estimating loads that combines the period-weighted approach and the regression-model method. In the composite method, a regression model is used to predict concentration variations between samples due to changing hydrologic conditions and season. A period-weighted approach is then used to adjust the predicted regression model concentrations to the actual sample concentrations when a sample is collected, and applies the residuals (the difference between the model predicted and observed concentrations) to the concentration model in a piecewise linear manner to periods between sample collections.

5.3 Rules of Thumbs for choosing load estimate methods

We will not make a comprehensive assessment of the utility of the various estimating equations in tables 1 and 2 since this is well documented in the literature. The main observations are:

- Averaging techniques are simple and relatively robust although biases will result from inadequate representation of storm events. In instances where the correlation between discharge and concentration is positive (negative), loads will tend to be underestimated (overestimated). Weighted averaging is a simple device that, to some extent, overcomes this drawback. A substantial decline in precision associated with averaging methods has been observed as the sample size, *n* decreases (ie. the time interval over which samples are obtained increases) (Walling and Webb (1981)).
- Stratification can potentially improve both the accuracy and precision of load estimates (Preston et al. 1989).
- Ratio estimators work best when discharge and concentration are linearly related (passing through the origin) with non-constant variance. They are considered more suited to situations where there is less intensively sampled concentration data. The Beale ratio estimator (Beale 1962) is widely used.

A tangible outcome of our research has been the development of a software tool. GUMLEAF (Generator for Uncertainty Measures and Load Estimates using Alternative Formulae) (Tan et al. 2005a), was developed to facilitate the computation of annual pollutant loads (incorporating sampling and method uncertainties) and visualisation of data and results, using the 22 methods. Details of the structure and application of this software is documented in the GUMLEAF v0.1alpha User Guide (Tan et al. 2005b). A complete listing of the 22 methods is given in Appendix A.

6 APPLICATION TO DRAINS IN THE MID

Using the twenty two methods described in Appendix A, separate estimates of annual load were calculated for each of the six sites in the MID for each year of available data[2]. And, unless some other information or analysis is presented to limit the validity of particular estimation techniques, it is reasonable to assume that each of these estimates is equally valid. For example, twenty two different estimates of the annual TP load at CG02 in 2000 and 2004 are shown in Figures 20 and 21 respectively. Estimates vary considerably across the twenty-two methods even though sampling was daily in 2000 (although there is some data missing) and every second day in 2004. These results show considerable differences for some estimates, and demonstrate that the 'true' load cannot be calculated.

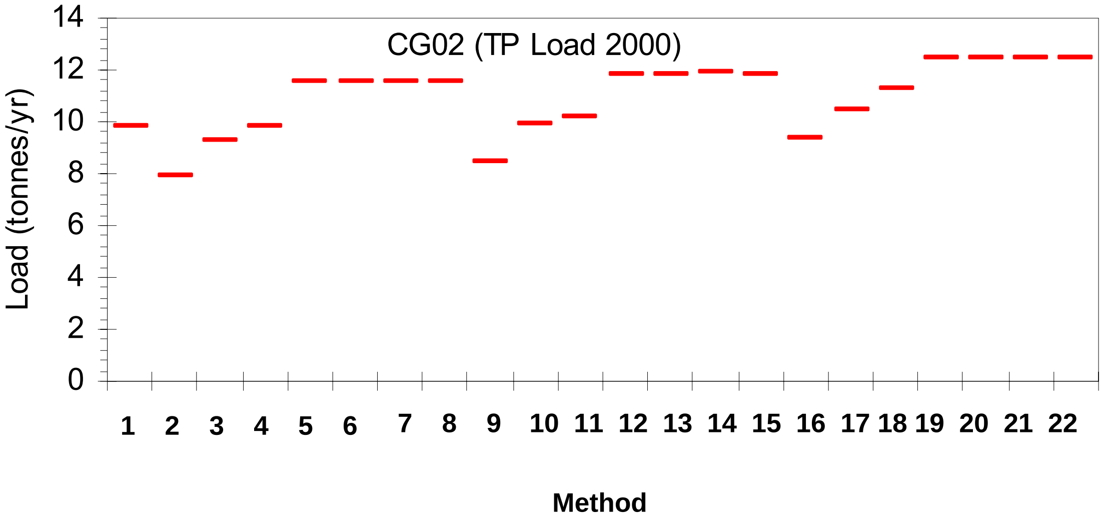


Figure 20 Annual TP Load Estimates for CG02 using twenty two different estimation techniques for 2000

[2] Not all twenty two methods could be applied in all cases (for all sites in all years). In particular, some seasonal and flow stratification calculations could not be completed where insufficient data was available. Details of the number of samples and flow distribution for each site and year are presented in Appendix B.

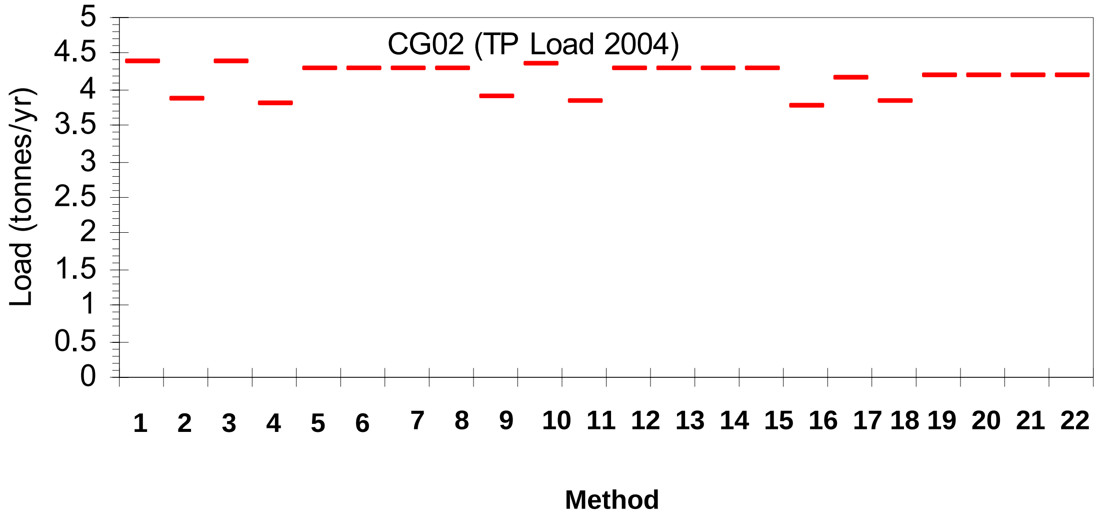


Figure 21 Annual TP Load Estimates for CG02 using twenty two different estimation techniques for 2004

Future research will focus on improving our understanding of uncertainty beyond historical load estimation to incorporate considerations of sampling also. The design of sampling protocols should be developed with a corresponding load estimation technique in order that the uncertainty of estimates is minimised. Future research will provide guidance on sampling and load estimation to minimise uncertainty (with a minimum of water quality samples).

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 and ratio methods, that sampling is representative of general conditions. In practice, determining the pollutant concentration during high flow events is particularly important since a large proportion of the annual load is transported during these events, and frequently, higher than average concentrations occur then.

Using the each estimate of annual load for each site in 2000 and 2004 a five year percentage reduction to 2004 has been calculated (Table 6). On the basis of these calculations, there can be some confidence in concluding that at almost all sites there has been a significant reduction in nutrients. Furthermore, the standard deviation of some reductions is quite low giving a reasonable degree of certainty at particular sites (e.g. CG02 and Newry Ck). Strictly speaking, such an assessment of load reduction should be informed by the magnitude of flow or rainfall in those years (since dry years will necessarily have lower flows and therefore relatively lower loads). Future research will address the formulation of load targets to consider the magnitude of flows.

Table 6 Five year reductions in estimated loads between 2000 and 2004

Method	CG02	CG03	CG04	LWMD	Serp	Newry
Mean	**61%**	**19%**	**n/a**	**16%**	**13%**	**38%**
Sd	**5%**	**10%**	**n/a**	**5%**	**18%**	**5%**
1	55%	26%		13%	12%	40%
2	51%	38%		12%	45%	26%
3	53%	32%		6%	35%	38%
4	61%	24%		24%	14%	32%
5	63%	15%		18%	-1%	43%
6	63%	15%		18%	-1%	43%
7	63%	15%		18%	-1%	43%
8	63%	15%		18%	-1%	43%
9	54%	40%		19%	47%	26%
10	56%	33%		10%	35%	35%
11	62%	23%		25%	17%	30%
12	64%	13%		18%	-1%	38%
13	64%	13%		18%	-1%	38%
14	64%	13%		18%	-1%	38%
15	64%	13%		18%	-1%	38%
16	60%	24%		9%	45%	40%
17	60%	21%		10%	35%	40%
18	66%	7%		17%	14%	40%
19	66%	7%		18%	-1%	40%
20	66%	7%		18%	-1%	40%
21	66%	7%		18%	-1%	40%
22	66%	7%		18%	-1%	40%

6.2 Quantification of the Uncertainty of Annual TP Load Estimates

The quantification of the uncertainty of load estimates should reflect the three sources of uncertainty: knowledge, variability and measurement uncertainty. However, since no information is available regarding data uncertainty, this source will not be considered in this analysis.

The procedure used to quantify uncertainty uses Monte-Carlo simulation[3] where the knowledge uncertainty and stochastic uncertainty were considered. The knowledge uncertainty was reflected since the one method for calculation (from the twenty two possible methods) was randomly selected, providing a particular mean and variance for consideration. Then, stochastic uncertainty was considered by assuming the estimate was normally distributed around the mean, generating a random normal variate with the relevant mean and variance. One thousand repetitions were generated and histograms produced to represent the resulting range of load estimates. Specifically, the method to quantify uncertainty for each site in each year consisted of six steps:

1. Select random integer, j, between 1 and 22, corresponding to a particular method of load estimation (described in Section 2);
2. Determine corresponding mean, μ_j, and variance, σ^2_j, of the estimated annual load , for the randomly selected method and for the particular site and year;
3. Randomly generate a standard normal variate for each repetition k, $t_k \sim N(0,1)$;
4. Calculate the simulated load for each repetition k (L_k), such that:

$$L_k = \mu_j + t_k.\sigma_j$$

5. Repeat for $k = 1 \ldots 1000$
6. Present histogram of L for each site in each year.

The uncertainty of estimated loads is presented in three forms. In Table 4, the median estimated annual TP loads are presented along with the 5th, 25th, 75th and 95th percentile values. Also, in Appendix C, a Box-Plot is presented for each site showing these results along with a corresponding Box-Plot of daily flow. Finally, in Appendices D through I, the histograms showing the frequency of simulated loads are given for each site in each year.

[3] Monte-Carlo simulation relies on generating many example solutions to a problem to provide an approximate a numerical solution.

Table 7 Percentiles of Load Estimated Annual TP Loads (Tonnes)

Site	Year	Load - 5th Percentile	Load - 25th Percentile	Median Load	Load - 75th Percentile	Load - 95th Percentile
CG02	2000	8.2	9.8	11.3	11.9	13.2
	2001	32.6	38.8	42.6	44.0	47.7
	2002	8.6	9.8	10.8	11.4	12.4
	2003	1.1	1.1	1.2	1.3	1.3
	2004	3.8	3.9	4.2	4.3	4.5
CG03	1998	5.4	5.9	7.6	8.1	9.6
	1999	7.1	8.1	8.5	8.8	9.4
	2000	7.2	7.9	8.9	9.2	9.7
	2001	9.4	11.1	12.1	12.5	13.2
	2002	6.7	7.9	8.7	8.9	9.3
	2003	4.1	4.7	4.8	4.9	5.1
	2004	4.6	6.1	7.5	8.0	9.0
CG04	2001	2.6	3.9	4.8	5.8	7.4
	2002	8.5	10.4	11.8	13.2	15.5
	2003	2.7	3.7	4.1	4.6	5.8
	2004	1.5	2.0	2.5	2.9	3.6
LWMD	1998	2.8	5.5	6.4	7.0	8.3
	1999	5.3	5.9	6.9	7.1	7.5
	2000	2.6	2.9	3.1	3.3	3.4
	2001	15.7	17.7	19.0	20.2	22.2
	2002	5.8	6.1	6.2	6.4	6.9
	2003	0.5	0.5	0.6	0.6	0.6
	2004	2.2	2.3	2.6	2.7	3.0
Serp	2000	1.5	1.7	1.8	2.1	2.3
	2001	1.7	1.8	1.9	2.0	2.2
	2002	1.8	2.0	2.5	2.8	3.4
	2003	0.4	0.5	0.7	0.8	1.0
	2004	1.1	1.4	1.6	1.8	2.1
Newry	2000	1.5	2.1	2.3	2.4	2.7
	2001	3.3	4.3	5.2	5.5	6.2
	2002	2.9	3.3	3.6	3.8	4.1
	2003	0.6	0.7	0.7	0.8	0.8
	2004	1.1	1.3	1.4	1.5	1.6

7 DISCUSSION

Overall, there are significant sources of uncertainty in the estimation of nutrient loads, arising from the choice of estimation technique (knowledge uncertainty), stochastic and measurement uncertainty.

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(or similar logic) is applied to select appropriate techniques. 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, it is essential that the same estimation technique is applied to determine all annual estimates for comparative purposes (i.e. to give an apples to apples comparison).

A quantification of uncertainty was presented for Total Phosphorous for six sites in the Macalister Irrigation District for all available years. The results of this quantification showed that, whilst some results were quite reliable, others varied widely and caution should be applied in the application of those estimates. A method for quantifying uncertainty has been described in Section 4 and it is recommended that this methodology be applied wherever robust estimates are required which consider the potential effects of uncertainty.

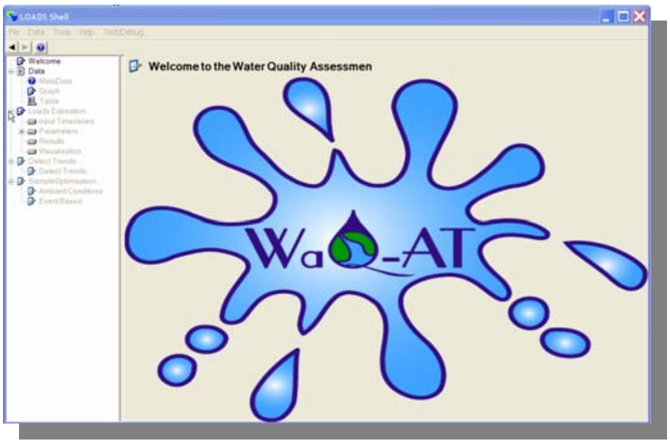
Finally, given the linkages between sampling regimes and appropriate load estimation techniques, it is clear that sampling regimes and protocols should be accompanied by details of corresponding estimation techniques. Future work will be focused on articulating sampling protocols and corresponding load estimation techniques to reduce overall uncertainty of load estimates as much as possible without significantly increasing the number of samples taken.

7.1 Key findings

A number of important observations and results have emerged during the course of this research. Firstly, the statistical decomposition of empirical flow data has provided a rational and consistent way of applying stratified sampling techniques which potentially lead to more accurate load estimates. Furthermore, important insights into the underlying flow regimes afforded by this decomposition can inform the allocation of limited monitoring resources to help identify 'optimal' sampling strategies. Our work has resulted in the development of new statistical algorithms for load sampling and estimation and these have been embodied in two software tools. The size-biased sampling algorithm developed by Fox extends the earlier work of Thomas (1985) in a novel and significant way and enables water quality practitioners to construct flow-biased sampling schemes even for previously ungauged waterways. The GUMLEAF software is the first of its kind in Australia. It is a significant development which not only automates the routine load calculations, but importantly enables comparisons between different computational methodologies as well as providing error estimates. This latter feature is unique and hitherto inaccessible to most practitioners.

7.2 Implications

We believe the work reported on here has the potential to have a pronounced impact on the way natural resources managers approach the related problems of: data collection; analysis; and interpretation in the context of sediment-nutrient load estimation. Our work has already been applied to other systems including tropical river systems, trade waste disposal via sewage effluent, and historical contaminant loads discharged to the coastal waters off Adelaide. The important work on error and uncertainty analysis for the first time provides the necessary statistical background against which aspirational and compliance targets can be meaningfully assessed. We expect that in due course, these results will be incorporated into other modelling frameworks such as *TIME* (The Invisible Modelling Environment) and the Water Quality Assessment Tool (WaQ_AT) currently being developed by the Queensland EPA.



7.3 Application and implementation

Much of the work presented here is highly technical and it is recognised that a necessary next step involves disseminating the results in a more user-friendly manner. The software tools already developed and those currently under development will greatly facilitate this task. We envisage running a number of workshops and training sessions to assist in the uptake and adoption of methods described in this report. Preliminary discussions with colleagues have confirmed the desirability of providing autonomous samplers which have been programmed to implement the sampling strategies and load computations described in this report.

7.4 Further Work

Future research will focus on the following areas:

- the estimation of loads (and associated error estimates) for entire catchments based on limited data for gauged rivers and streams;
- the performance of various sampling protocols in terms of the uncertainty of annual load estimates;
- the formulation of nutrient reduction targets to incorporate considerations such as the magnitude of flow; and
- using data wisely to optimise the estimation of nutrient loads in waterways and across basins. In particular, there are several ungauged sites of interest in the MID and numerical techniques will be applied to determine the potential range of load discharge along with an indication of the corresponding uncertainty;
- development of user-friendly software tools.

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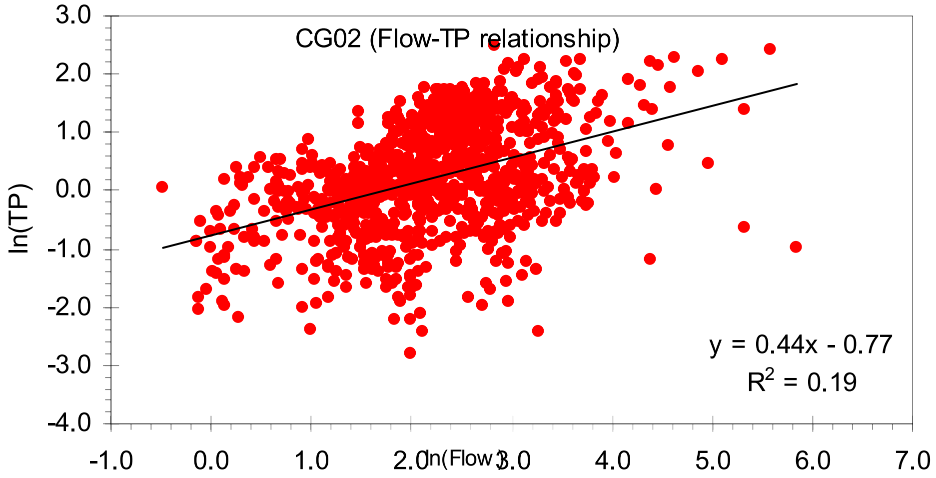
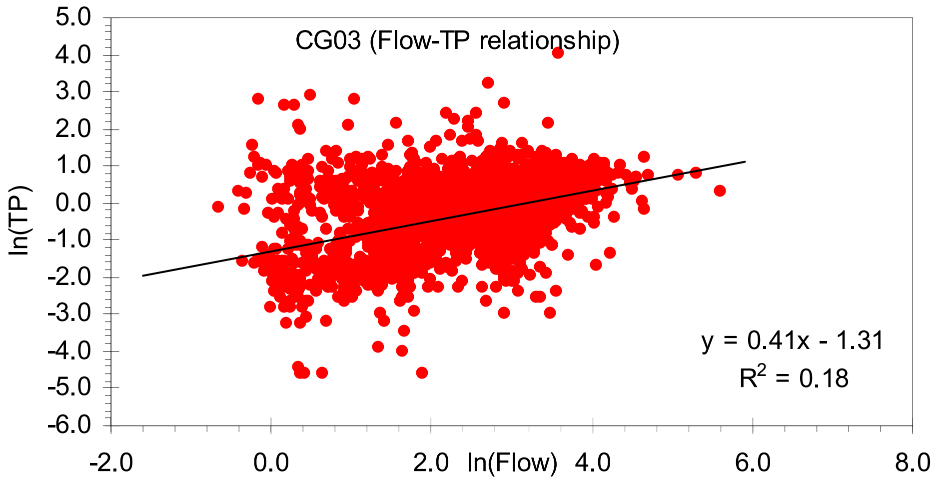
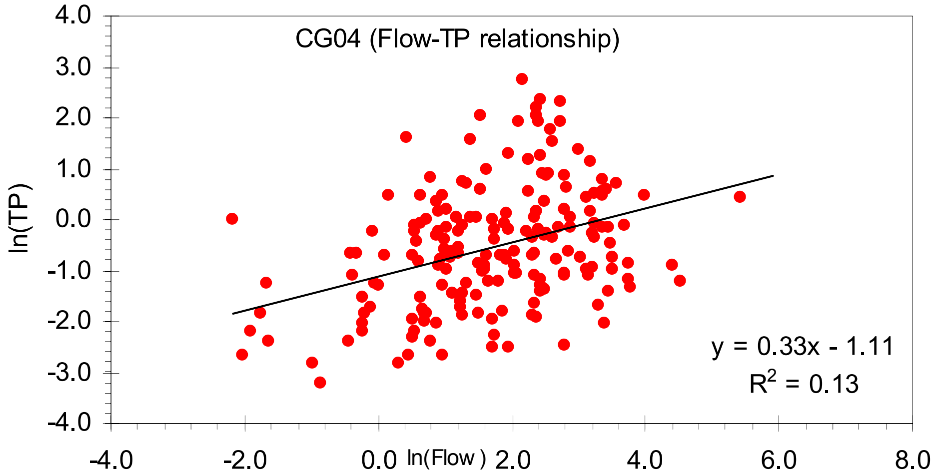
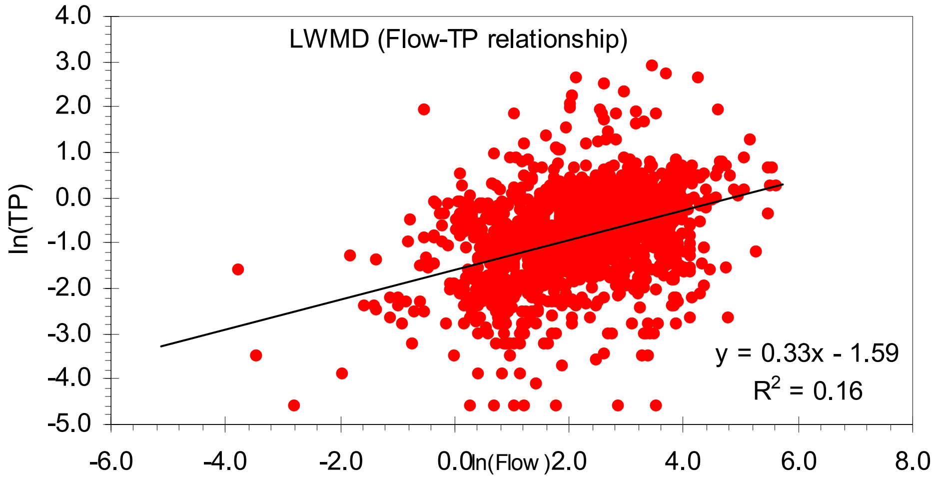
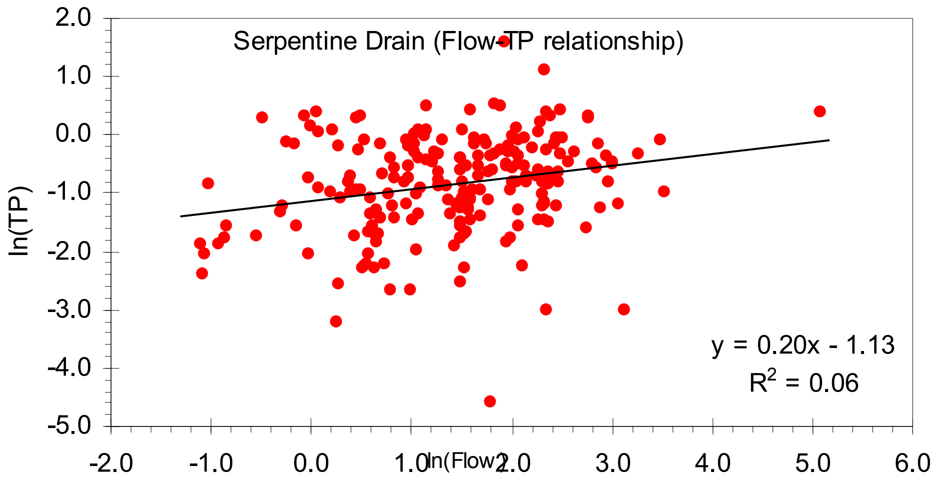
Appendix A: Relationship between Flow and TP for MID sites

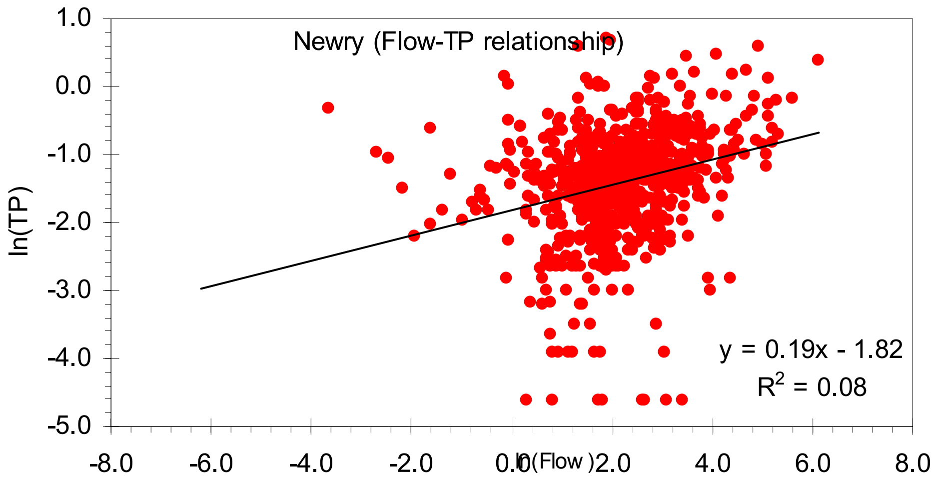







LWMD (Flow-TP relationship)
y = 0.33x - 1.59
R2 = 0.16
ln(TP)
ln(Flow)
4.0
3.0
2.0
1.0
0.0
-1.0
-2.0
-3.0
-4.0
-5.0
-6.0
-4.0
-2.0
0.0
2.0
4.0
6.0
8.0


Serpentine Drain (Flow-TP relationship)
y = 0.20x - 1.13
R2 = 0.06
ln(TP)
ln(Flow)
2.0
1.0
0.0
-1.0
-2.0
-3.0
-4.0
-5.0
-2.0
-1.0
0.0
1.0
2.0
3.0
4.0
5.0
6.0


Newry (Flow-TP relationship)
y = 0.19x - 1.82
R2 = 0.08
ln(TP)
ln(Flow)
1.0
0.0
-1.0
-2.0
-3.0
-4.0
-5.0
-8.0
-6.0
-4.0
-2.0
0.0
2.0
4.0
6.0
8.0

Appendix B: 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	$\sum_{S=1}^{T_S}\left(k\bar{c}_S Q_S\right)$	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	$\sum_{S=1}^{T_S}\left(k\hat{R}_S Q_S\right)$	Seasonal form of Walling & Webb (1981); Method 5 (Littlewood 1992); Method 4 (Letcher et al. 1999)	$\sum_{S=1}^{T_S}\left[\frac{kN_S\left(\sum_{i=1}^{n_S} q_i^{\,2}\right)}{\left(\sum_{i=1}^{n_S} q_i\right)^2} Var\left[L_S\right]\right]$	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)	$\sum_{S=1}^{T_S}\left[\left(k\hat{R}_s Q_s\right)^2 Var\left[\tau_s\right]\right]$	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)	$k^2\sum_{R=1}^{T_R}\left[\left(\frac{N_R}{n_R}\right)^2 Var\left[L_R\right]\right]$	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)	$k^2\sum_{R=1}^{T_R}\left[\frac{N_R{}^2\left(\sum_{i=1}^{n_R}q_i{}^2\right)}{n_R\left(\sum_{i=1}^{n_R}q_i\right)^2}Var\left[L_R\right]\right]$	Fox (2005b)[1]
	18	R_ AvCmFd	Flow regime-stratified mean sample conc-mean flow averaging	$k\sum_{R=1}^{T_R}\left(\bar{c}_RQ_R\right)$	Flow regime form of Ferguson (1987); Table 1 Method 5 (Preston 1989); Method 13 (Letcher et al. 1999)	$k\sum_{R=1}^{T_R}\left[\frac{N_R}{n_R}Var\left[L_R\right]\right]$	Derived based on Fox (2005b)[1]
	19	R_ FWMC	Flow regime-stratified flow-weighted mean conc	$k\sum_{R=1}^{T_R}\left(\hat{R}_RQ_R\right)$	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	$k\sum_{R=1}^{T_R}\left(\hat{R}_RQ_R\right)$	Flow regime form of Cochran (1977); Table 2 Method 1 (Preston 1989); Method 15 (Letcher et al. 1999)	$k^2\sum_{R=1}^{T_R}\left[N_R{}^2\left(\frac{1-\frac{n_R}{N_R}}{n_R\left(n_R-1\right)}\right)\left(\sum_{i=1}^{n_R}\left(l_i-\hat{R}_Rq_i\right)^2\right)\right]$	Cooper & Watts (2002)
	21	R_ RtoKen	Flow regime-stratified Kendall's ratio estimator	$k\sum_{R=1}^{T_R}\left(\left[\left(\frac{N_R-1}{n_R-1}\right)\left(\bar{l}_R-\bar{c}_R\bar{q}_R\right)\right]\hat{R}_RQ_R\right)$	Flow regime form of (Kendall et al., 1983)	$k^2\sum_{R=1}^{T_R}\left[\left(\frac{\hat{R}_RQ_R}{n_R}\right)^2\left(\frac{Var\left[l_R\right]}{\bar{l}_R{}^2}+\frac{Var\left[q_R\right]}{\bar{q}_R{}^2}-\frac{2Cov\left[lq\right]_R}{\bar{l}_R\bar{q}_R}\right)\right]$	Cooper & Watts (2002)

	22	R_ RtoBea	Flow regime-stratified Beale's ratio estimator	$k\sum_{S=1}^{T_S}\left(\left[\dfrac{1+\left(\dfrac{1}{n_R}-\dfrac{1}{N_R}\right)\left(\dfrac{[S_{lq}]_R}{\bar{l}_R\bar{q}_R}\right)}{1+\left(\dfrac{1}{n_R}-\dfrac{1}{N_R}\right)\left(\dfrac{[S_q]_R^{\;2}}{\bar{q}_R^{\;2}}\right)}\right]\hat{R}_R Q_R\right)$	Beale (1962); Table 2 Method 5 (Preston 1989); Method 20 (Letcher et al. 1999)	$k^2\sum_{R=1}^{T_R}\left[\left(\hat{R}_R Q_R\right)^2 Var[\tau_R]\right]$	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)

$\hat{R} = \dfrac{\bar{l}}{\bar{q}}, \hat{R}_S = \dfrac{\bar{l}_S}{\bar{q}_S}, \hat{R}_R = \dfrac{\bar{l}_R}{\bar{q}_R}$ = 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

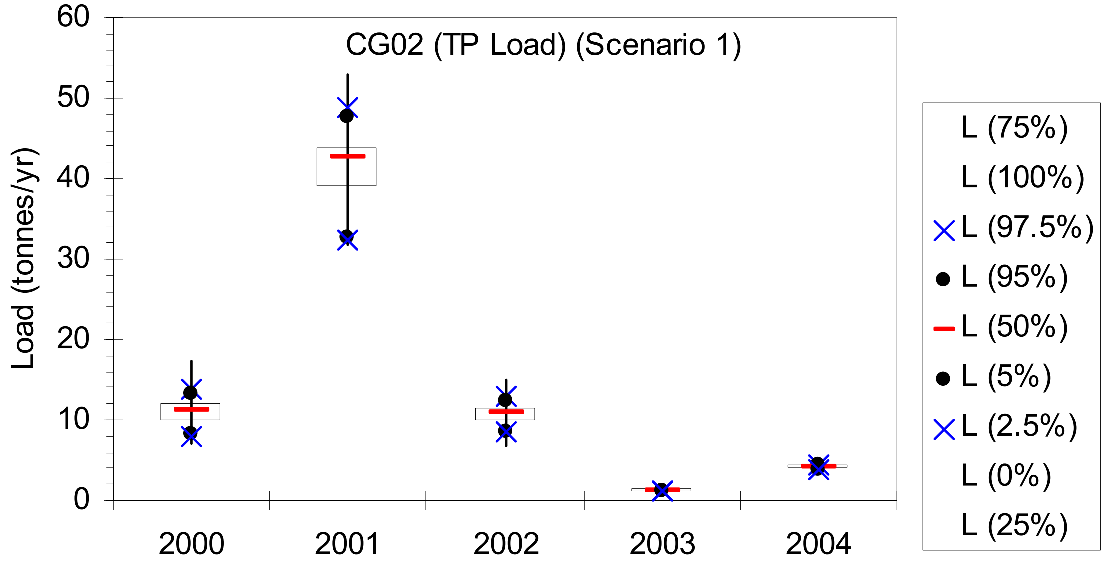
Notes:
[1] Variances for all averaging methods are based on bi-variate log-normal distribution of concentration and flow,
where $Var[L] = E[L^2] - (E[L])^2$, see Fox (2005b) for theoretical expressions of $E[L]$ and $E[L^2]$.

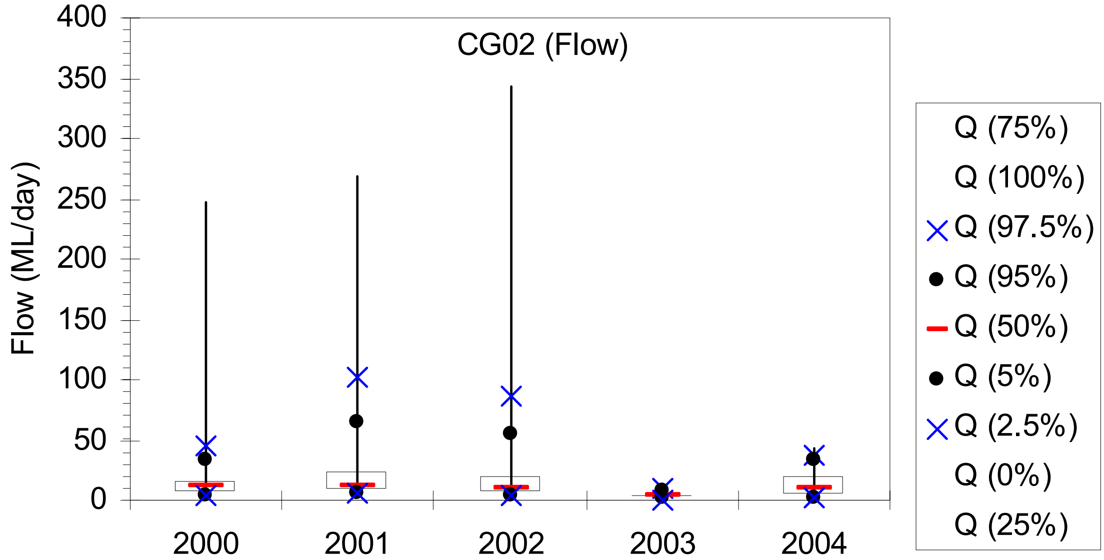
[2] Variance for Beale's ratio method is based on bi-variate normal distribution of load and flow,
see Appendix: Variance of the Beale Estimator in Cooper & Watts (2002) for theoretical expression of $Var[\tau]$.
[3] Modified variance and covariance for Beale's ratio method are based on bi-variate normal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

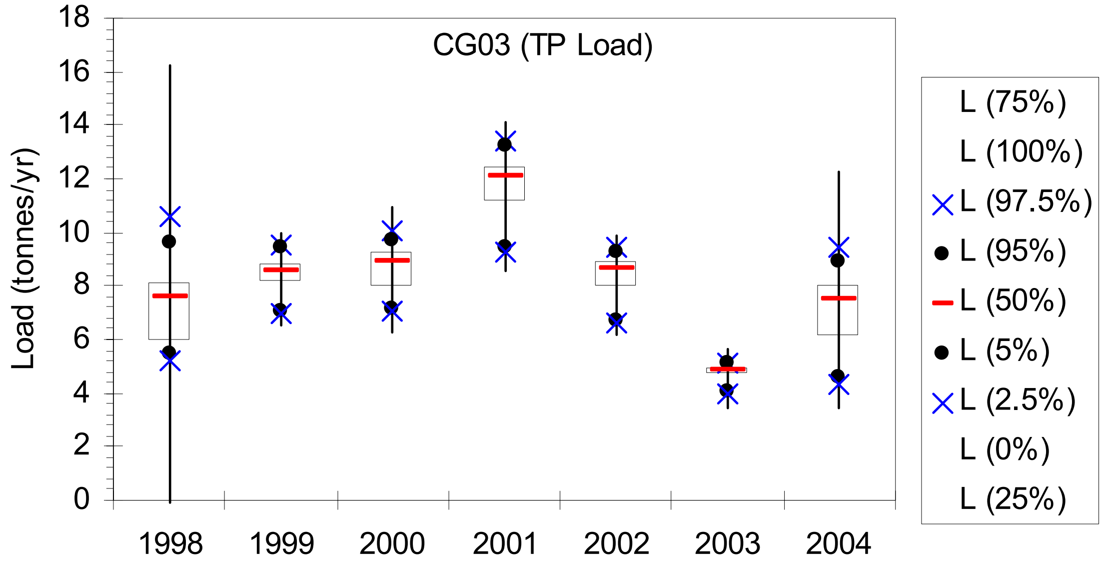
Appendix C: Number of Samples and Daily Flow Characteristics for MID drain data

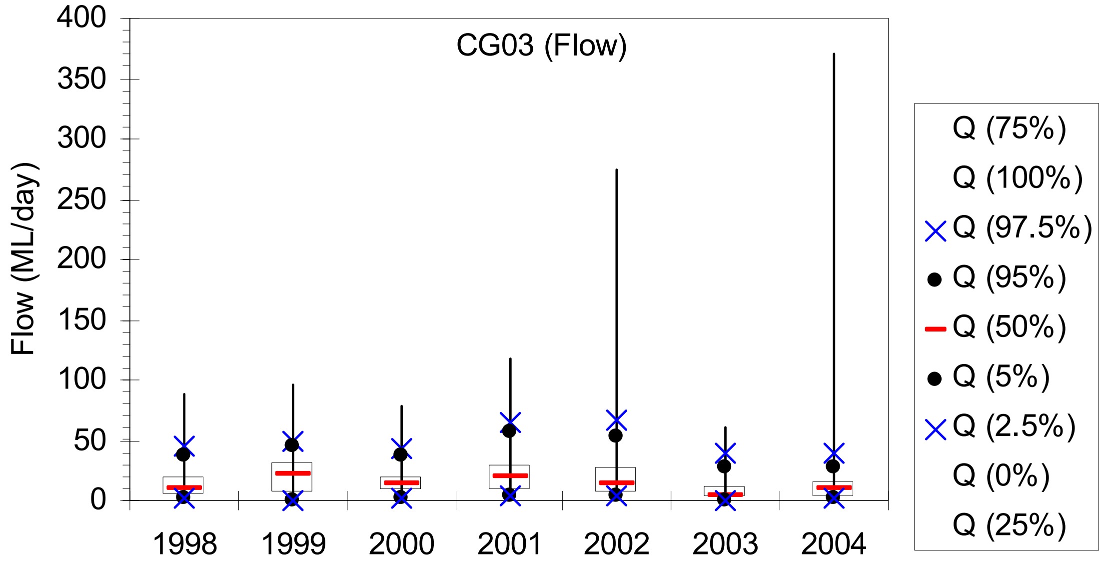
			Daily Flow Characteristics (ML/day)				
Site	Year	# TP Samples	5th Percentile	25th Percentile	Median	75th Percentile	95th Percentile
CG02	2000	4.6	6.7	11.1	15.6	33.2	4.6
	2001	6.3	8.7	12.4	23.5	63.8	6.3
	2002	3.7	6.7	10.0	20.1	55.6	3.7
	2003	1.0	1.6	2.9	4.2	8.1	1.0
	2004	2.7	4.7	10.8	18.9	33.9	2.7
CG03	1998	2.3	3.6	9.8	19.8	36.3	2.3
	1999	0.0	6.6	22.1	30.9	45.2	0.0
	2000	2.5	7.0	14.3	20.4	36.9	2.5
	2001	4.3	7.7	19.0	29.9	56.7	4.3
	2002	4.3	5.8	13.7	27.6	53.4	4.3
	2003	0.9	1.5	4.6	12.0	27.2	0.9
	2004	1.1	2.8	10.2	15.2	27.1	1.1
CG04	2001	0.6	2.3	6.7	16.5	52.9	0.6
	2002	0.1	1.7	8.3	16.9	36.6	0.1
	2003	0.8	1.9	4.5	10.9	38.7	0.8
	2004	0.8	1.9	4.2	8.5	22.4	0.8
LWMD	1998	0.8	2.8	8.8	24.6	62.1	0.8
	1999	1.5	6.4	13.6	28.4	49.4	1.5
	2000	2.1	4.4	9.2	22.9	51.0	2.1
	2001	3.6	7.9	15.2	32.0	73.6	3.6
	2002	2.9	6.6	14.8	31.6	74.8	2.9
	2003	0.4	1.3	2.1	3.9	10.0	0.4
	2004	2.1	5.3	10.0	17.5	43.0	2.1
Serp	2000	4.6	5.8	7.1	10.3	16.9	4.6
	2001	4.2	4.8	7.2	10.9	18.6	4.2
	2002	1.1	2.3	4.1	9.7	20.3	1.1
	2003	0.3	0.7	1.5	3.1	7.8	0.3
	2004	0.9	1.8	3.0	6.6	19.1	0.9
Newry	2000	3.0	4.8	7.4	15.1	38.1	3.0
	2001	4.4	7.3	11.8	25.1	124.0	4.4
	2002	1.2	6.8	13.2	25.2	69.5	1.2
	2003	0.4	2.0	4.4	10.3	22.2	0.4
	2004	1.8	4.1	6.4	12.5	31.8	1.8

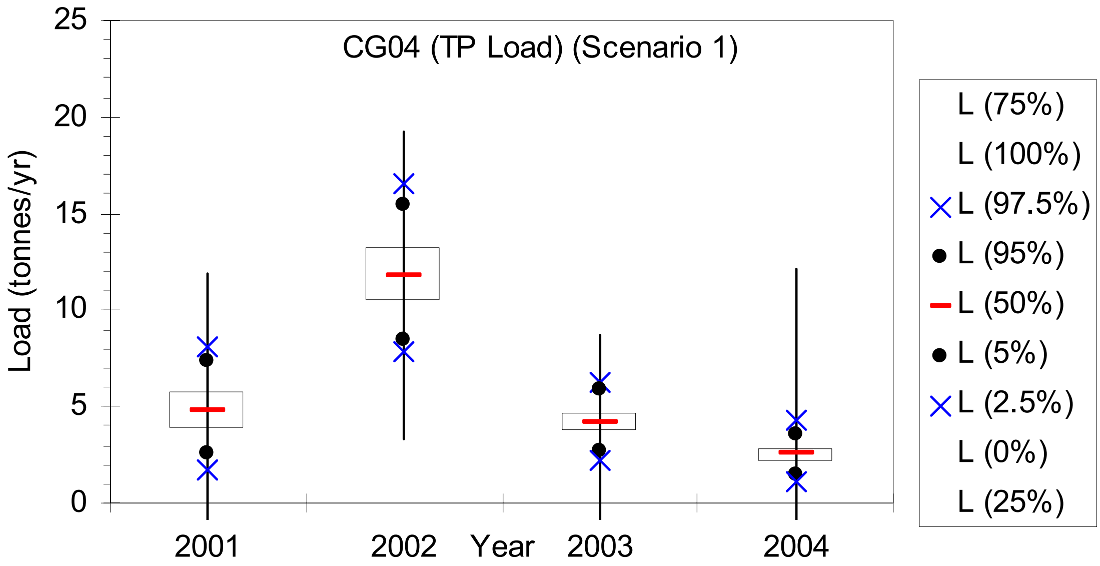
Appendix D: Box Plots of Estimated Annual TP Load and Flows in MID drains

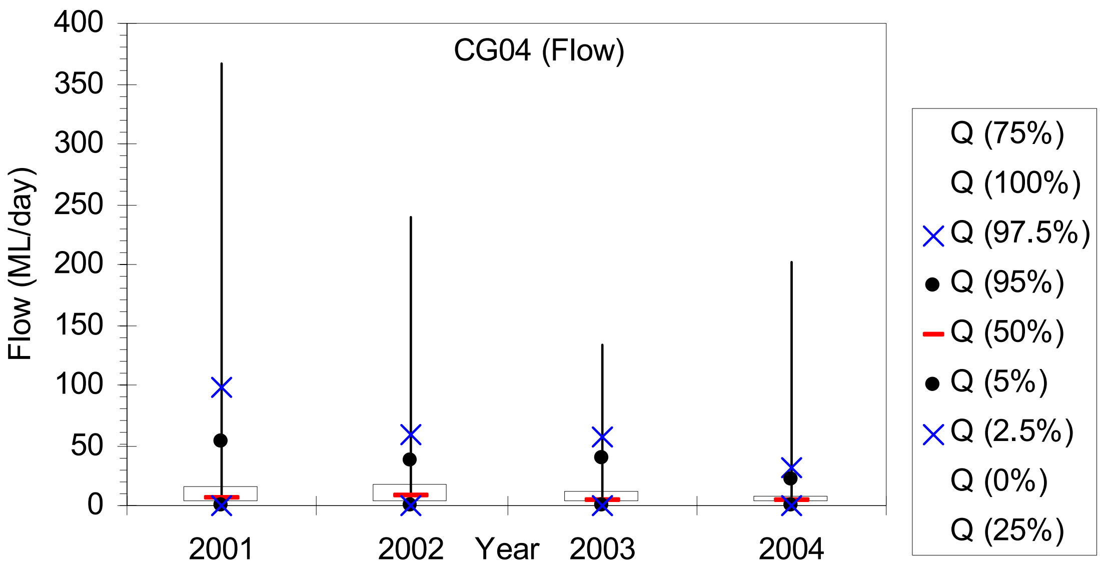


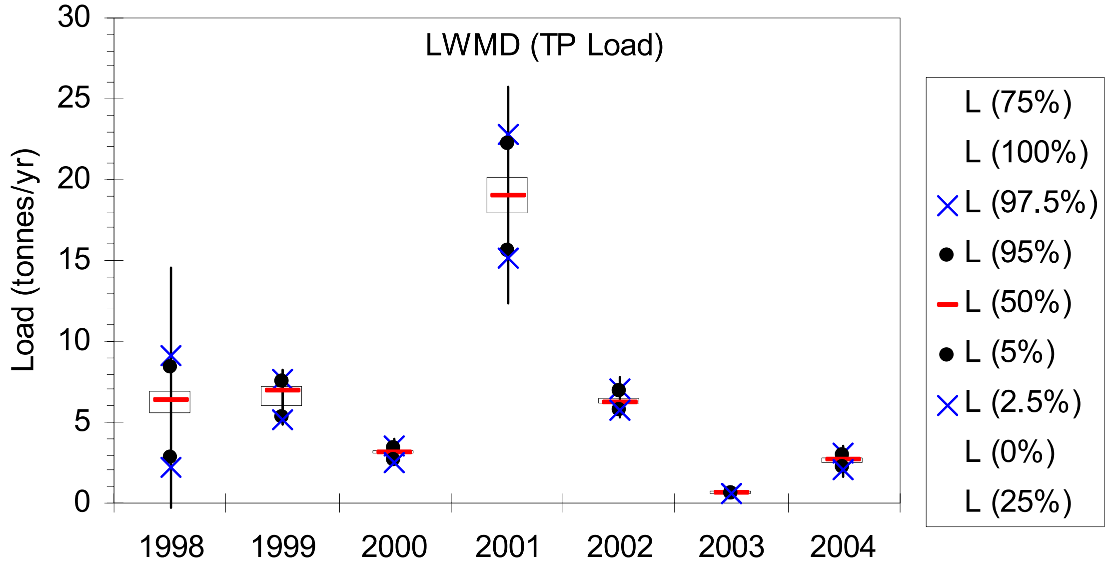


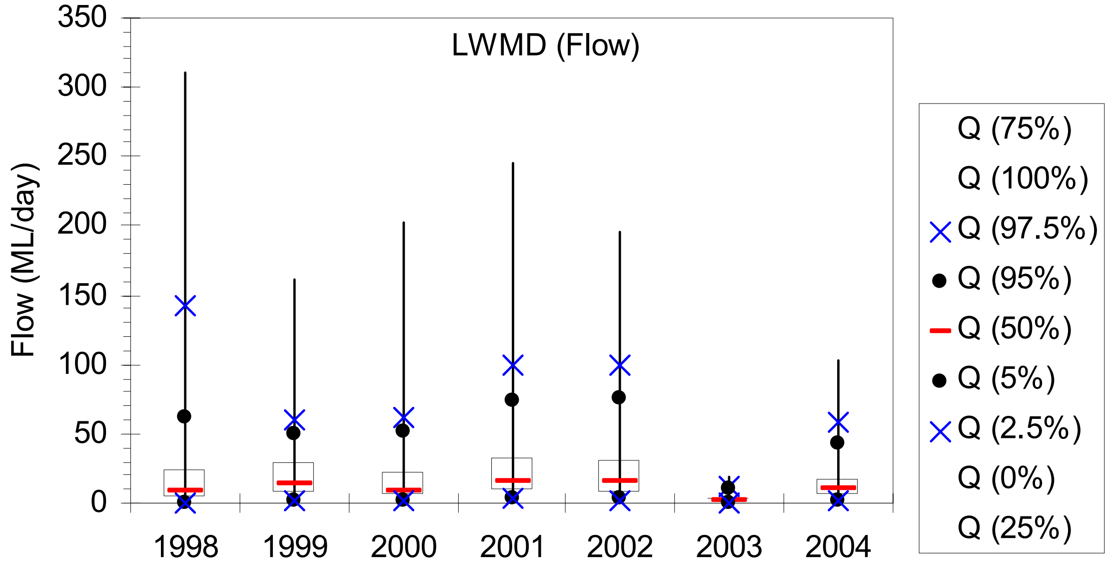

CG03 (TP Load)
Load (tonnes/yr)
0
2
4
6
8
10
12
14
16
18
1998
1999
2000
2001
2002
2003
2004
L (75%)
L (100%)
L (97.5%)
L (95%)
L (50%)
L (5%)
L (2.5%)
L (0%)
L (25%)

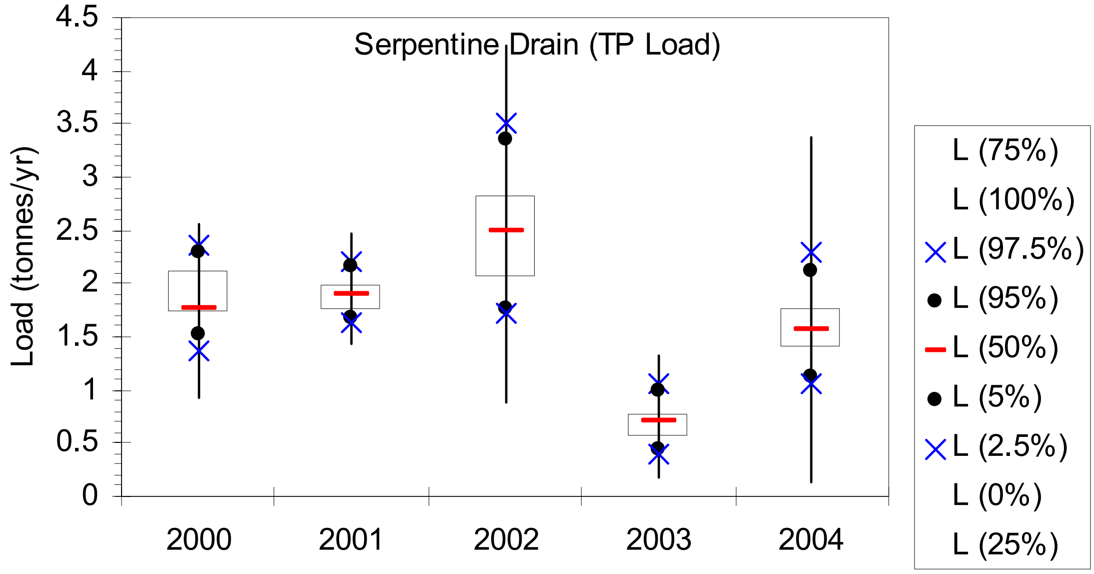

CG03 (Flow)
Flow (ML/day)
0
50
100
150
200
250
300
350
400
1998
1999
2000
2001
2002
2003
2004
Q (75%)
Q (100%)
Q (97.5%)
Q (95%)
Q (50%)
Q (5%)
Q (2.5%)
Q (0%)
Q (25%)

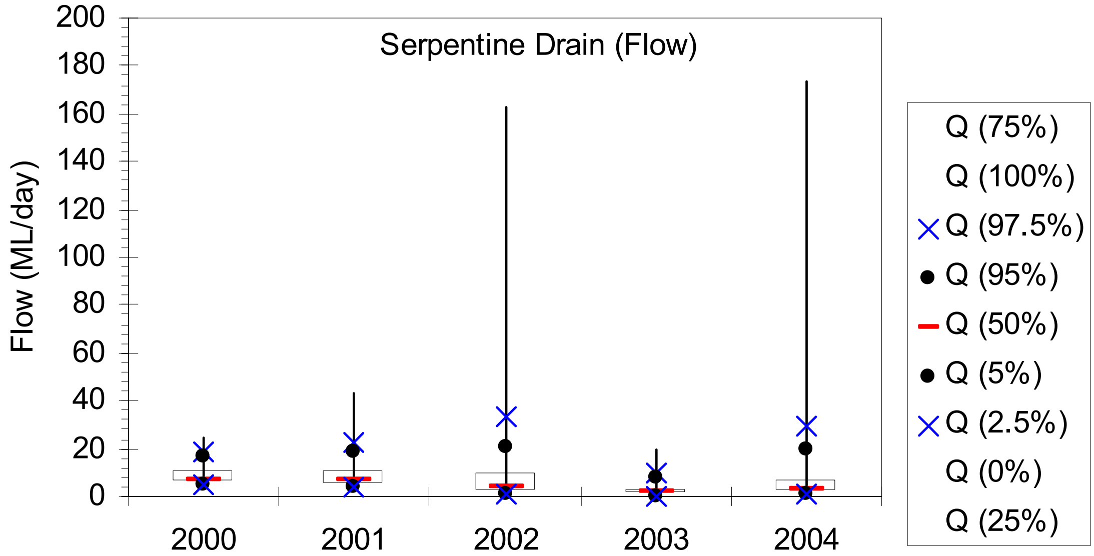

CG04 (TP Load) (Scenario 1)
Load (tonnes/yr)
0
5
10
15
20
25
2001
2002
Year
2003
2004
L (75%)
L (100%)
L (97.5%)
L (95%)
L (50%)
L (5%)
L (2.5%)
L (0%)
L (25%)

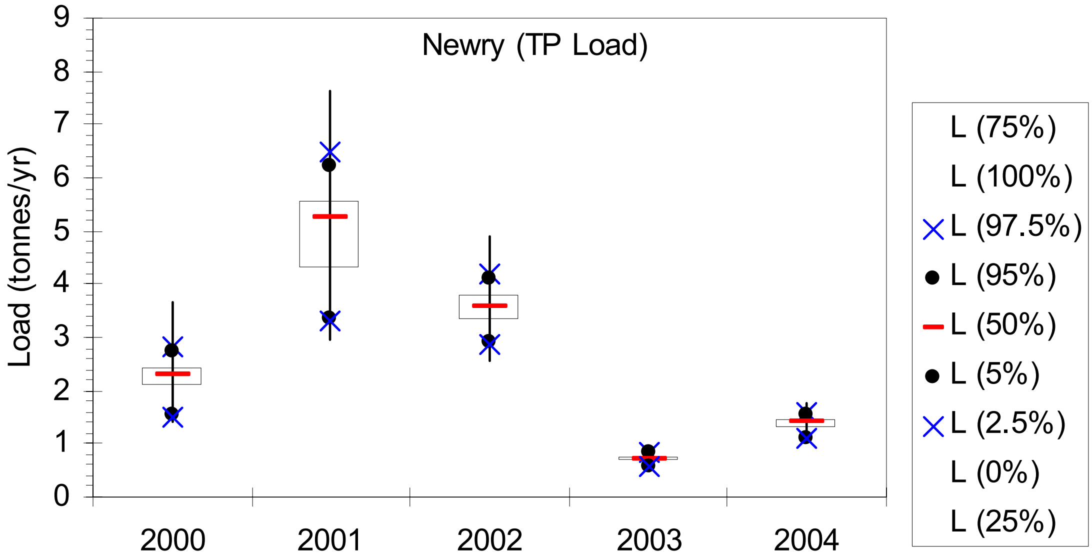

CG04 (Flow)
Flow (ML/day)
0
50
100
150
200
250
300
350
400
2001
2002
Year
2003
2004
Q (75%)
Q (100%)
Q (97.5%)
Q (95%)
Q (50%)
Q (5%)
Q (2.5%)
Q (0%)
Q (25%)

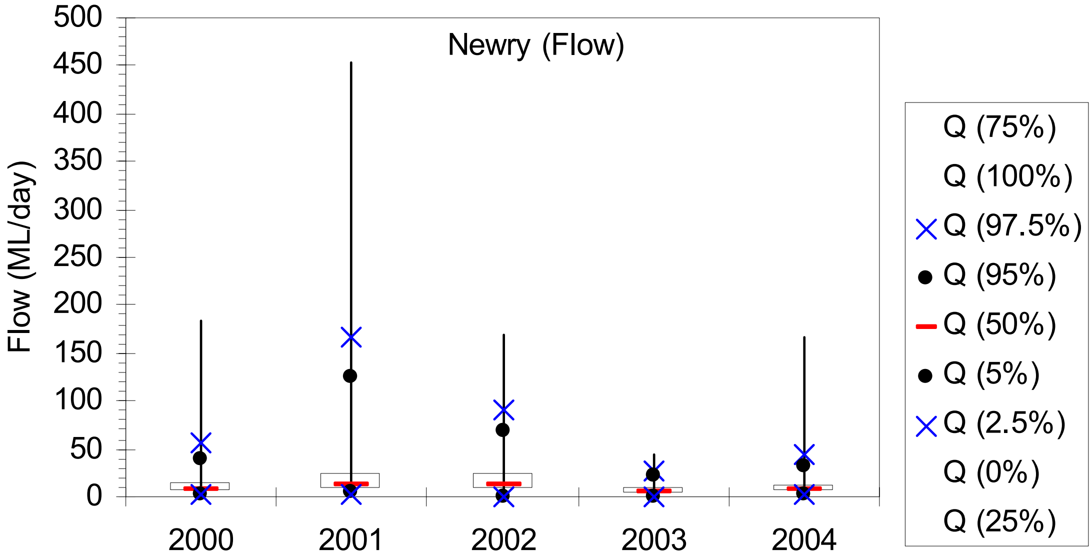

LWMD (TP Load)
Load (tonnes/yr)
30
25
20
15
10
5
0
1998
1999
2000
2001
2002
2003
2004
L (75%)
L (100%)
L (97.5%)
L (95%)
L (50%)
L (5%)
L (2.5%)
L (0%)
L (25%)


LWMD (Flow)
Flow (ML/day)
350
300
250
200
150
100
50
0
1998
1999
2000
2001
2002
2003
2004
Q (75%)
Q (100%)
Q (97.5%)
Q (95%)
Q (50%)
Q (5%)
Q (2.5%)
Q (0%)
Q (25%)

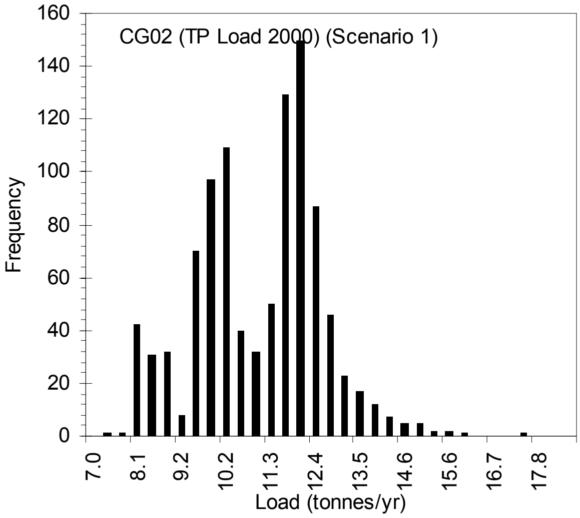

Serpentine Drain (TP Load)
Load (tonnes/yr)
4.5
4
3.5
3
2.5
2
1.5
1
0.5
0
2000
2001
2002
2003
2004
L (75%)
L (100%)
L (97.5%)
L (95%)
L (50%)
L (5%)
L (2.5%)
L (0%)
L (25%)

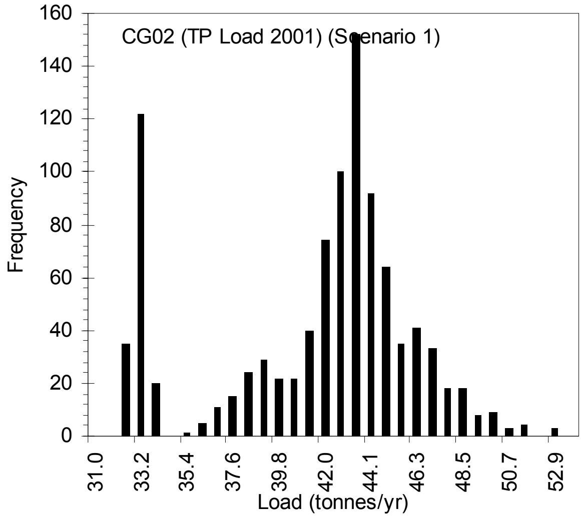

Serpentine Drain (Flow)
Flow (ML/day)
200
180
160
140
120
100
80
60
40
20
0
2000
2001
2002
2003
2004
Q (75%)
Q (100%)
Q (97.5%)
Q (95%)
Q (50%)
Q (5%)
Q (2.5%)
Q (0%)
Q (25%)

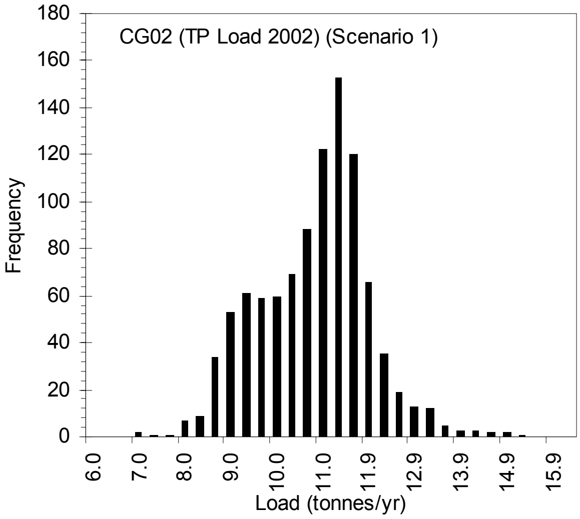

Newry (TP Load)
Load (tonnes/yr)
0
1
2
3
4
5
6
7
8
9
2000
2001
2002
2003
2004
L (75%)
L (100%)
L (97.5%)
L (95%)
L (50%)
L (5%)
L (2.5%)
L (0%)
L (25%)

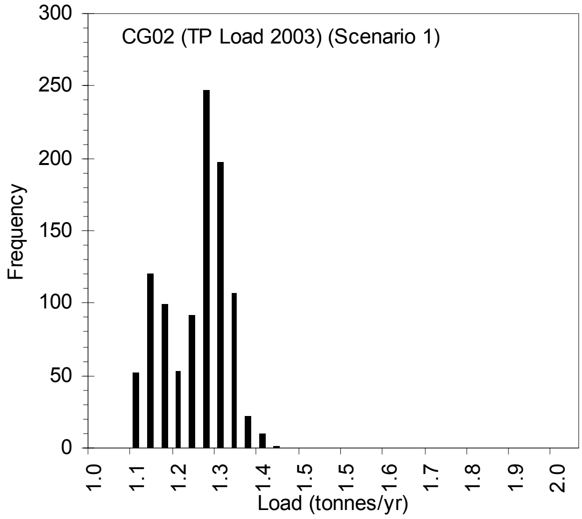

Newry (Flow)
Flow (ML/day)
0
50
100
150
200
250
300
350
400
450
500
2000
2001
2002
2003
2004
Q (75%)
Q (100%)
Q (97.5%)
Q (95%)
Q (50%)
Q (5%)
Q (2.5%)
Q (0%)
Q (25%)

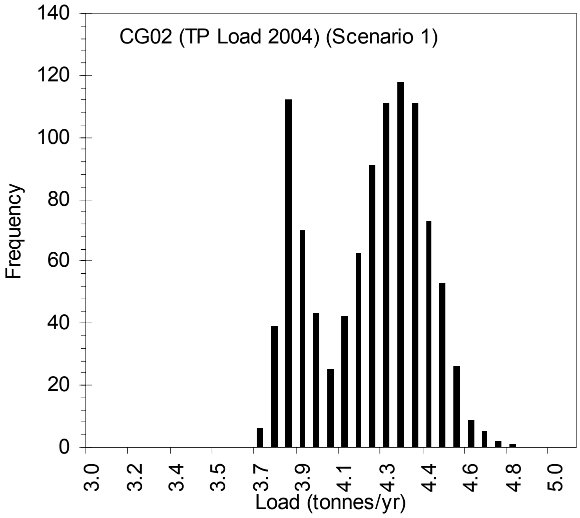
Appendix E : Histograms of estimated annual TP loads for site CG02



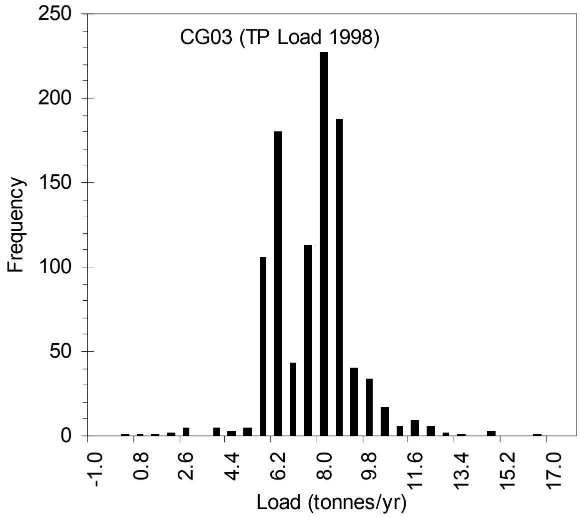


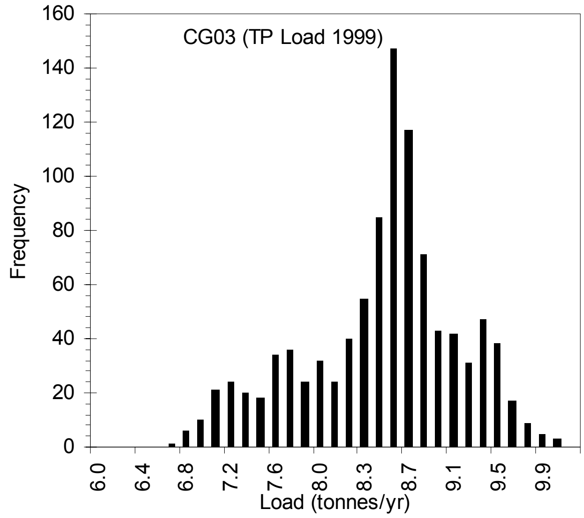


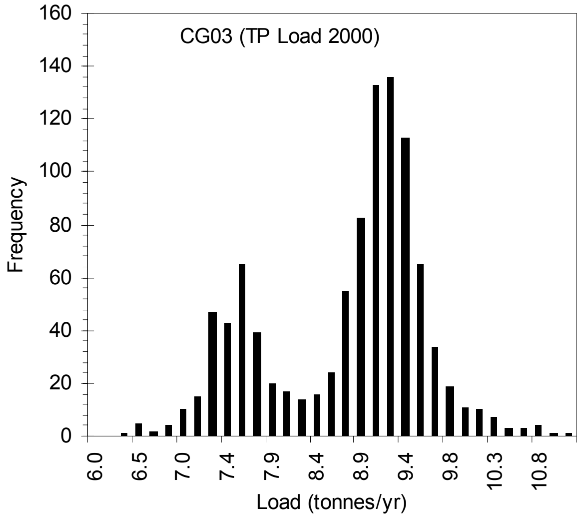


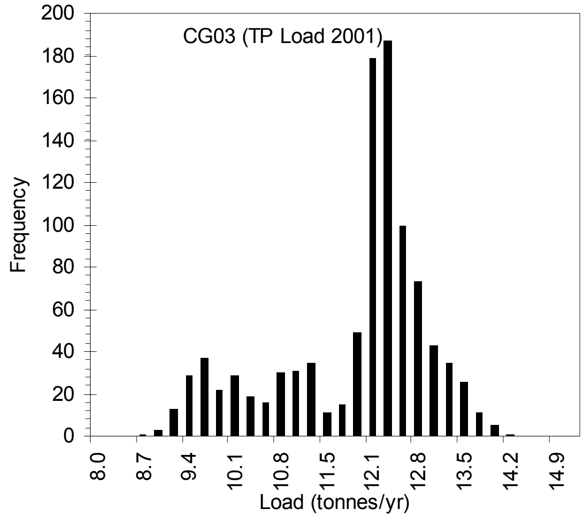


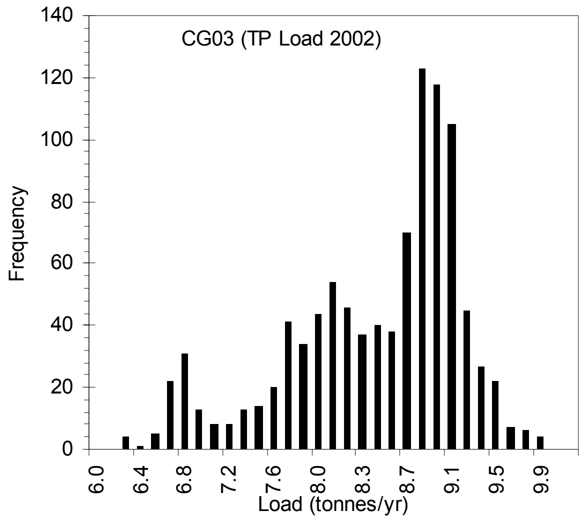
Appendix F: Histograms of estimated annual TP loads for site CG03

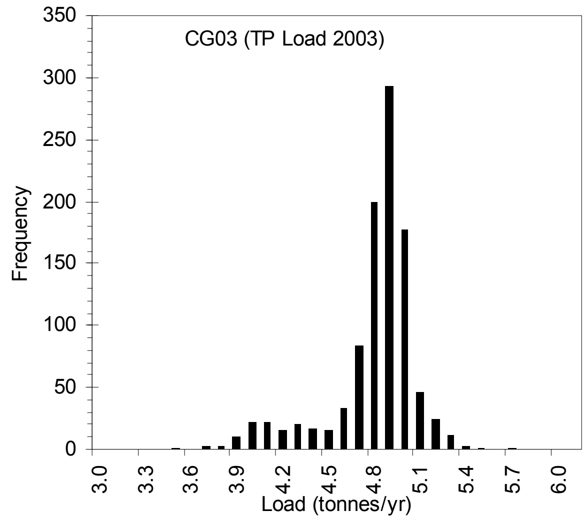


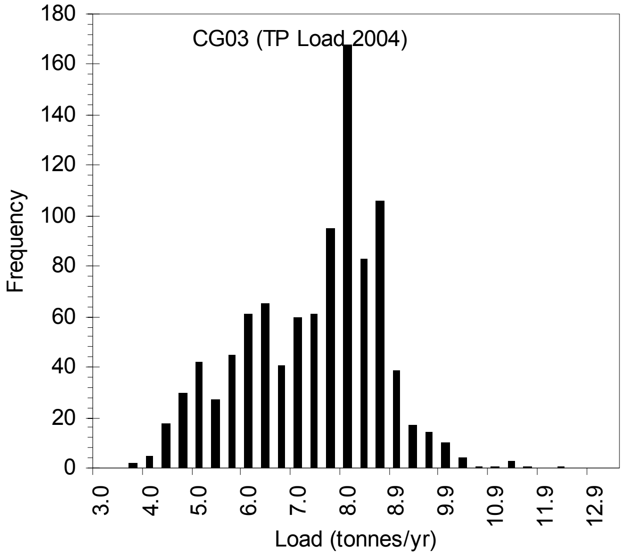




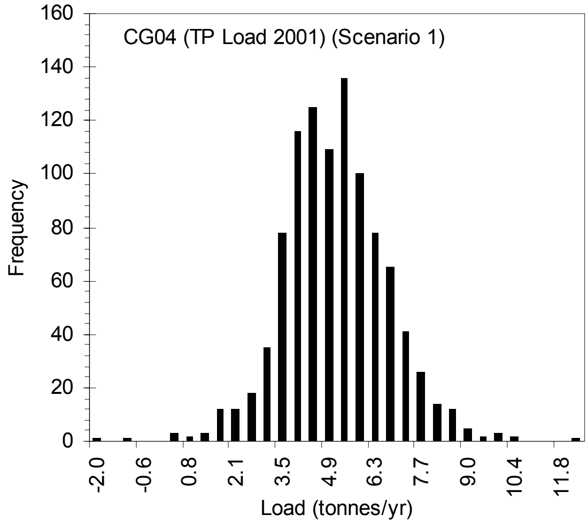


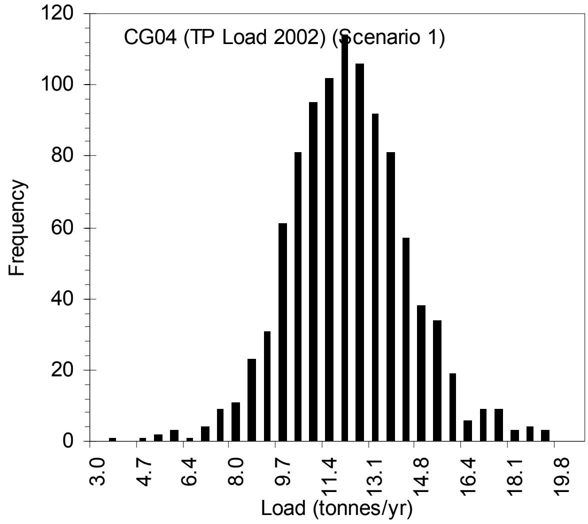


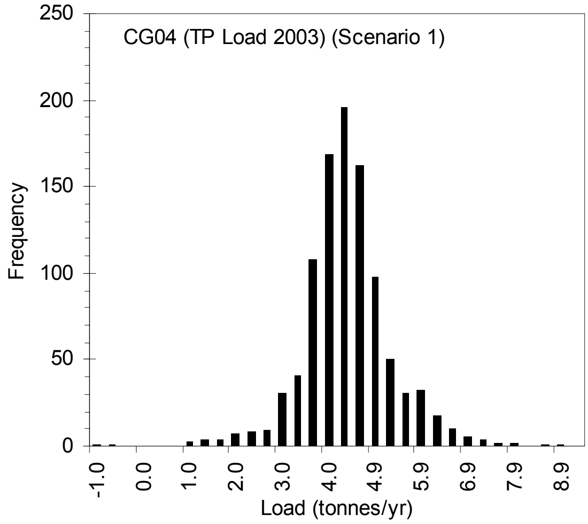


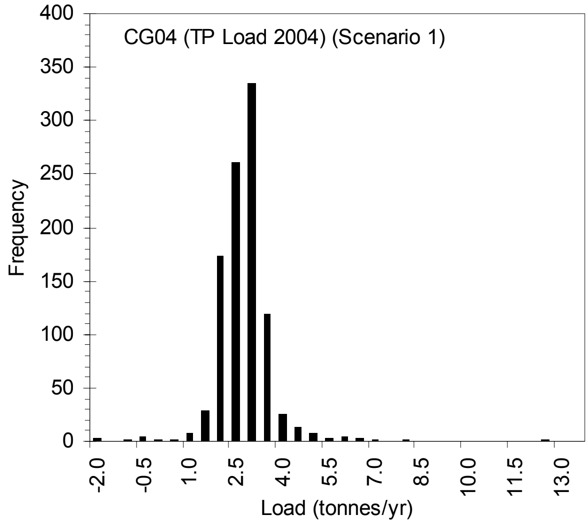

CG03 (TP Load 2004)
Frequency
180
160
140
120
100
80
60
40
20
0
3.0
4.0
5.0
6.0
7.0
8.0
8.9
9.9
10.9
11.9
12.9
Load (tonnes/yr)

Appendix G: Histograms of estimated annual TP loads for site CG04

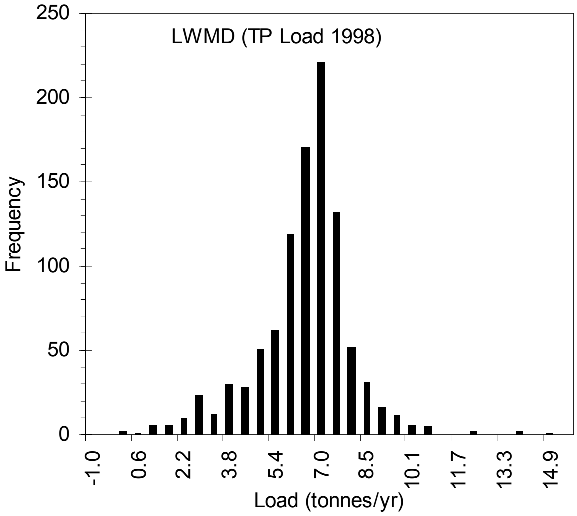


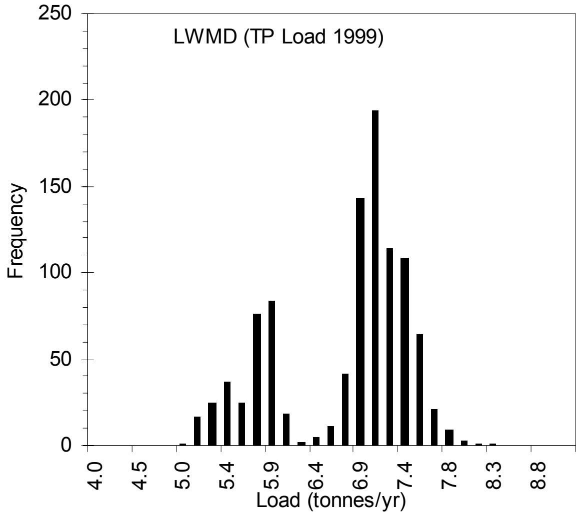


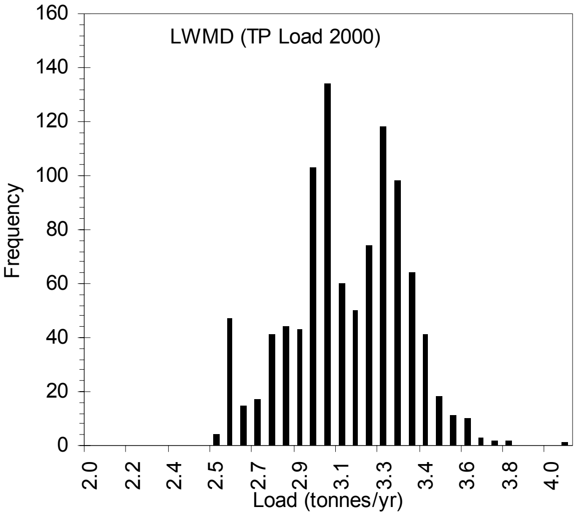


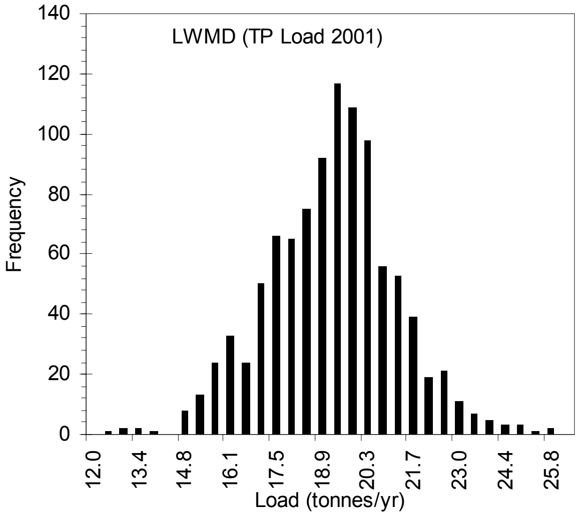


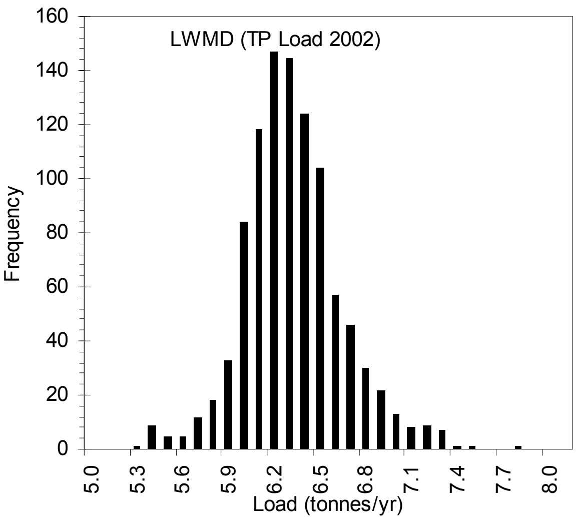
Appendix H: Histograms of estimated annual TP loads for LWMD

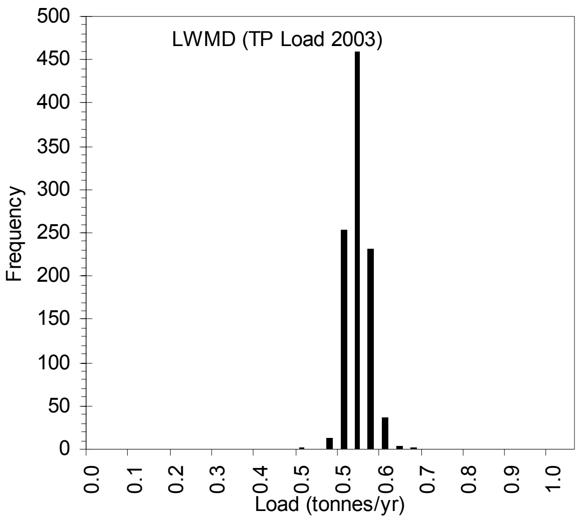


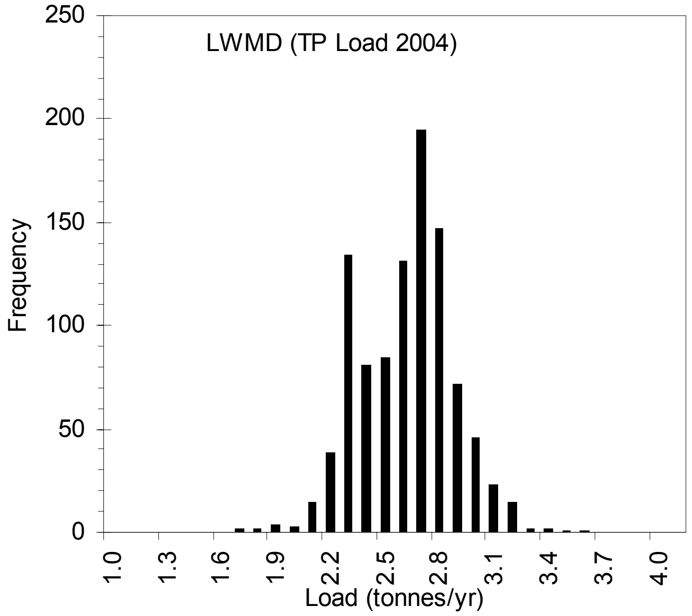




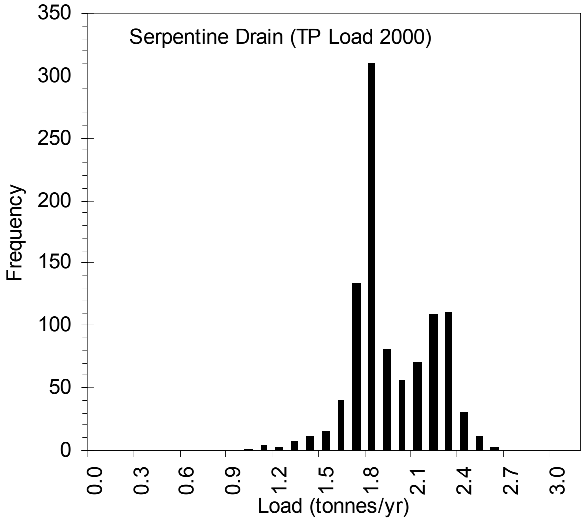


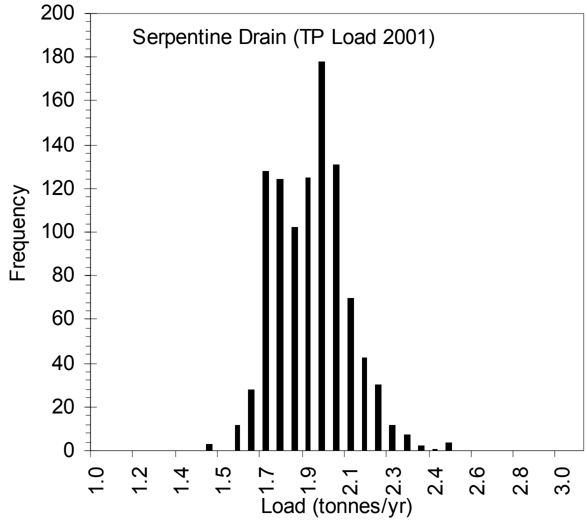


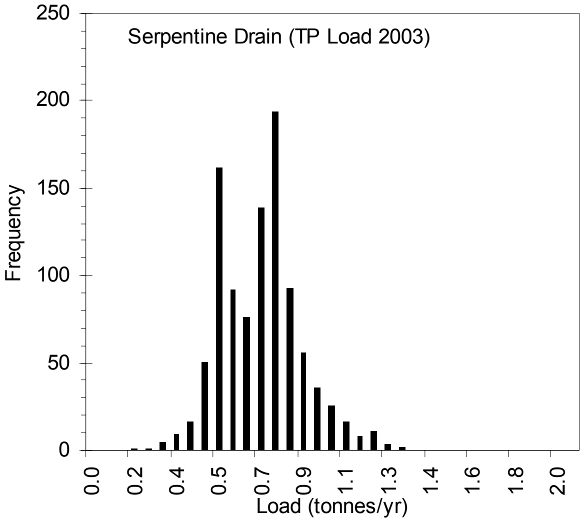


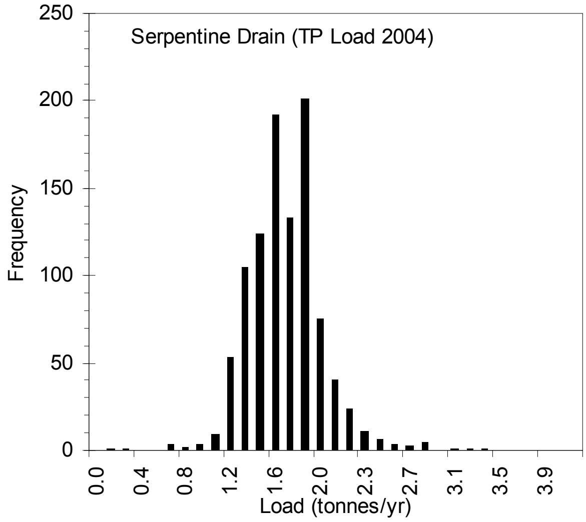

LWMD (TP Load 2004)
Frequency
250
200
150
100
50
0
1.0
1.3
1.6
1.9
2.2
2.5
2.8
3.1
3.4
3.7
4.0
Load (tonnes/yr)

Appendix I: Histograms of estimated annual TP loads for Serpentine

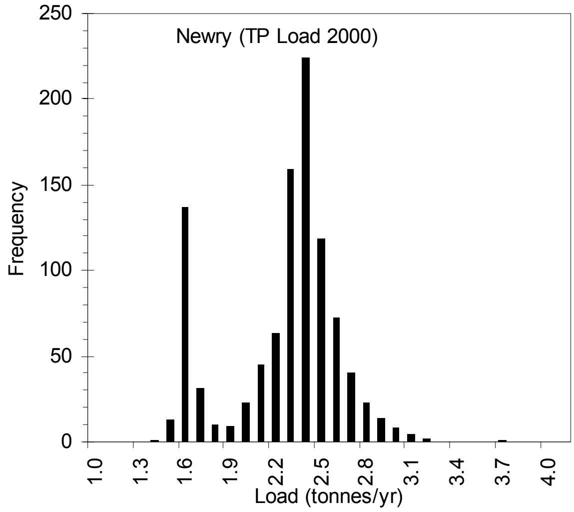


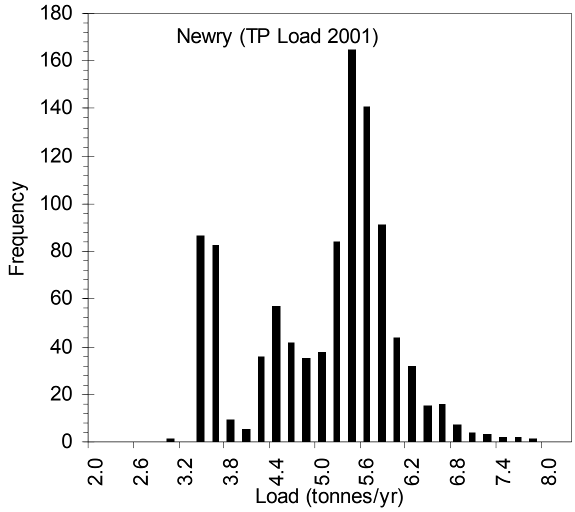


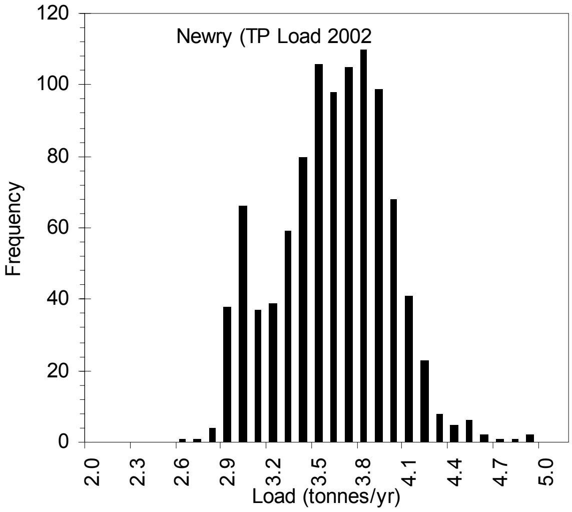


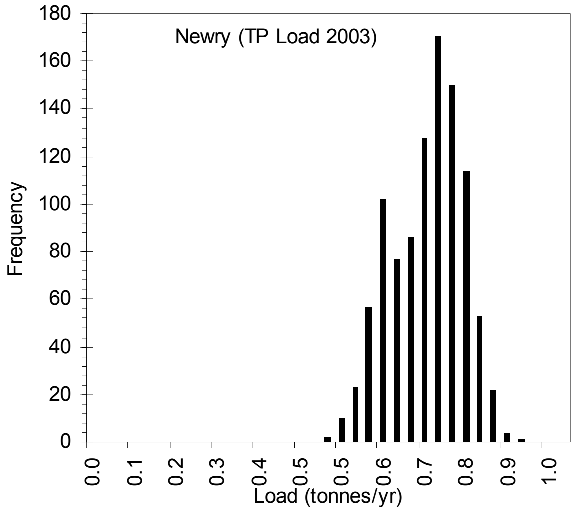


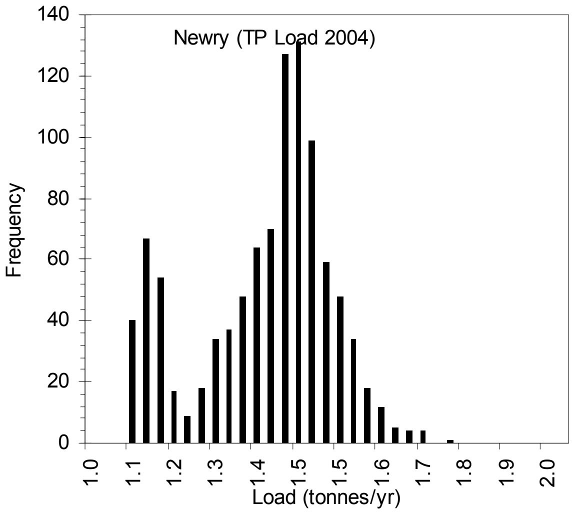
Appendix J: Histograms of estimated annual TP loads for Newry Ck











Appendix K: Simulation results for the Fox Sampling Strategy (FSS) for estimating nutrient loads

Progress Report

Prof. David R. Fox
Dr. Bryan Beresford-Smith

Australian Centre for Environmetrics

August 2004

Important: *The information and results contained herein have not been subject to peer review and accordingly no reliance should be made on them. This document shall not be cited without the express permission of the author.*

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- Dr Petra Kuhnert (Qld. EPA);
- Mr. Geoff Gordon (NSW EPA).

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1. Introduction

The accurate estimation of total loads of sediments and nutrients is a problem that is attracting considerable attention among natural resource managers, environmental protection agencies, governments, landowners, and the general community. The delivery of sediments from Queensland catchments has been identified as a threat to the ecosystem of the Great Barrier Reef, while point and diffuse sources of land-based nutrients are implicated in the increased frequency and severity of algal blooms in water bodies around the country. Accordingly, there has been a growing trend towards the expression of aspirational and compliance targets for nutrients and sediments in terms of either a relative or absolute reduction in total *load*. For example, a 20% nutrient reduction target has been imposed on Queensland catchments impacting the Great Barrier Reef while the Victorian EPA has required a 40% reduction in the total phosphorous load from the McAlister Irrigation District by 2005 and a commensurate 40% reduction in total nutrient loads to the Gippsland Lakes by 2022.

This project seeks to identify 'optimal' sampling and estimation strategies for sediment-nutrient load estimation. The first stage of the project has been associated with the development of a probabilistic sampling strategy (FSS[4]) which is both efficient (in terms of the amount of sampling undertaken) and robust (provides reliable load estimates under a variety of discharge regimes). A more detailed report is currently in preparation. The purpose of this progress report is to document results of simulation studies associated with the FSS load estimation technique and to describe the essential features of the companion software tool which has been developed by the Australian Centre for Environmetrics.

[4] Fox Sampling Strategy

2. Overview of the simulation study

For the purpose of assessing the efficacy of the FSS we have used a dataset provided by Southern Rural Water which has daily measurements on flow and total phosphorus over a one year period. We have assumed that the total annual phosphorus load obtained by summing the daily values of load x TP concentration is the 'true' annual load which is to serve as the basis for comparing load estimates obtained under FSS sampling.

In the following analysis the complete flow record is denoted as $F = \{ f_i : i = 1, \ldots N \}$ and the concentration record as $C = \{ c_i : i = 1, \ldots N \}$. Let $n < \frac{N}{2}$ be the target number of samples for which measurements will be taken. A primary input to the FSS method is either an historical flow record or estimates for the 10^{th}, 50^{th}, and 90^{th} percentiles for the flow distribution. The mathematical details of the FSS method are to be detailed in a separate report. An important output from the FSS method is the selection probability, π_i for the i^{th} day (ie. the probability that a water quality measurement for day *i* will be required for the sample). At the end of this process (i.e. after N days) the *actual* number of samples taken will be *m* and this number may differ from the target number *n* due to the probabilistic nature of the FSS.

An estimator of the total annual load is:

$$\hat{L} = \frac{n}{m} \sum_{i=1}^{m} \frac{f_i c_i}{\pi_i}$$

The estimated variance of $\hat{L}$ is calculated using the following formula:

$$\hat{Var}\left[\hat{L} \right] = \frac{n}{m} \sum_{i=1}^{m} (1 - \pi_i) \left(\frac{f_i c_i}{\pi_i} - \frac{\hat{L}}{n} \right)^2$$

Results from a number of simulations are presented in the following sections. In each case N flows are randomly generated from an appropriate log-normal distribution. For convenience, the corresponding concentrations are assumed to be proportional to the flows. The algorithm is then run a total of K times (with a target sample size of 0.1N i.e. 10% for example) and the resulting estimated loads and standard deviations along with the actual sample size of measurements taken are analysed by displaying their histograms. In addition the fraction of results for which the actual load is *not* within 2 standard deviations of the estimated load is calculated.

The lognormal distribution can be specified by giving the 10^{th} percentile L, the 50^{th} percentile (median) M and the 90^{th} percentile U. The paper "Using Tenth and Ninetieth Percentiles and the Mode to Characterize Lognormal Distributions", Lloyd S. Nelson, The American Statistician, Vol 31, No 1 (Feb 1977), 26-27+30 also shows how the mode can be used to estimate the median (given L and U). It is important to note that for left-skewed distributions it is necessary for $L < M < U$ and $M < \frac{U+L}{2}$ and $Mode < \frac{U+L}{2}$. Right-skewed lognormal distributions for flow have *not* been included in the program since these are rarely encountered in practice.

3. Software description

A software tool has been developed that implements the FSS as a macro in MS-Excel (Figure 1). The user specifies the time step (eg. daily) and the target number of samples to be taken over the estimation period (Figure 2). The software then creates a template for the entry of flow readings. As soon as a new flow is entered (Figure 3), a decision is made based on the FSS as to whether or not a water quality sample is to be taken (Figure 4). Time periods which are selected for water quality sampling are highlighted in the spreadsheet and data is entered once it becomes available (Figure 5). After all water quality results have been entered, an estimate of total load for the period of interest is produced together with an estimated standard error (Figure 6.)

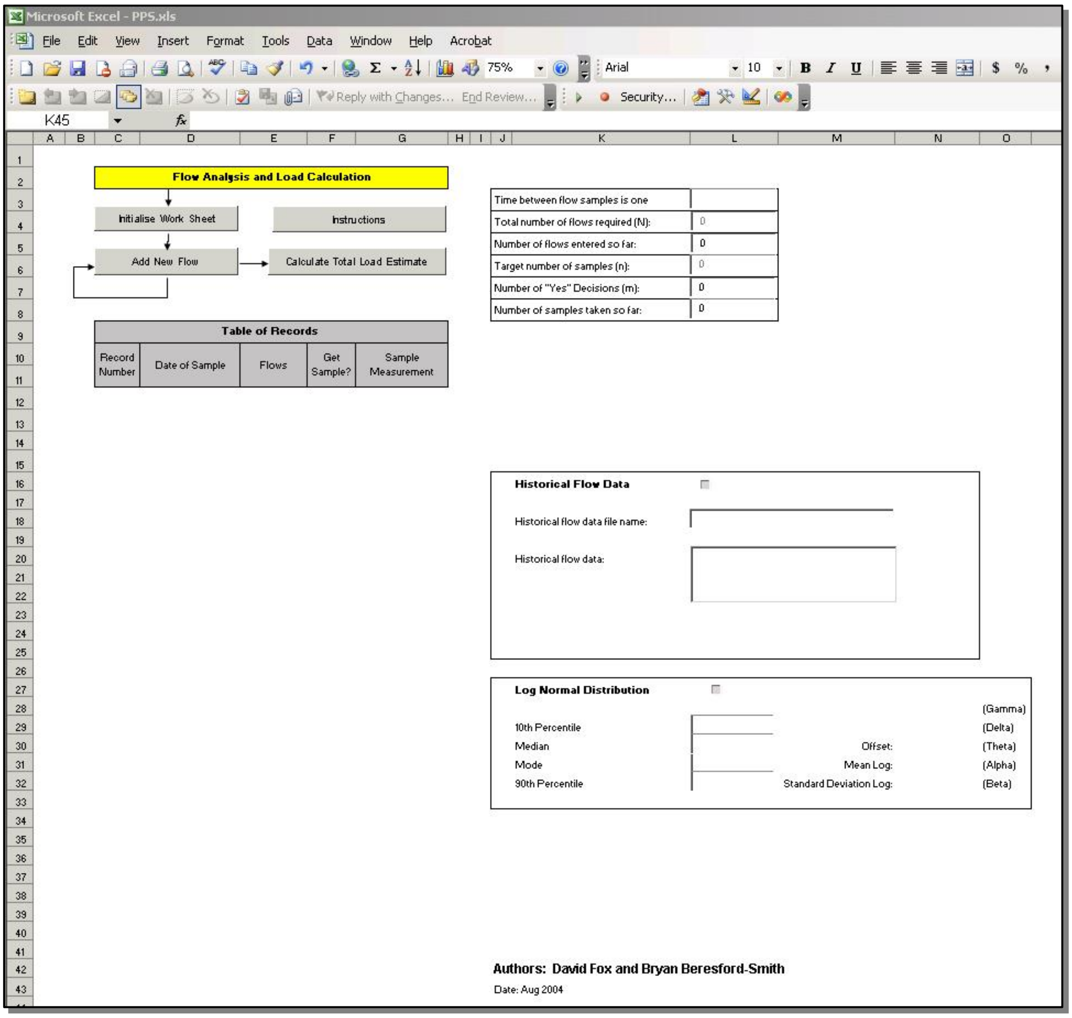

Figure 22. FSS Initial Screen

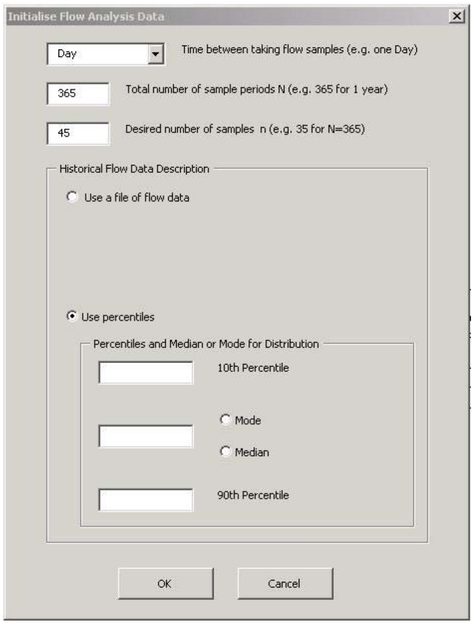

Figure 2. Initialisation of flow characteristics based either on historical data or user-defined percentiles.

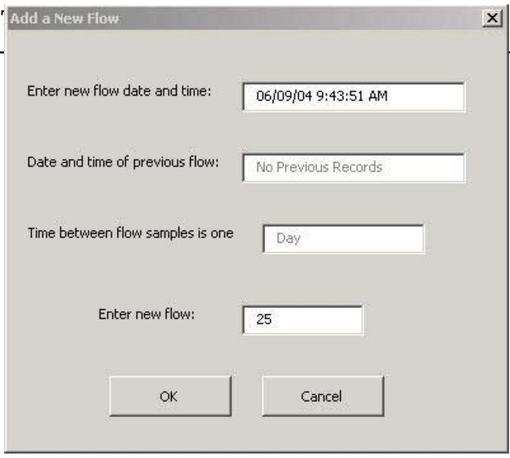

Figure 3. Data entry screen

Table of Records				
Record Number	Date of Sample	Flows	Get Sample?	Sample Measurement
1	06/09/04 9:43	25	No	

Figure 4. Decision-making dialogue box.

Table of Records				
Record Number	Date of Sample	Flows	Get Sample?	Sample Measurement
1	06/09/04 9:47	10.191	No	
2	06/09/04 9:47	17.466	No	
3	06/09/04 9:47	12.221	No	
4	06/09/04 9:47	3.607	No	
5	06/09/04 9:47	4.162	No	
6	06/09/04 9:47	9.141	No	
7	06/09/04 9:47	5.796	Yes	0.63
8	06/09/04 9:47	4.486	No	
9	06/09/04 9:47	5.584	No	
10	06/09/04 9:47	10.695	No	
11	06/09/04 9:47	12.904	Yes	0.67
12	06/09/04 9:47	3.479	No	
13	06/09/04 9:47	2.659	No	
14	06/09/04 9:47	1.922	No	
15	06/09/04 9:47	1.835	No	
16	06/09/04 9:47	4.259	No	
17	06/09/04 9:47	4.002	No	
18	06/09/04 9:47	1.912	No	
19	06/09/04 9:47	2.005	No	
20	06/09/04 9:47	2.354	No	
21	06/09/04 9:47	7.569	No	
22	06/09/04 9:47	4.369	No	
23	06/09/04 9:47	4.784	Yes	0.87
24	06/09/04 9:47	5.81	No	
25	06/09/04 9:47	3.327	No	
26	06/09/04 9:47	7.33	No	
27	06/09/04 9:47	2.689	No	
28	06/09/04 9:47	3.295	No	
29	06/09/04 9:47	4.632	No	
30	06/09/04 9:47	17.575	No	
31	06/09/04 9:47	15.151	No	
32	06/09/04 9:47	18.28	No	
33	06/09/04 9:47	8.938	No	
34	06/09/04 9:47	12.192	No	
35	06/09/04 9:47	5.425	No	
36	06/09/04 9:47	15.625	No	

Figure 5. Table of input data and selected sampling occasions (highlighted)

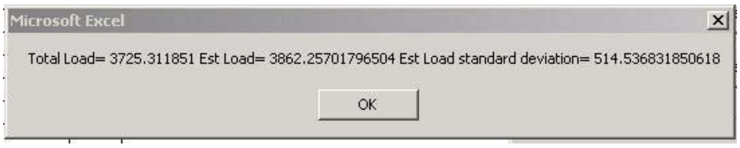

Figure 6. Estimated annual load with standard error of estimate.

4. Simulation Results

Historical flow and TP concentration data from Souther Rural Water's Central Gippsland Drain #3 (CG3) have been used to test the FSS. The empirical and fitted distributions for this flow data are shown in figure 7.

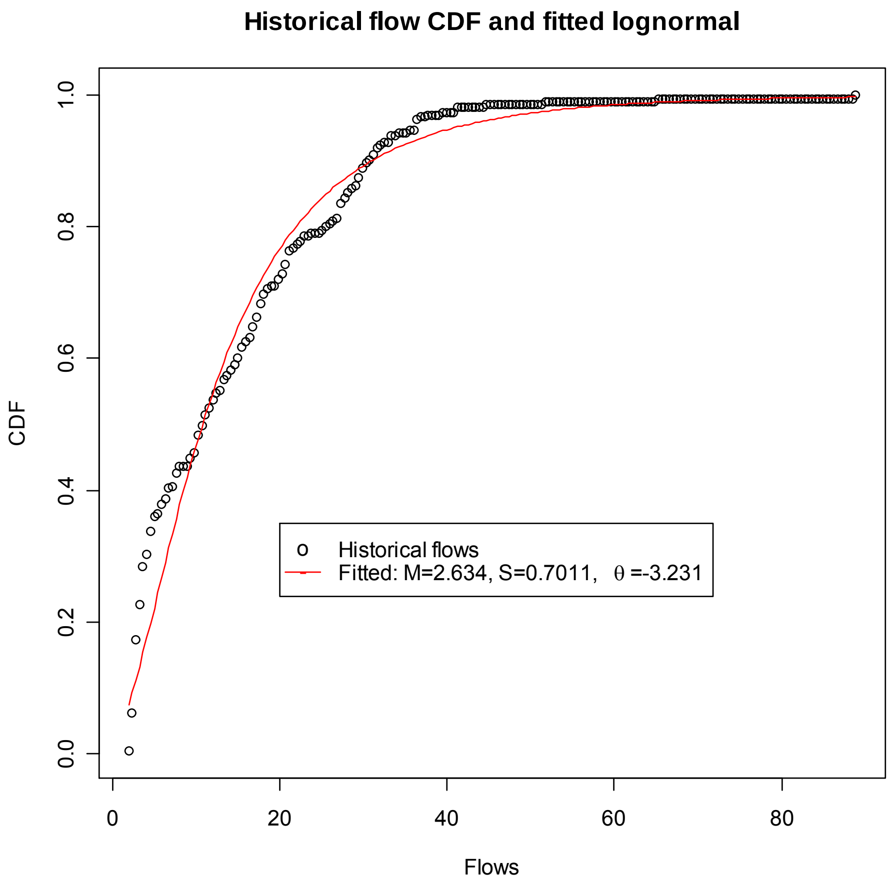

Figure 7. Comparison of empirical cdf (open circles) and fitted log-normal distribution (solid line).

Scenraio #1: Simulated rlnorm: Meanlog= 0 SDlog= 1 Target fraction= 0.1

Number of runs= 1000 Number of sample flows N = 365
Fraction of runs for which abs(real load - estimated load) > 2*standard deviation = 0.208

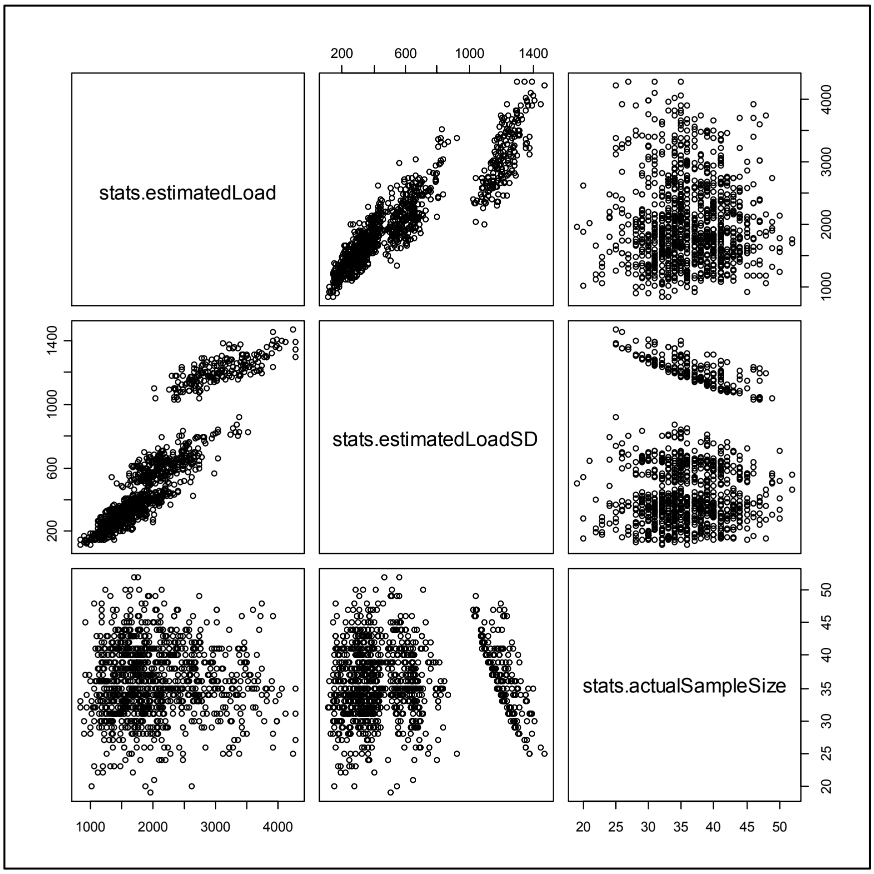

Figure 8. Matrix plot of simulation results for estimated load, standard error, and actual sample size – scenario #1.

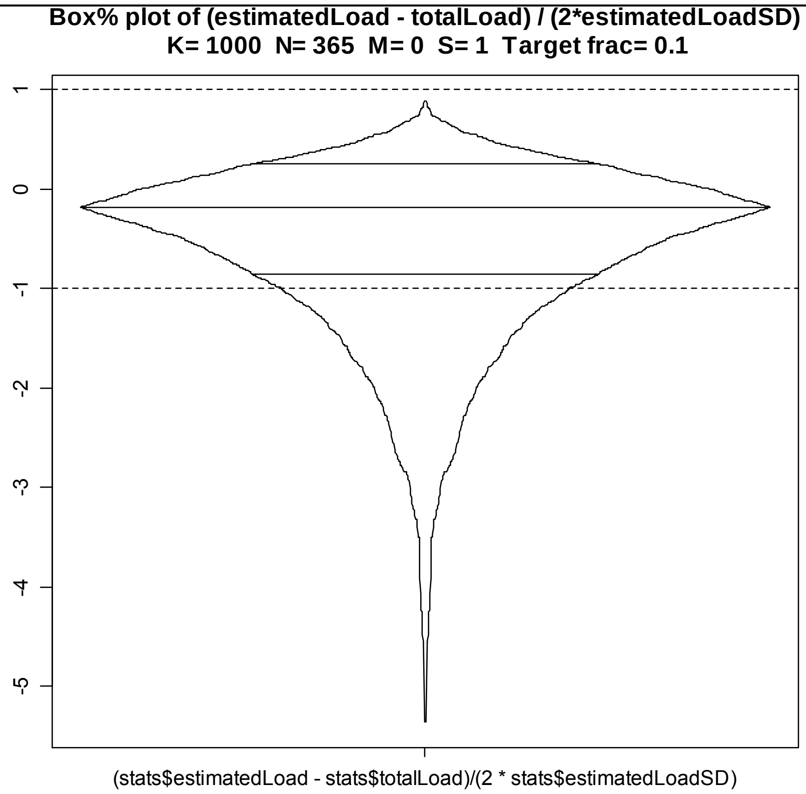

Figure 9. Box plot of standardised bias in annual load estimated under scenario 1.

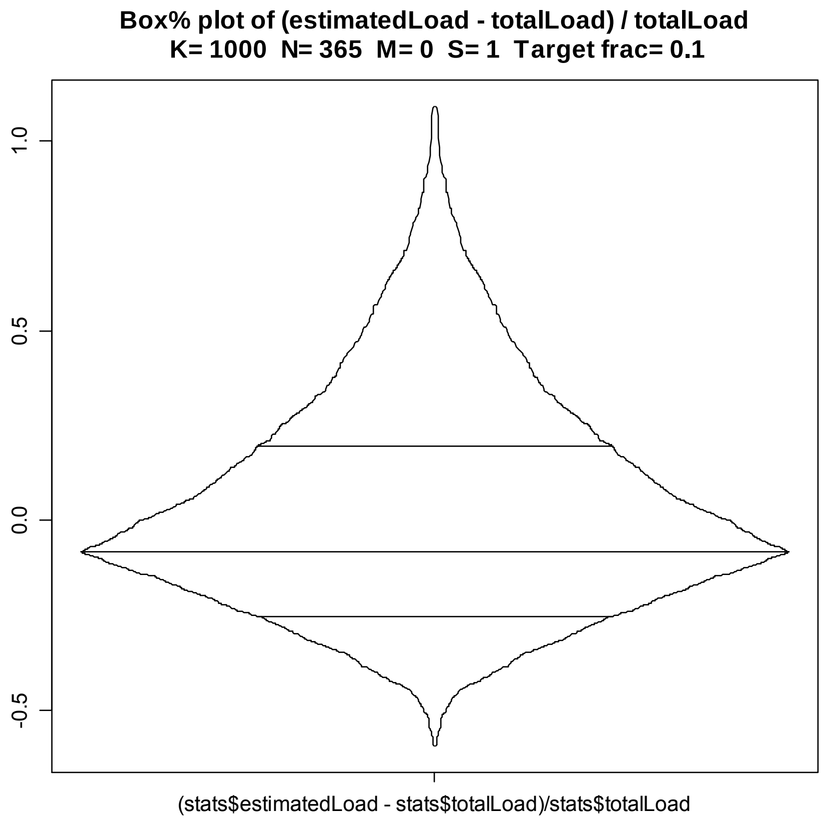

Figure 10. Box plot of proportional bias in annual load estimated under scenario #1.

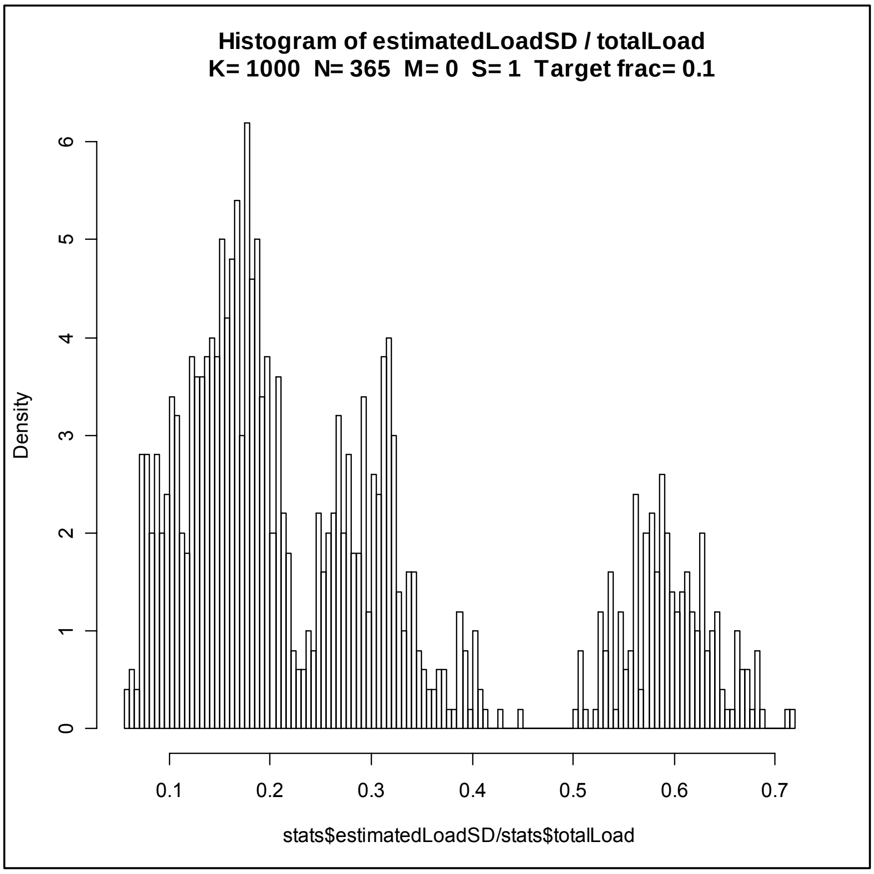

Figure 11. Histogram of ratio of estimated load to true load under scenario #1.

Scenario #2: Simulated rlnorm: Meanlog= 0 SDlog= 1 Target fraction= 0.2

Number of runs= 1000 Num sample flows N= 365
Fraction of runs for which abs(real load - estimated load) > 2*standard deviation = 0.122

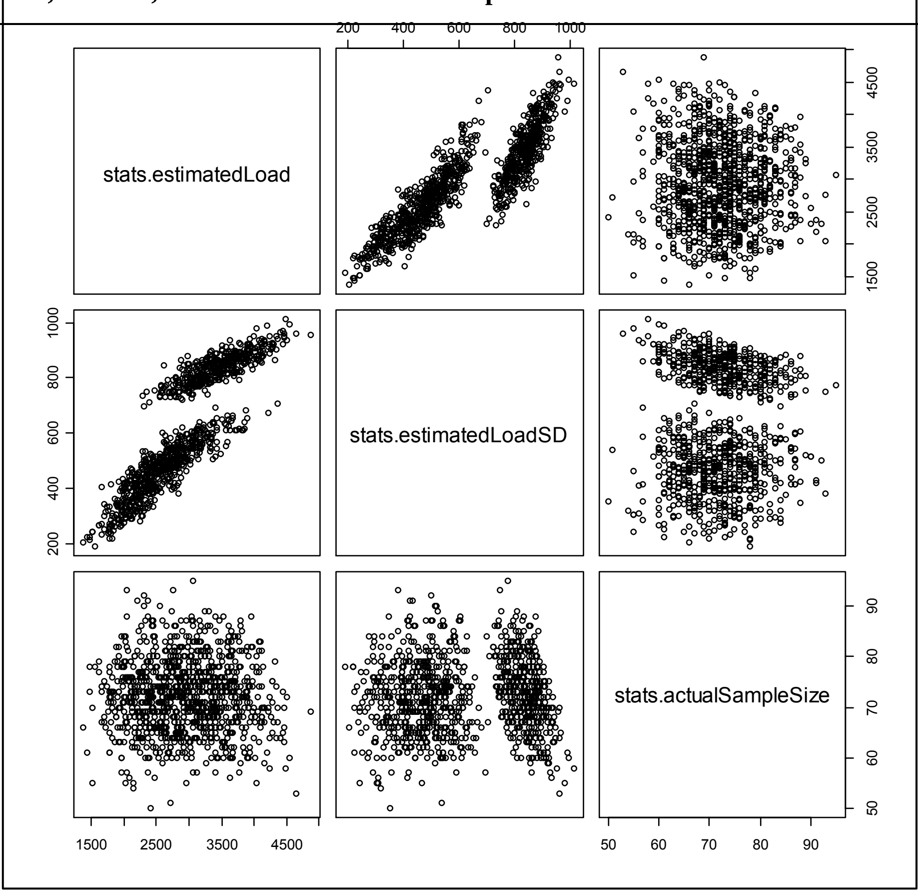

Figure 12. Matrix plot of simulation results for estimated load, standard error, and actual sample size – scenario #2.

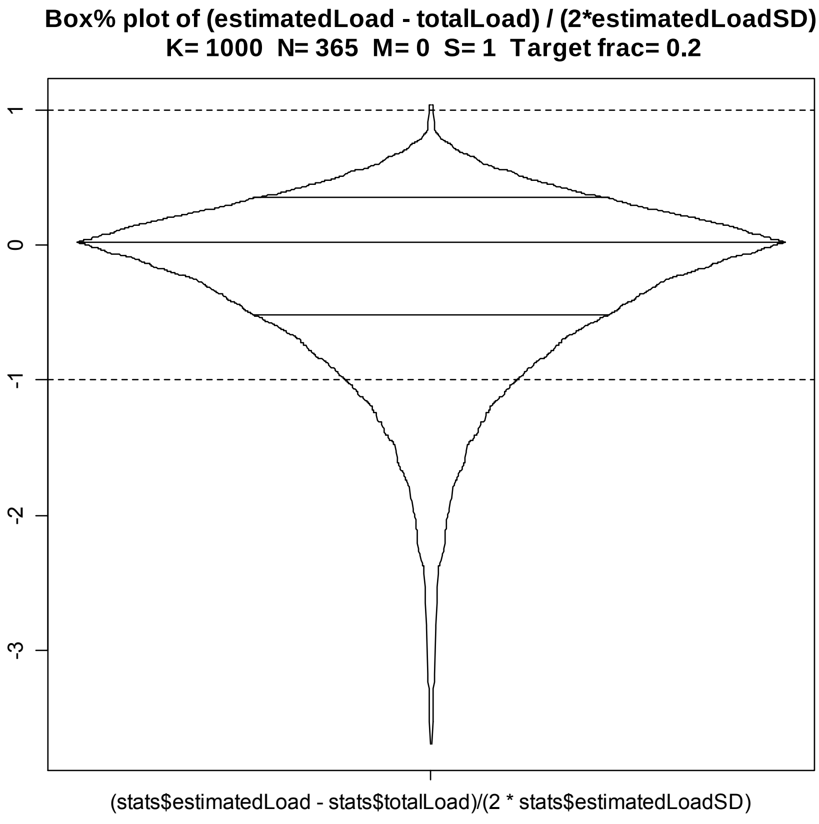

Figure 13. Box plot of standardised bias in annual load estimated under scenario #2.

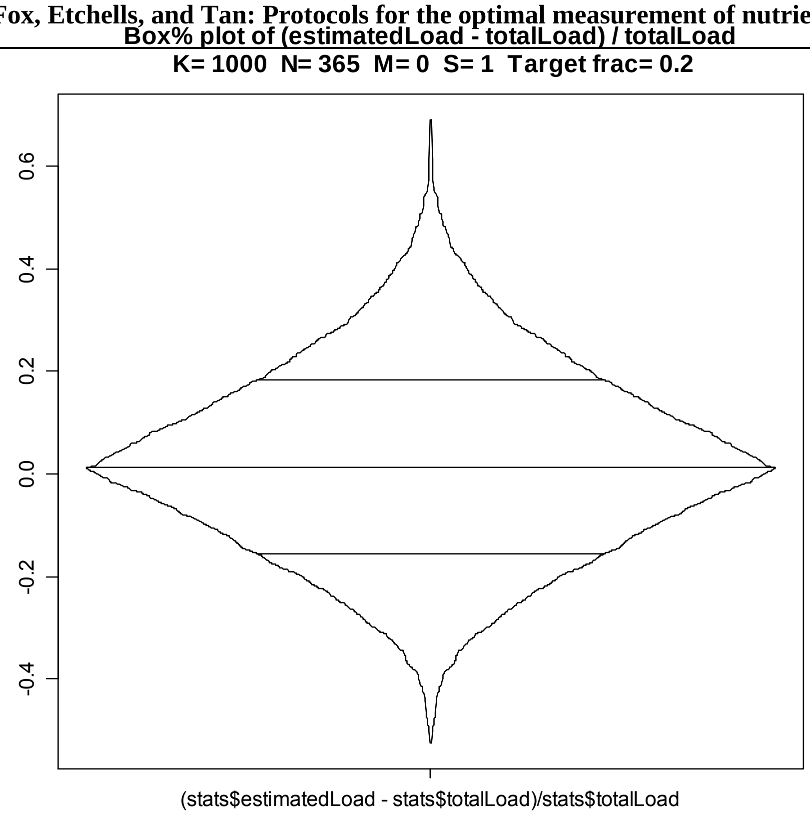

Figure 14. Box plot of proportional bias in annual load estimated under scenario #2.

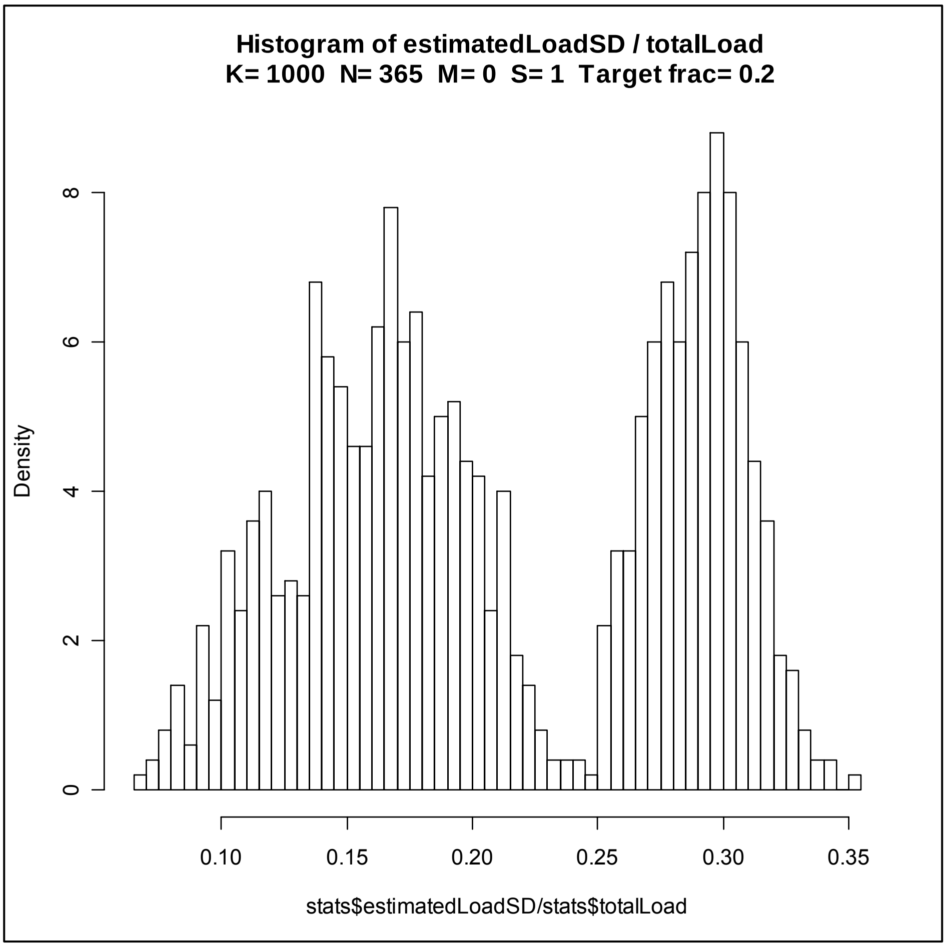

Figure 15. Histogram of ratio of estimated load to true load under scenario #2.

Scenario #3: Simulated rlnorm: Meanlog= 0 SDlog= 1 Target fraction= 0.3

Number of runs= 1000 Num sample flows N= 365
Fraction of runs for which abs(real load - estimated load) > 2*standard deviation = 0.084

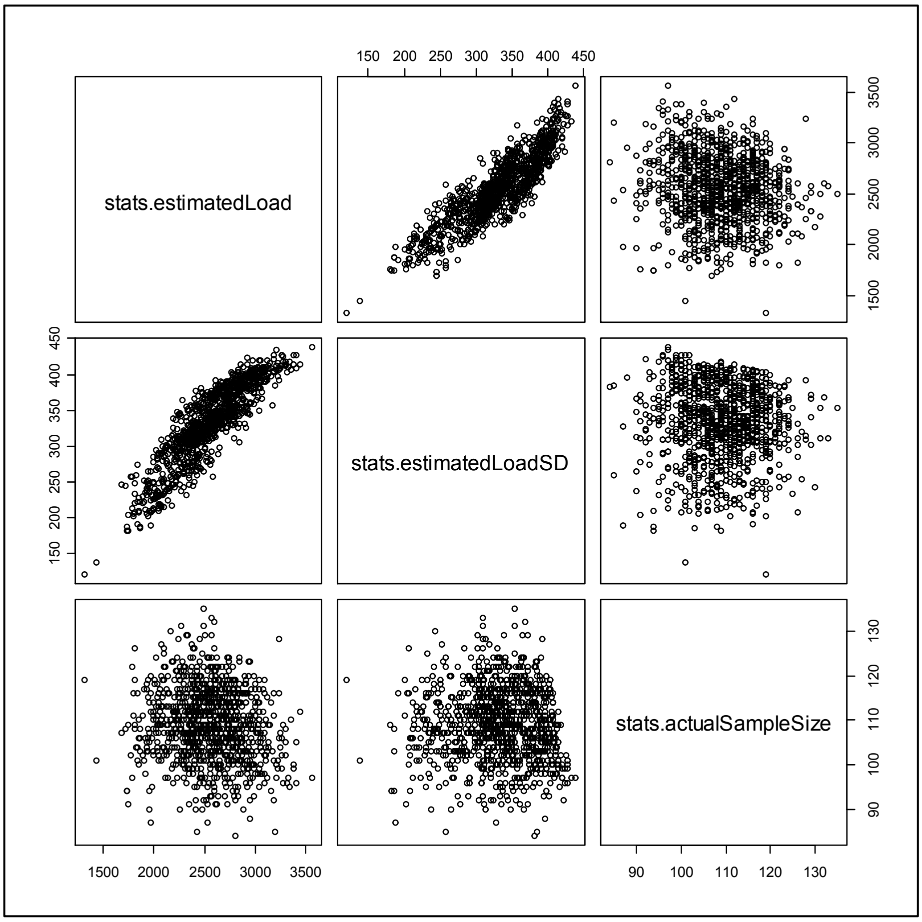

Figure 16. Matrix plot of simulation results for estimated load, standard error, and actual sample size – scenario #3.

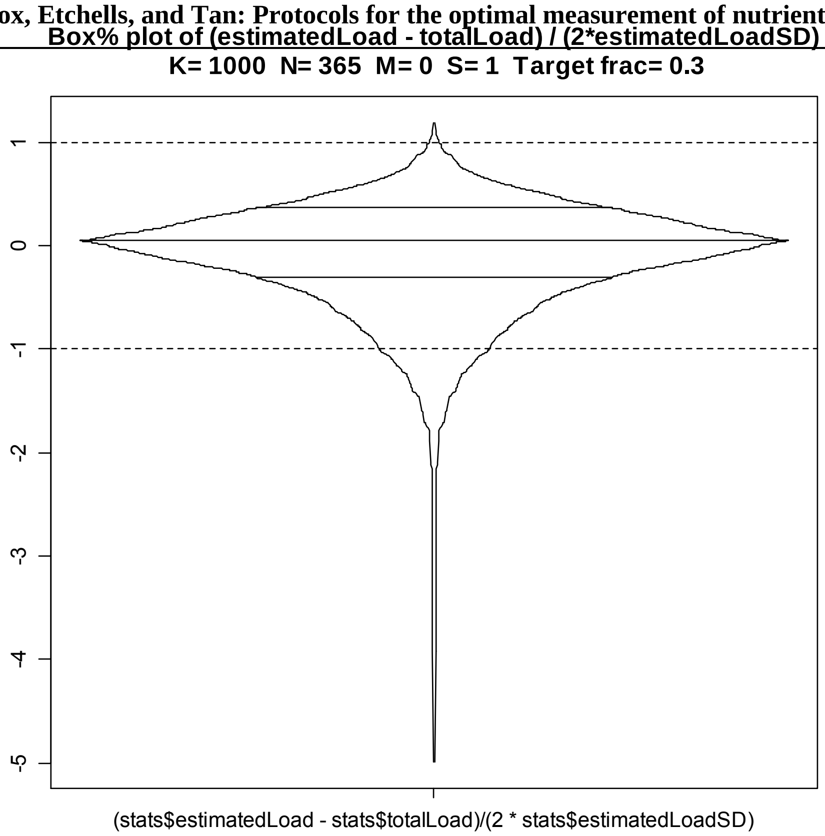

Figure 17. Box plot of standardised bias in annual load estimated under scenario #3.

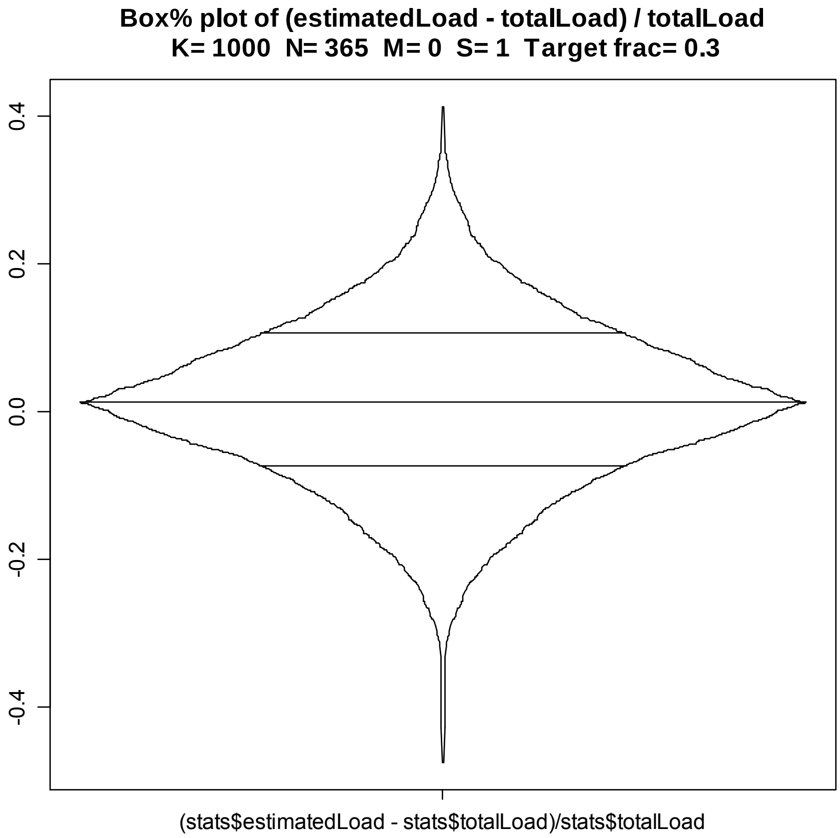

Figure 18. Box plot of proportional bias in annual load estimated under scenario #3.

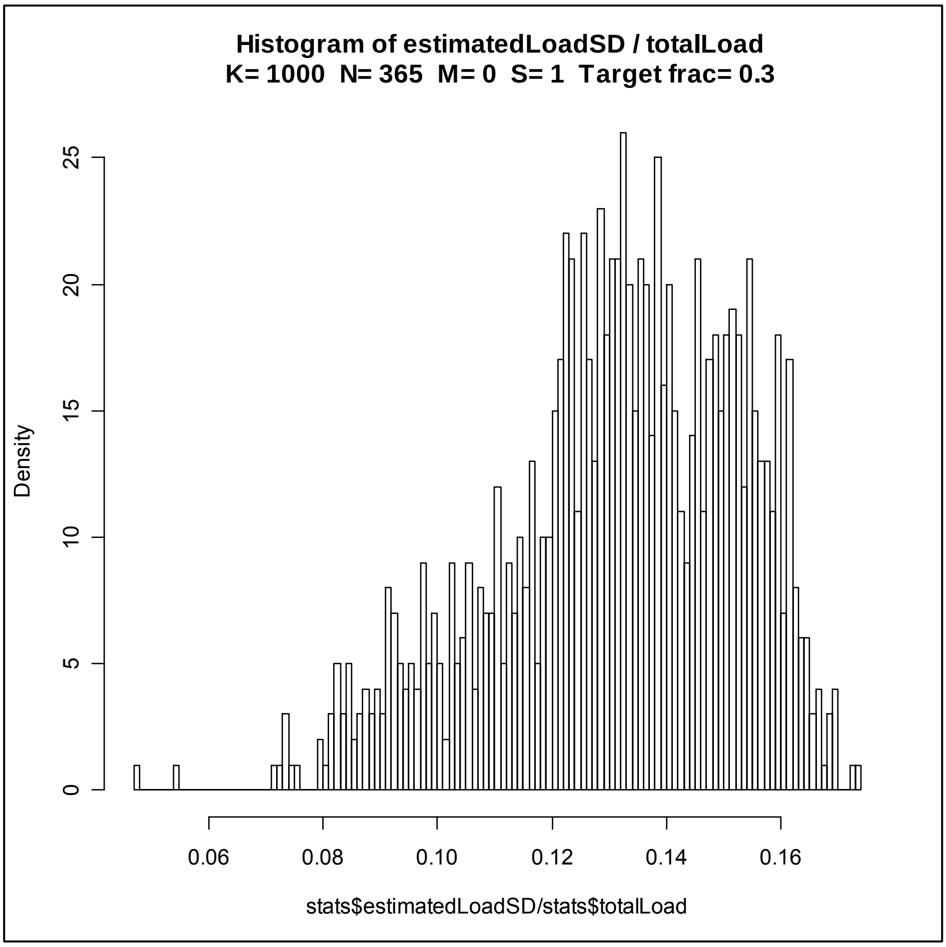

Figure 19. Histogram of ratio of estimated load to true load under scenario #3.

Scenario #4: Simulated rlnorm: Meanlog= 0 SDlog= 1 Target fraction= 0.4

Number of runs= 1000 Num sample flows N= 365
Fraction of runs for which abs(real load - estimated load) > 2*standard deviation = 0.095

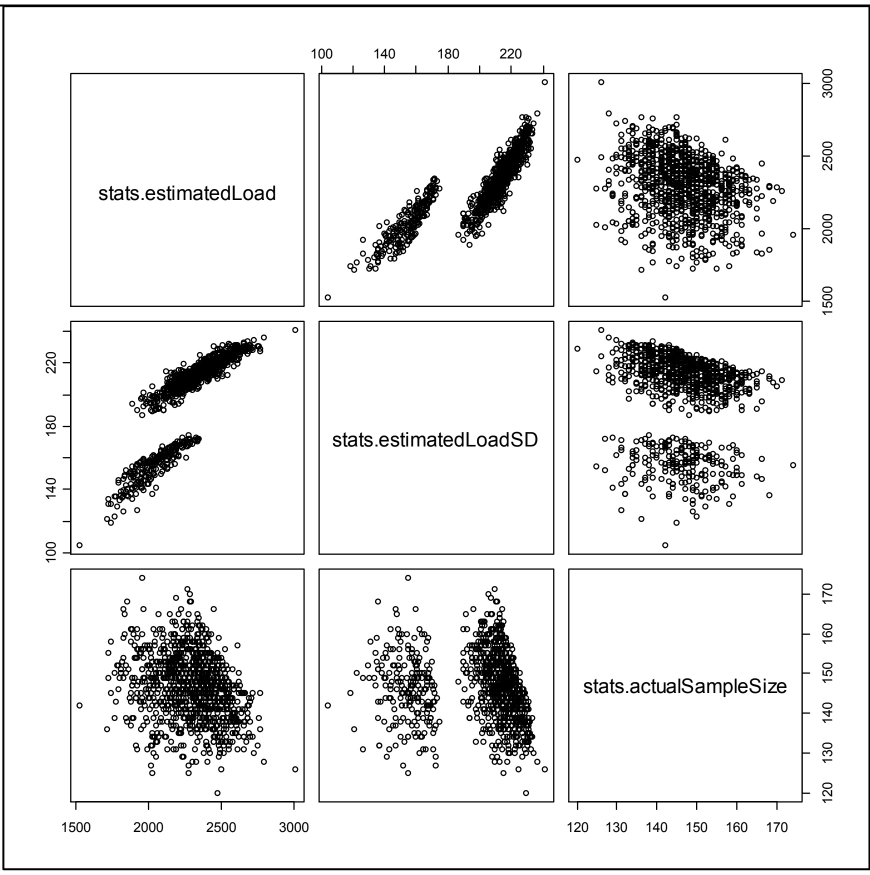

Figure 20. Matrix plot of simulation results for estimated load, standard error, and actual sample size – scenario #4.

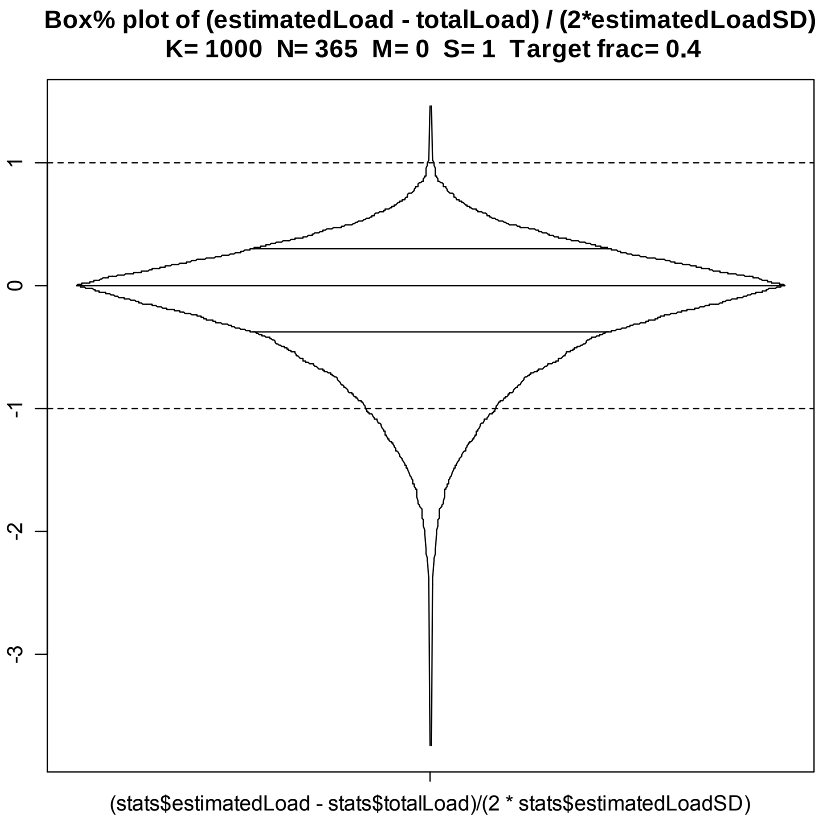

Figure 21. Box plot of standardised bias in annual load estimated under scenario #4.

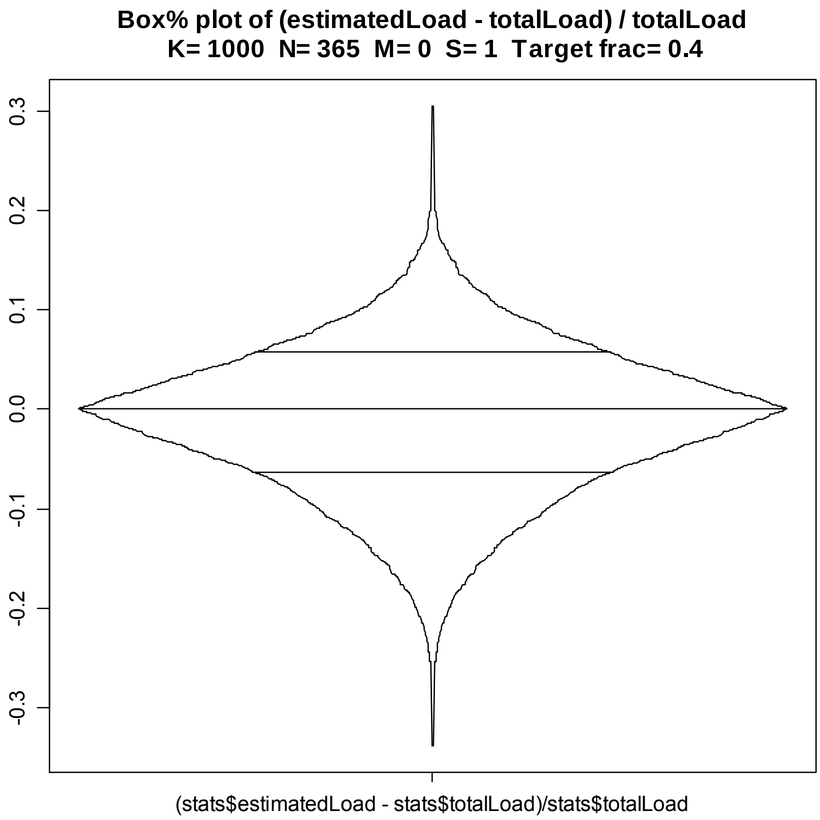

Figure 22. Box plot of proportional bias in annual load estimated under scenario #4.

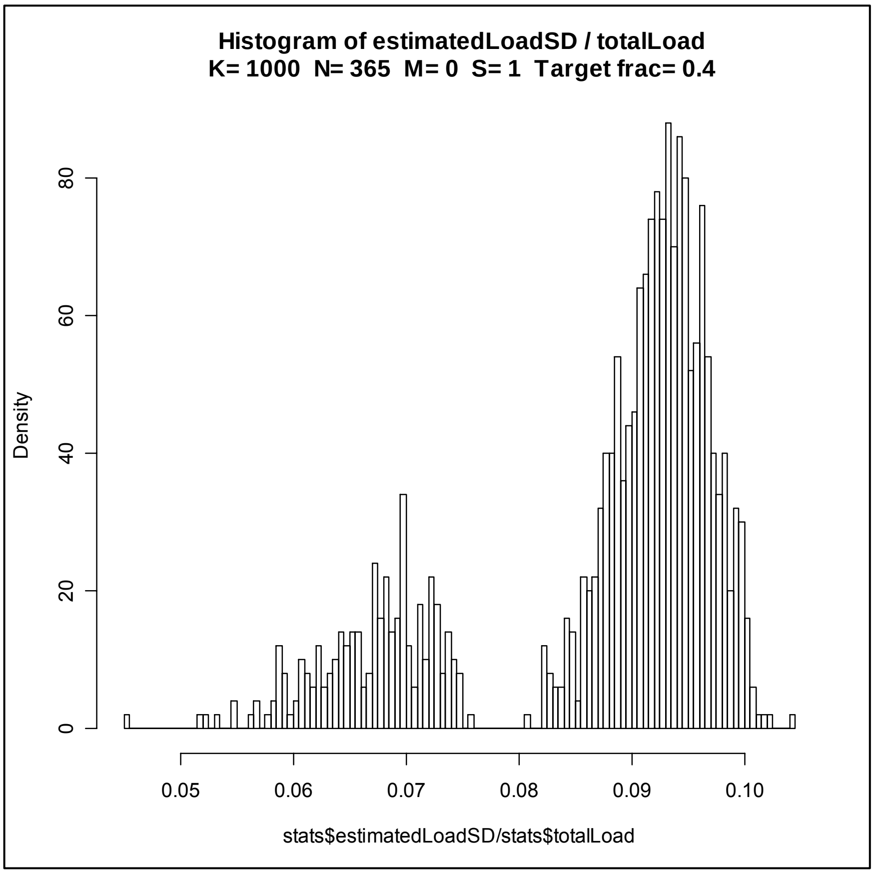

Figure 23. Histogram of ratio of estimated load to true load under scenario #4.

Scenario #5: Simulated rlnorm: Meanlog= 0 SDlog= 0.5 Target fraction= 0.1

Number of runs= 1000 Num sample flows N= 365
Fraction of runs for which abs(real load - estimated load) > 2*standard deviation = 0.134

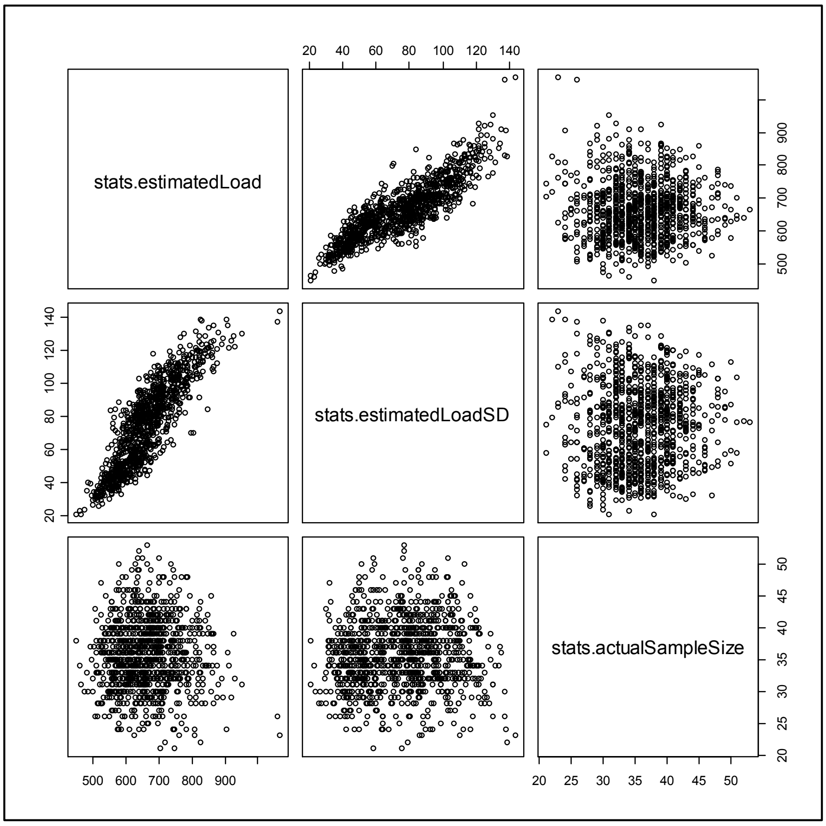

Figure 24. Matrix plot of simulation results for estimated load, standard error, and actual sample size – scenario #5.

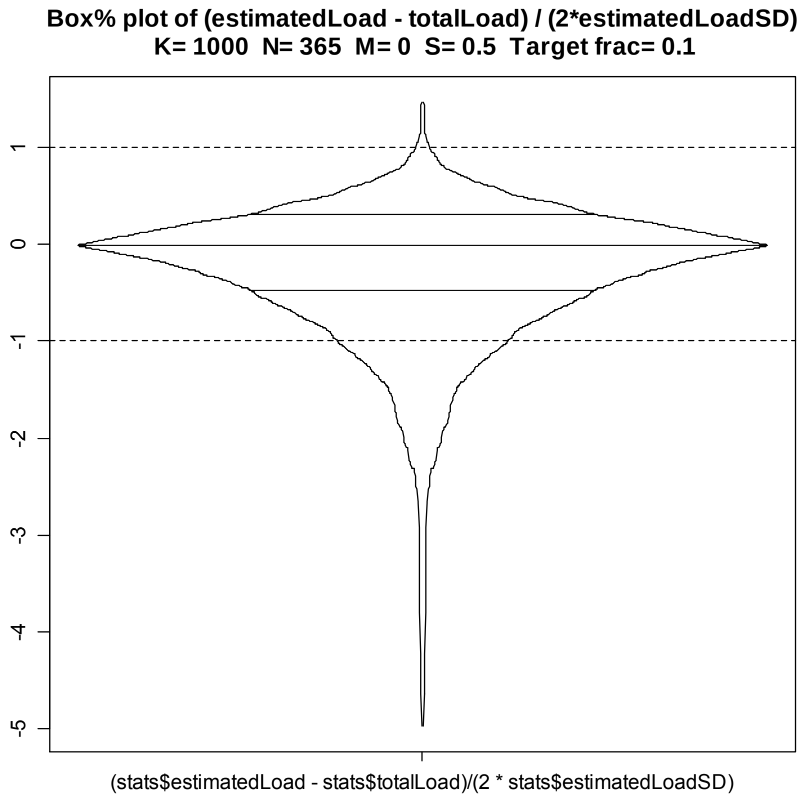

Figure 25. Box plot of standardised bias in annual load estimated under scenario #5.

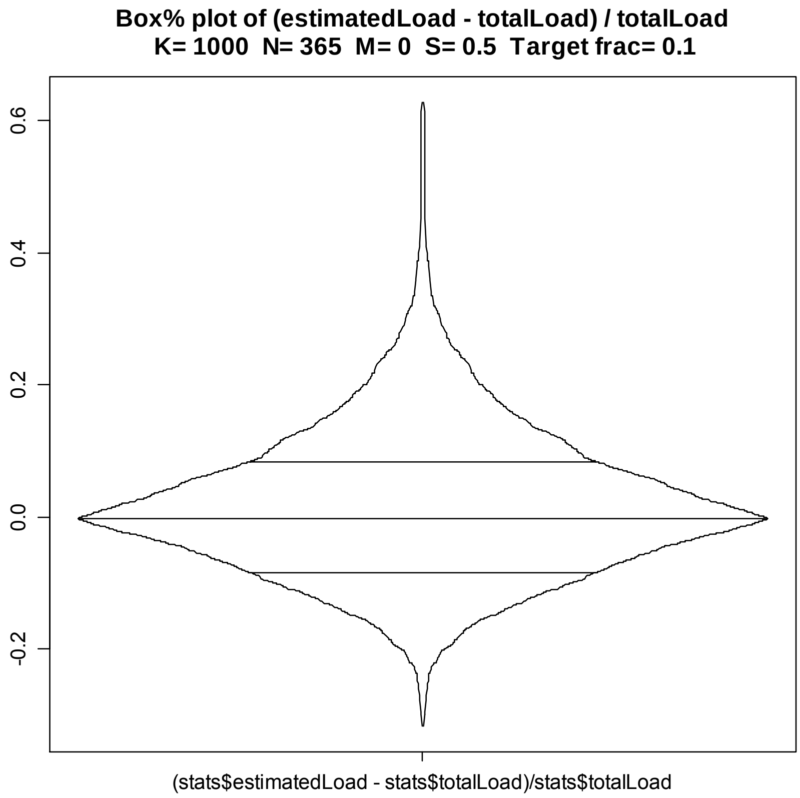

Figure 26. Box plot of proportional bias in annual load estimated under scenario #5.

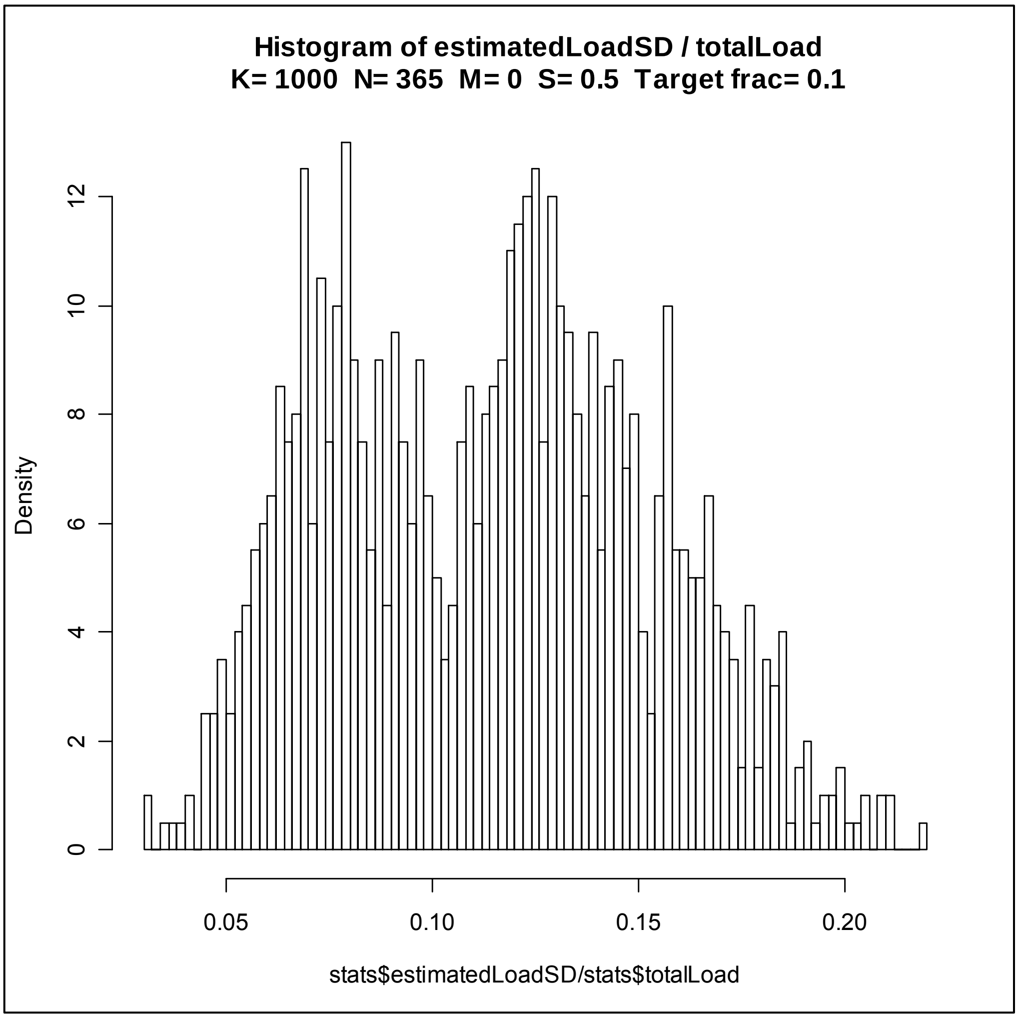

Figure 27. Histogram of ratio of estimated load to true load under scenario #5.

Scenario #6: Simulated rlnorm: Meanlog= 0 SDlog= 0.5 Target fraction= 0.2

Number of runs= 1000 Num sample flows N= 365
Fraction of runs for which abs(real load - estimated load) > 2*standard deviation = 0.106

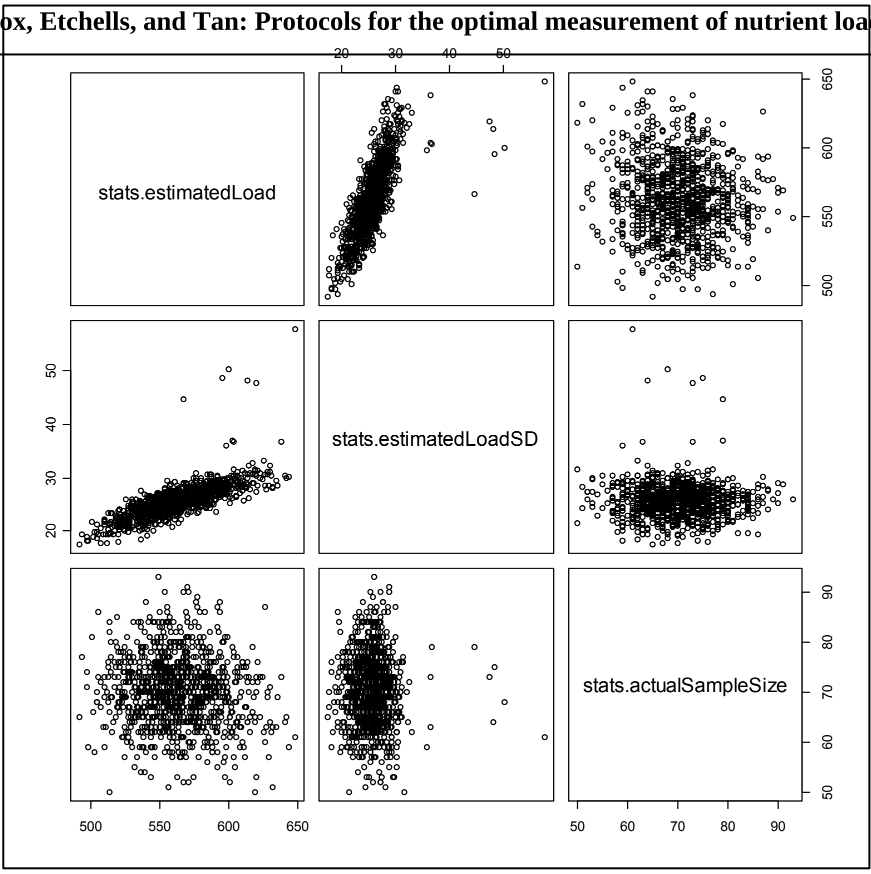

Figure 28. Matrix plot of simulation results for estimated load, standard error, and actual sample size – scenario #6.

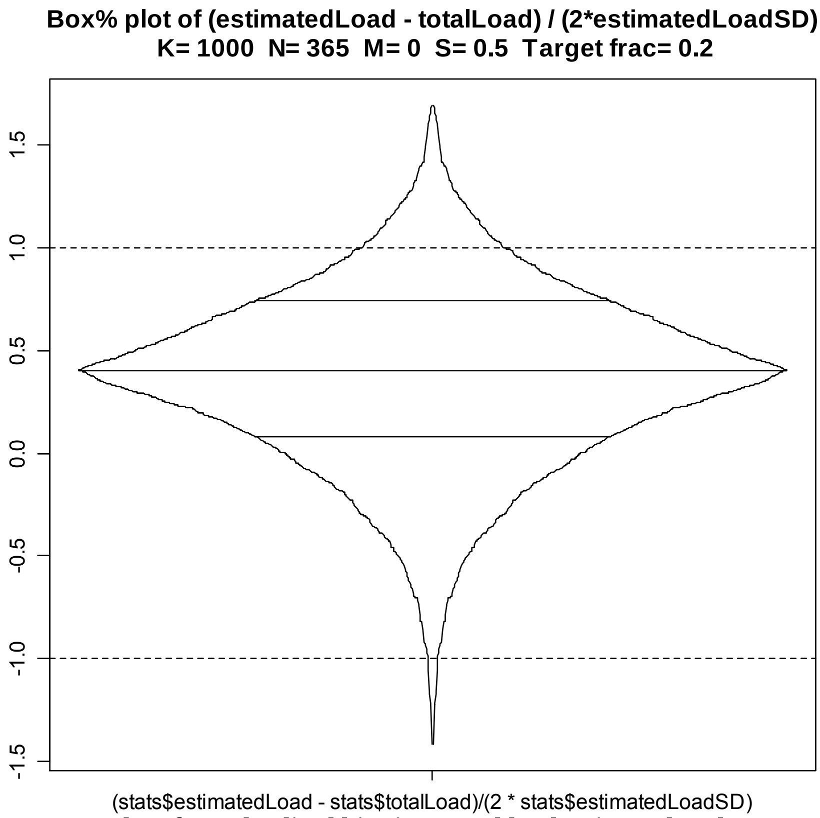

Figure 29. Box plot of standardised bias in annual load estimated under scenario #6.

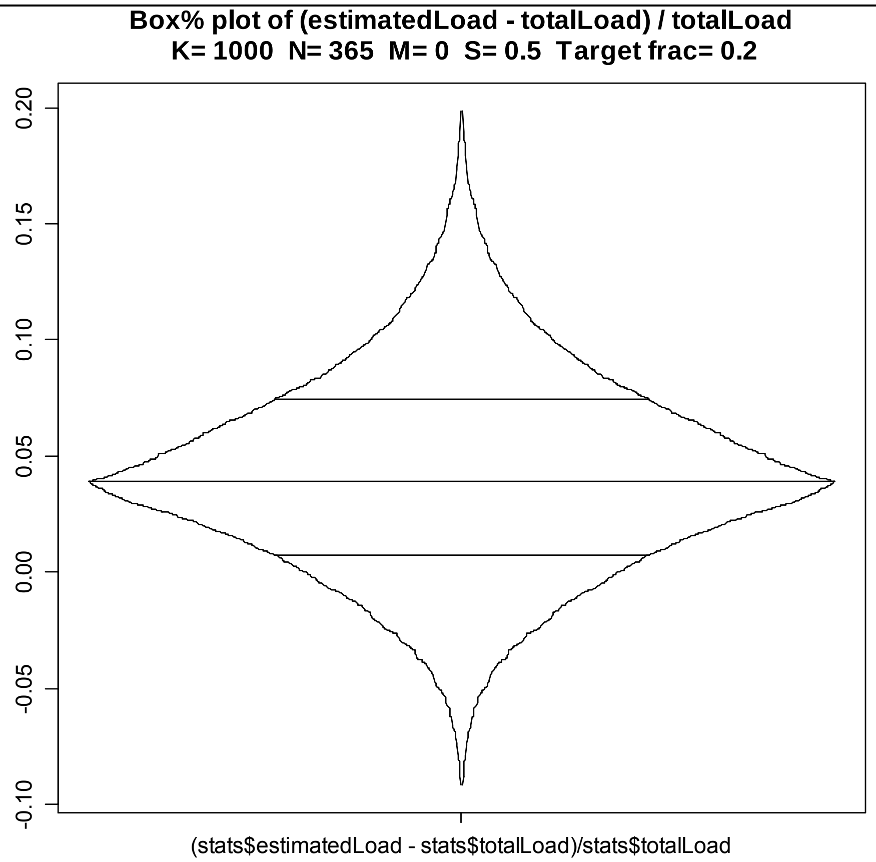

Figure 30. Box plot of proportional bias in annual load estimated under scenario #6.

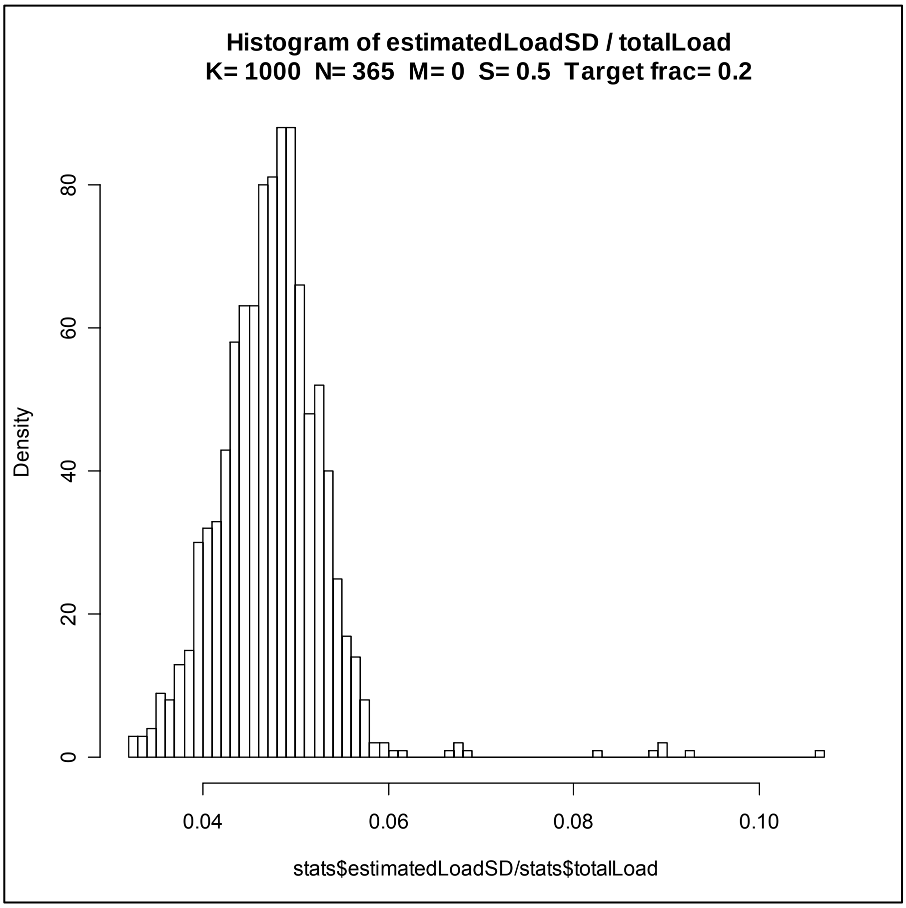

Figure 31. Histogram of ratio of estimated load to true load under scenario #6.

Scenario #7: Simulated rlnorm: Meanlog= 0 SDlog= 0.5 Target fraction= 0.3

Number of runs= 1000 Num sample flows N= 365
Fraction of runs for which abs(real load - estimated load) > 2*standard deviation = 0.07

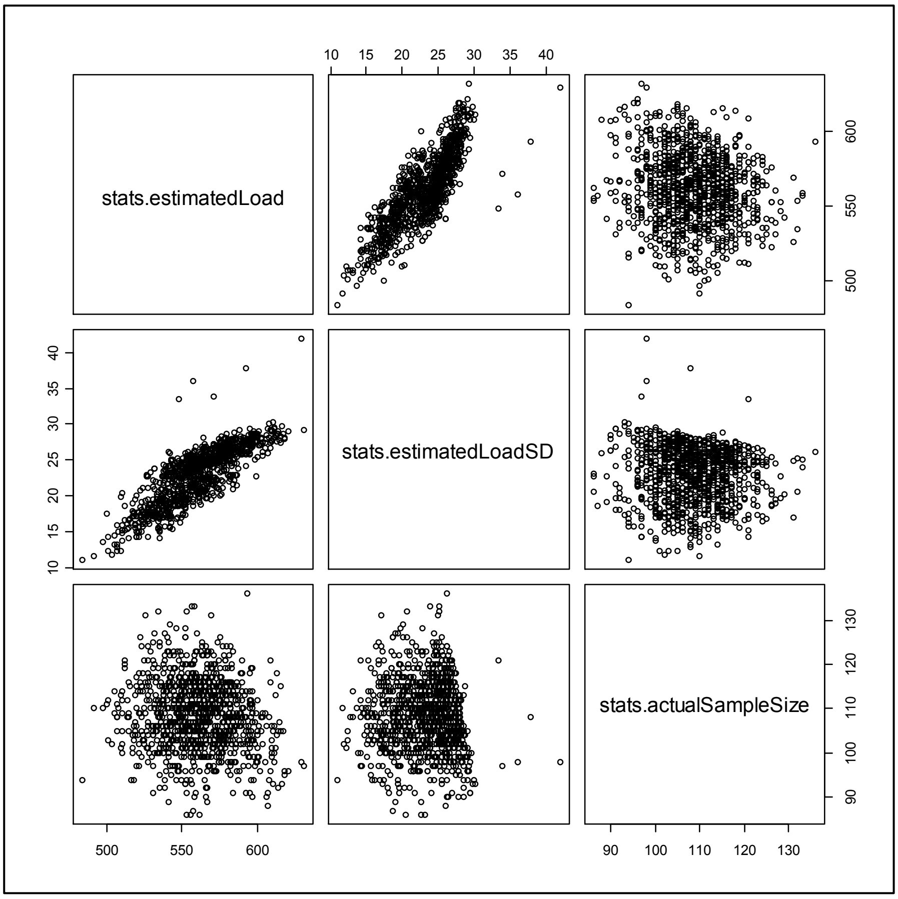

Figure 32. Matrix plot of simulation results for estimated load, standard error, and actual sample size – scenario #7.

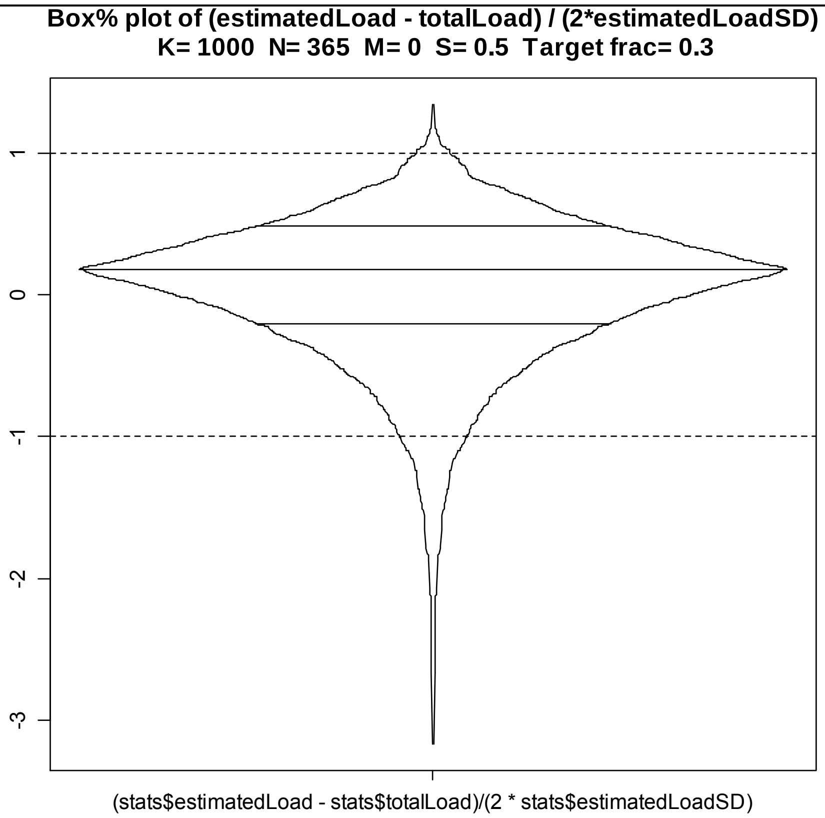

Figure 33. Box plot of standardised bias in annual load estimated under scenario #7.

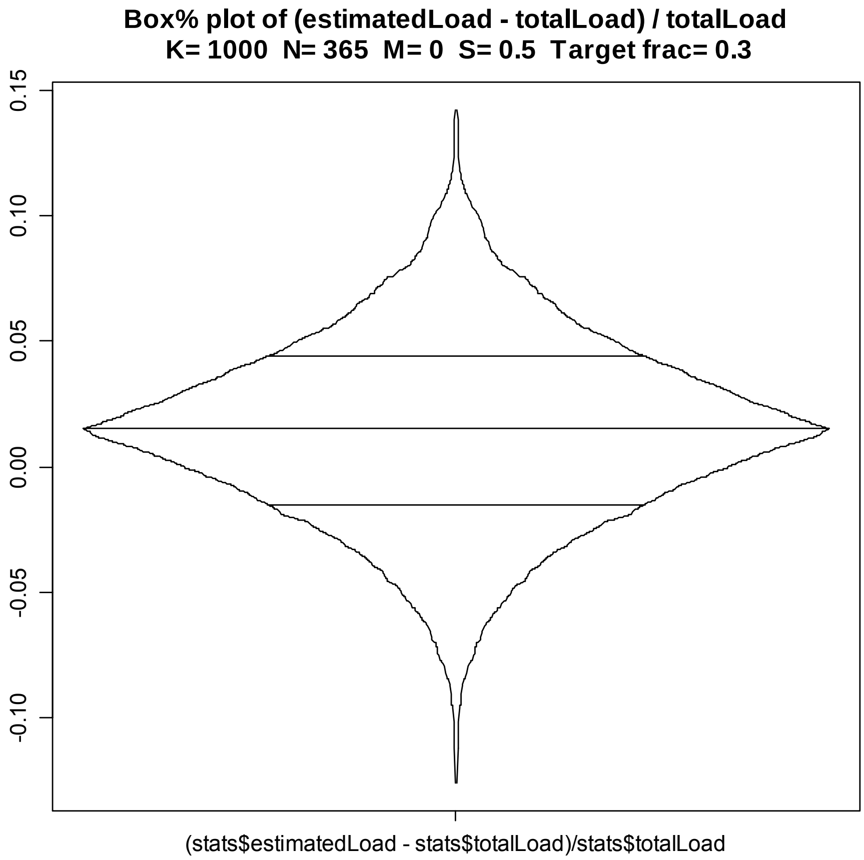

Figure 34. Box plot of proportional bias in annual load estimated under scenario #7.

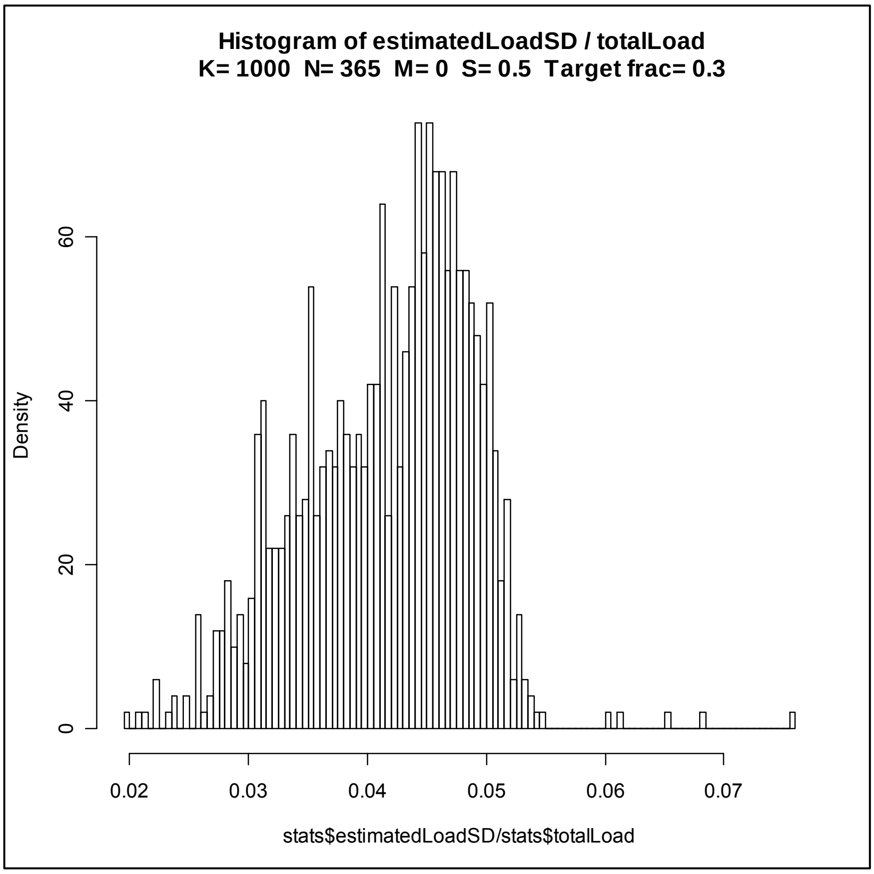

Figure 35. Histogram of ratio of estimated load to true load under scenario #7.

Scenario #8: Actual data: Target fraction= 0.1 (Outlier 57replaced by 1.111)

Number of runs= 1000 Num sample flows N= 261
Fraction of runs for which abs(real load - estimated load) > 2*standard deviation = 0.086

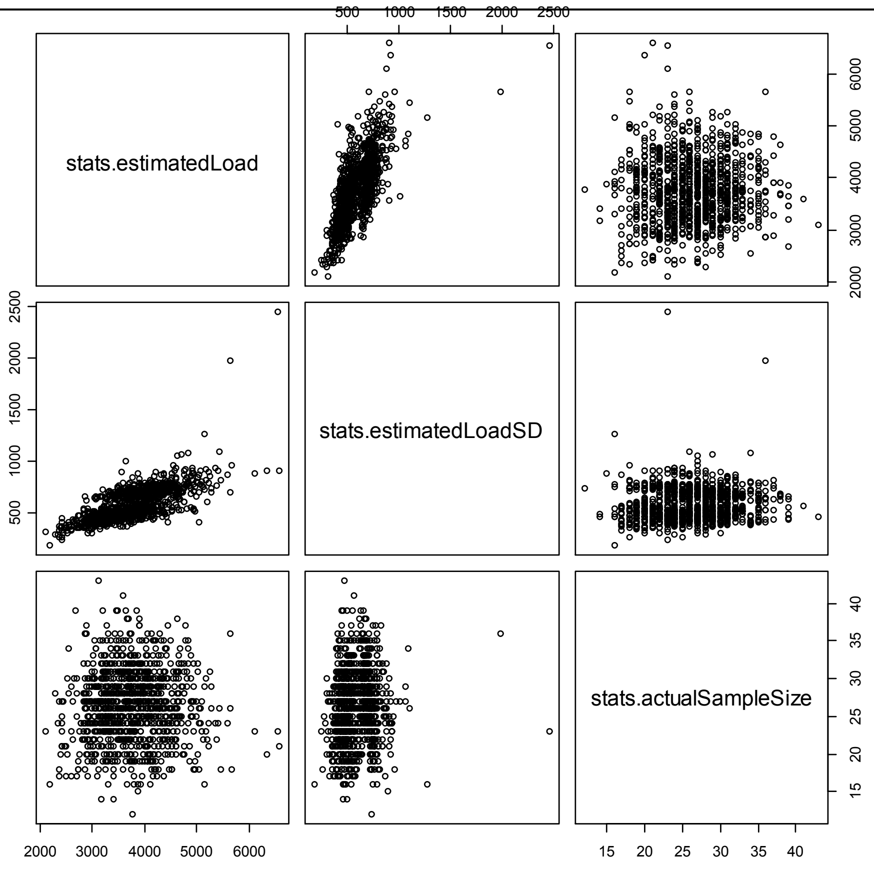

Figure 36. Matrix plot of simulation results for estimated load, standard error, and actual sample size – scenario #8.

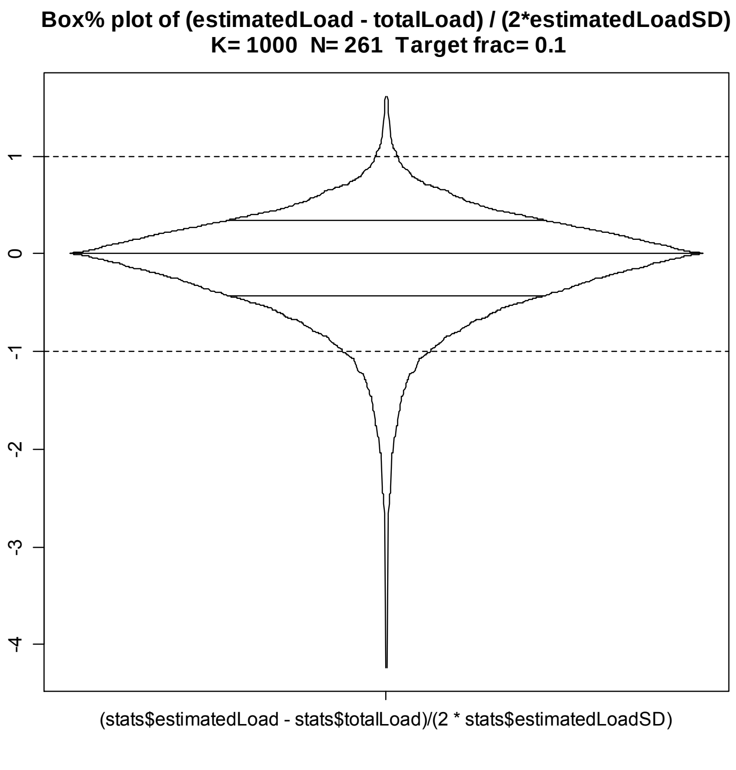

Figure 37. Box plot of standardised bias in annual load estimated under scenario #8.

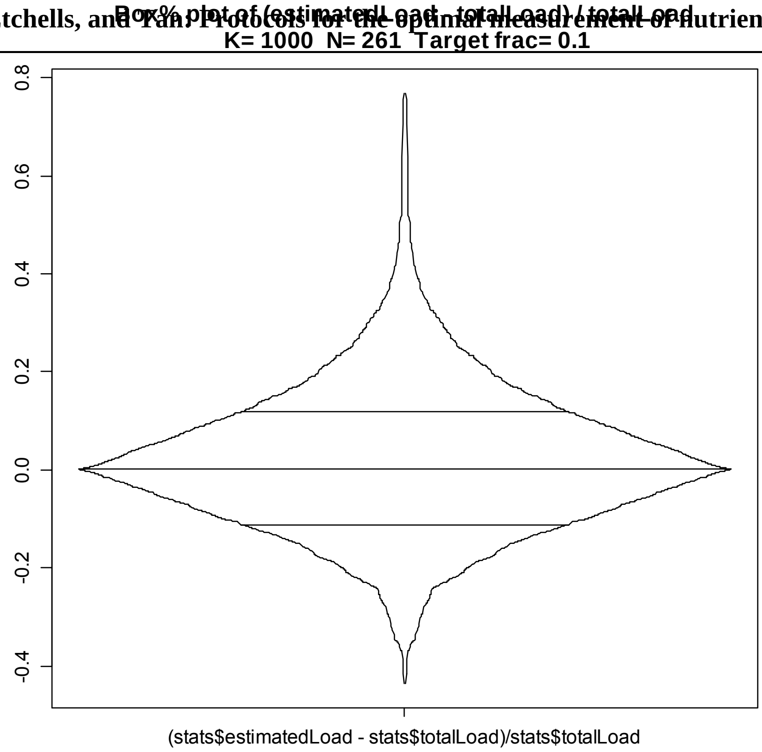

Figure 38. Box plot of proportional bias in annual load estimated under scenario #8.

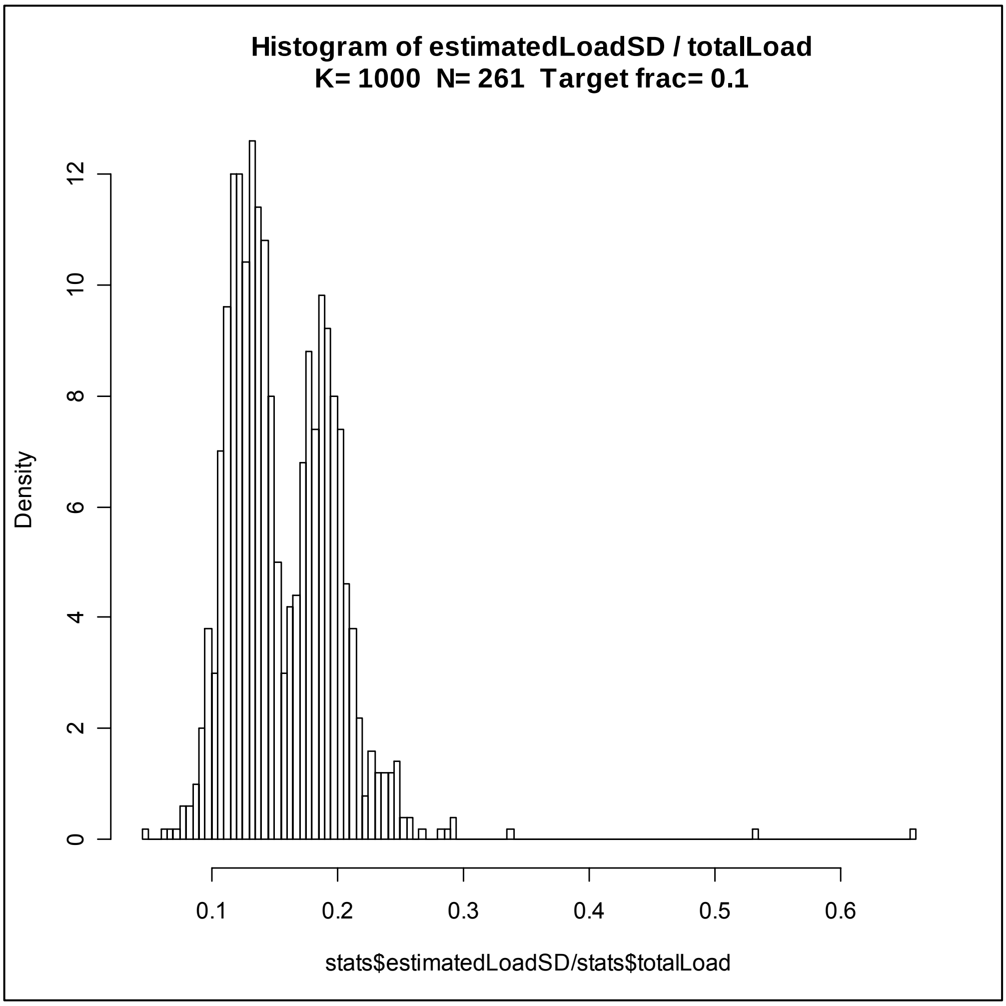

Figure 39. Histogram of ratio of estimated load to true load under scenario #8.

APPENDIX L: A Transfer Modelling Approach to Sediment-Nutrient Load Estimation[5]

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Introduction

The problem of estimating mass loads (of sediments &/or nutrients is not new). By definition, the instantaneous *flux rate* at time *t* is defined as the product of the sediment/nutrient concentration at time *t* and the instantaneous flow (discharge) at time *t*:

(1) $$F_t = C_t \cdot Q_t$$

The total load or mass transported in the interval [0,T] is obtained by integrating the instantaneous flux rate:

(2) $$Load = \int_0^T C_t \cdot Q_t \, dt$$

In practice, equation (1) is approximated by the summation

(3) $$L = K \sum_{i=1}^{n} C_i \cdot Q_i$$

where C_i and Q_i are measurements of concentration and flow respectively and *K* is a constant.

Many papers have been published on the dual problems of: (i) how to gather the flow-concentration data ie. sampling strategies; and (ii) the estimation process itself. Equation (2) is the simplest estimator and accords with intuition as it is essentially the discrete analog of equation (1). However, numerous other estimating equations have been proposed (see for example Letcher et al. (1999). The simplest sampling strategy is *systematic sampling* whereby a water sample is obtained once every *k* time periods. The main advantage of this approach is a logistical one since it is easy to implement and lends itself to automation. The disadvantage is that the intensity of sampling bears no relation to the hydrology of the water body being sampled. It is well known that for most catchments, significant amounts of material are transported during 'peak' flow events (eg. storms). In recognition of this phenomenon, more sophisticated sampling strategies have been devised which aim to capture these high-flow/high-load events. These strategies are either *deterministic* whereby sampling occurs whenever the flow (stage height) exceeds some threshold, or *probabilistic* in which case a statistical algorithm is used to bias the sampling events towards high-flow events. In either case, a common problem is that resource constraints are such that typically only about 12 - 30 water quality samples (ie. C_i values) can be obtained.

In contrast to the usual paucity of concentration data, information on flows is much more abundant since these can be obtained from in-situ data loggers. Thus, it is invariably the case that flows and concentrations are <u>not</u> measured

[5] This paper presented at International Statistical Institute, 55th Session 2005, Sydney.

contemporaneously. The analyst is then faced with the issue of estimating, for example, an annual load using daily flow information and monthly concentrations. Common strategies involve linearly interpolating the monthly concentrations and resampling to a daily time base, or alternatively, to assume the 'spot' monthly concentration reading is indicative of the average for the month and to apply this to the total volume of water over the month. Neither of these approaches is satisfactory as large errors arise.

In this paper, we address the data paucity and estimation issues simultaneously by using a transfer function model whose parameters are estimated from *monthly* water quality data. Having fitted the model and estimated other key parameters such as the variance of the random error or shock component, simulated *daily* time-series for the water quality parameter of interest can be constructed. The simulated concentrations are then matched with *actual* flows and a straightforward application of equation (3) provides an estimate of load for the period of interest. A critical modification to the (assumed) monthly monitoring for water quality is required. Instead of taking a *single* sample once a month for analysis, the procedure outlined here requires that an *average* concentration be obtained from a *composite* monthly sample.

A transfer model for daily concentration data

For the catchments we have investigated, there is evidence to suggest that the (log) concentration at time *i* is strongly related to the (log) flow at time *i* and the (log) concentration in the immediately two preceding time periods. Let C_i and Q_i denote the natural logarithms of concentration and flow respectively. Our model (equation 4) is an extension of the first-order transfer model adopted by Littlewood (1995):

$$(4) \qquad C_i = \frac{\alpha_0 + \alpha_1 Q_i}{\left(1 + B \cdot \beta_1 + B^2 \cdot \beta_2\right)} + \varepsilon_i$$

where the αs and βs are model parameters; *B* is the backward shift operator and ε_i is a random error or 'shock' component.

Results

Having estimated the model parameters, equation 4 may be used recursively (given initial values for C_1 and C_2) to generate sequences of daily concentration data (Figure 1). For each generated sequence, an estimate of total load is obtained using equation 3. Statistics (eg. Mean and standard error) are then computed for the collection of N load estimates to provide an interval estimate for the true total load. An application of the methodology estimated the phosphorous load in an irrigation channel in Gippsland, Victoria to within 3% of the true load. This is compared with a 30% over-estimate using monthly data.

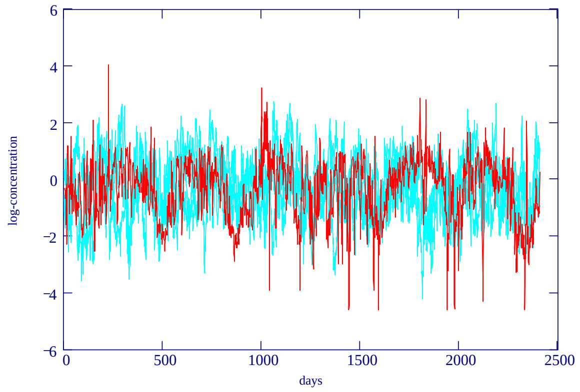

Figure 24. Simulated daily series (cyan lines) and actual daily series (red line)

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Appendix M: Error Approximations

Technical Report

Prof. David R. Fox
Australian Centre for Environmetrics

Report 03/05

April 2005

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Acknowledgements

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1. Introduction

The accurate estimation of total loads of sediments and nutrients is a problem that is attracting considerable attention among natural resource managers, environmental protection agencies, governments, landowners, and the general community. The delivery of sediments from Queensland catchments has been identified as a threat to the ecosystem of the Great Barrier Reef, while point and diffuse sources of land-based nutrients are implicated in the increased frequency and severity of algal blooms in water bodies around the country. Accordingly, there has been a growing trend towards the expression of aspirational and compliance targets for nutrients and sediments in terms of either a relative or absolute reduction in total *load*. For example, a 20% nutrient reduction target has been imposed on Queensland catchments impacting the Great Barrier Reef while the Victorian EPA has required a 40% reduction in the total phosphorous load from the McAlister Irrigation District by 2005 and a commensurate 40% reduction in total nutrient loads to the Gippsland Lakes by 2022. As noted by Henderson and Bui (2004), the quantification of errors and uncertainty is particularly important in the context of ecological risk assessments as a failure to do so may lead to risks being significantly under or over-estimated.

This report focuses on the quantification of errors associated with a number of common load estimation techniques. We also point out the duality between simple mean-based load estimators and ratio estimation techniques.

2. Load Estimation

A list of some 24 computational techniques for estimating a load was provided in Letcher et al. (2002). Most of these formulae can be classified as belonging to one of the groupings: mean-based estimators; ratio estimators; and regression estimators. In this paper we consider a class of load estimators given by equation 1.

$$\hat{L} = K\left(\sum_{i=1}^{n_c} w_i c_i\right)\left(\sum_{j=1}^{n_q} v_j q_j\right) \tag{1}$$

where c_i is a measured concentration on the i^{th} occasion; q_j is a measured flow on the j^{th} occasion and w_i and v_j are weights[6]. *K* is a constant that reconciles the sampling time-step with the period of interest (eg. if concentrations and flows represent daily values and an annual load estimate is required, then *K=365*).

3. Theoretical mean and variance

Before turning our attention to the properties of load estimators, it will be useful to develop some theoretical results for the expected value and variance of a load under certain distributional assumptions. In what follows we assume (not unreasonably), that the distribution of concentration (C) and flow (Q) are well described by the bivariate lognormal distribution given by equation 2 and that load, $L = CQ$.

$$f_{C,Q}(c,q) = \frac{1}{2\pi cq\sigma_C\sigma_Q\sqrt{1-\rho^2}}\exp\left\{-\frac{1}{2(1-\rho^2)}\left[\left(\frac{\ln(c)-\mu_C}{\sigma_C}\right)^2 - 2\rho\left(\frac{\ln(c)-\mu_Q}{\sigma_C}\right)\left(\frac{\ln(q)-\mu_Q}{\sigma_Q}\right)+\left(\frac{\ln(q)-\mu_{2Q}}{\sigma_Q}\right)^2\right]\right\} \quad (2)$$

where μ and σ are the mean and standard deviation of the log-transformed data and ρ is the correlation between *log* concentration and *log* flow.

Fox (2004) showed that the expected load is given by equation 3.

$$E[L] = \exp\left\{(\mu_C+\mu_Q)+\frac{1}{2(1-\rho^2)}\left[(\rho\sigma_Q+\sigma_C)^2+(\rho\sigma_C+\sigma_Q)^2-2\rho(\rho\sigma_Q+\sigma_C)(\rho\sigma_C+\sigma_Q)\right]\right\} \quad (3)$$

Furthermore, it can be established that the second (uncorrected) moment is:

[6] The weights are somewhat arbitrary although values are usually determined by the nature of the sampling scheme. For example, a constant weight of 1/n implies a simple average while flow weighted averaging implies weights are determined on the basis of observed flow (higher flow implying higher weight).

$$E\left[L^2\right] = \exp\left\{2\left(\mu_C + \mu_Q\right) + \frac{2}{\left(1-\rho^2\right)}\left[\left(\rho\sigma_Q + \sigma_C\right)^2 + \left(\rho\sigma_C + \sigma_Q\right)^2 - 2\rho\left(\rho\sigma_Q + \sigma_C\right)\left(\rho\sigma_C + \sigma_Q\right)\right]\right\} \quad (4)$$

and so the variance is given as

$$Var\left[L\right] = E\left[L^2\right] - \left(E\left[L\right]\right)^2 \quad (5)$$

4. Uncertainty in load estimates

We next turn our attention to sampling properties of the estimator given by equation 1. In particular, it can be shown that an approximation[7] to the variance is:

$$Var\left[\hat{L}\right] = K^2\left(\sum_{i=1}^{n_c} w_i^2\right)\left(\sum_{j=1}^{n_q} v_j^2\right)Var\left[L\right] \quad (6)$$

For suitable choices of the weights w_i and v_j we can obtain variance approximations for a number of common load estimators. Furthermore, the duality between a ratio estimator of load and one obtained using flow-weighted mean concentrations can be established. These issues are covered under special cases 1-3 below.

Special Case #1 – The Naïve estimator (average flow x average concentration)

The simplest of all load estimators is a scaled product of the mean concentration and the mean discharge (flow). We refer to this as the ‘naïve’ estimator – its attractiveness lies in its computational simplicity, although serious biases (typically > 30%) result

[7] It is recognised that this approximation does not take into account autocorrelation between the *c* and *q* data, nor the cross-correlations between them. See Appendix A for a derivation.

(Fox, 2004). The naïve estimator is readily seen to be obtained by letting $w_i = \frac{1}{n_c}$ and $v_j = \frac{1}{n_q}$ giving

$$\hat{L}_1 = K \bar{C} \bar{Q} \tag{7}$$

and

$$Var\left[\hat{L}_1\right] = \frac{K^2 Var\left[L\right]}{n_c\, n_q} \tag{8}$$

Special Case #2 – Load estimator using flow-weighted mean concentrations and unknown total discharge

Unlike the naïve estimator which assigns equal weight to each observed concentration, the flow-weighted mean concentration (*fwmc*) uses weights that are proportional to the magnitude of the associated flow. In this sense, the naïve estimator may be thought of as a time-based average whereas the *fwmc* is a flow-based average. It is implicit in flow-weighted averaging that the flow and concentration data are contemporaneous whereas no such assumption was previously made. Thus, $n_c = n_q = n$ and the weights for *fwmc* are

$$w_i = \frac{q_i}{\sum_{i=1}^{n} q_i}; \quad v_i = 1 \quad \forall i$$

Thus,

$$\hat{L}_2 = K' \frac{1}{\sum_{i=1}^{n} q_i} \left(\sum_{i=1}^{n} c_i\, q_i \right) \left(\sum_{i=1}^{n} q_i \right)$$

$$\hat{L}_2 = K' \sum_{i=1}^{n} c_i\, q_i \tag{9}$$

where $K' = \frac{K}{n}$ (eg. if one month of daily concentration data are available to estimate an annual load using equation 9, then *K=365* and *n=30*). The K' factor is needed in this case because the total discharge, $\sum_{i=1}^{n} q_i$ is only known for the *sample* and not the entire period of interest.

Furthermore,

$$Var\left[\hat{L}_2\right] = K'^2 \sum_{i=1}^{n} \left(\frac{q_i}{\sum q_i^2} \right) n\, Var\left[L\right]$$

$$= \frac{K^2 Var\left[L\right]}{n\left(\sum_{i=1}^{n} q_i\right)^2} \sum_{i=1}^{n} q_i^2 \qquad (10)$$

Aside

It can be readily established that in the case $n_c = n_q = n$, the variance of $\hat{L}_2$ is greater than the variance of $\hat{L}_1$. To see this, we look at $Var\left[\hat{L}_2\right] - Var\left[\hat{L}_1\right]$.

$$Var\left[\hat{L}_2\right] - Var\left[\hat{L}_1\right] = \frac{K^2}{n\left(\sum_{i=1}^{n} q_i\right)^2} \sum_{i=1}^{n} q_i^2\, Var\left[L\right] - \left\{ \frac{K^2 Var\left[L\right]}{n^2} \right\}$$

$$= K^2 Var\left[L\right] \left\{ \frac{\sum_{i=1}^{n} q_i^2}{n\left(\sum_{i=1}^{n} q_i\right)^2} - \frac{1}{n^2} \right\}$$

Hence, $Var\left[\hat{L}_2\right] > Var\left[\hat{L}_1\right]$ if

$$\frac{\sum_{i=1}^{n} q_i^2}{n\left(\sum_{i=1}^{n} q_i\right)^2} - \frac{1}{n^2} > 0$$

$$\Rightarrow \sum_{i=1}^{n} q_i^2 - \frac{\left(\sum_{i=1}^{n} q_i\right)^2}{n} > 0$$

which is *always* true since the last expression is the sample variance of the measured flows.

Special Case #3 – Load estimator using flow-weighted mean concentrations and known total discharge

This case is identical to special case #2 with the exception that the *fwmc* is applied to the total (annual) discharge, $\sum_{i=1}^{K} q_i$. Thus, the weights are as before except that the $\{v_j\}$ weights span the period of interest *(j=1,..,K)* rather than the sample *(j=1,..,n)*.

Thus,

$$\hat{L}_3 = \frac{\sum_{i=1}^{n} c_i q_i}{\left(\sum_{i=1}^{n} q_i\right)} Q \tag{11}$$

where Q is the total (annual) discharge.

Furthermore,

$$Var\left[\hat{L}_3\right] = \frac{K \sum_{i=1}^{n} q_i^2}{\left(\sum_{i=1}^{n} q_i\right)^2} Var\left[L\right] \tag{12}$$

Note, if we have sampling fraction $f = \frac{n}{K}; \quad 0 < f < 1$ then equation 10 can be written as $Var\left[\hat{L}_2\right] = \frac{Var\left[\hat{L}_3\right]}{f}$ and it is evident that $Var\left[\hat{L}_3\right] < Var\left[\hat{L}_2\right]$.

5. The duality of the fwmc load estimator and a ratio estimator

Ratio estimation is a well known technique for potentially reducing the error (increasing the precision) of the estimate when an auxiliary variable that is correlated with the variable of interest is available. A full treatment of ratio estimators is given in Cochran (1977). In the present context, a ratio estimator is formed by assuming the ratio of the total load for the *sample* to the total discharge for the *sample* is the same as the corresponding quantities over the period of interest. That is

$$\frac{l}{q} = \frac{L}{Q}$$

Where *l (L)* is the sample (population) load and *q (Q)* is the sample (population) discharge. The ratio estimator is then

$$\hat{L}_{ratio} = \left(\frac{l}{q}\right)Q \tag{13}$$

Expanding equation 13, we have

$$\hat{L}_{ratio} = \frac{\left(\sum_{i=1}^{n} w_i c_i\right)\left(\sum_{i=1}^{n} v_i q_i\right)}{\sum_{i=1}^{n} q_i} \cdot \sum_{j=1}^{K} q_j \tag{14}$$

and letting $v_i = 1 \quad \forall i$ and $w_i = \frac{q_i}{\sum_{i=1}^{n} q_i}$ we see that $\hat{L}_{ratio} = \hat{L}_3$.

6. An Example

We consider the estimation of the total phosphorous (TP) load in a drain (designated CG3) in Gippsland, Victoria during the 2004 irrigation season[8]. The availability of daily flow and TP measurements enables us to compute the 'true' load as 5,517.10 kg. A random sample of *n*=29 observations were taken and the results used to demonstrate the methods outlined in this paper. The parameters given in table 1 were estimated from the *log*-transformed flow and concentration data.

Table 8. Parameters for log-flow and log-concentration

	Log-Flow	*Log-Concentration*
μ	2.5561	-0.02834
σ	0.6706	0.8008
ρ	0.482	

[8] Data courtesy of Southern Rural Water

By substituting the parameter estimates in table 1 into equations (3) and (4) we obtain (using equation (4)) estimate the load variance to be $Var\left[L\right]=3132.863$. We next obtain load estimates using methods 1-3.

Method#1

Our data yield: $n=29$, $\overline{c}=\frac{1}{n}\sum_{i=1}^{n}c_i=1.17225$, and $\overline{q}=\frac{1}{n}\sum_{i=1}^{n}q_i=11.4015$. The duration of the irrigation season is such that K=279 days. Thus

$$\hat{L}_1=(279)(1.17225)(11.4015)=3728.95\,\text{kg}$$

Compared to the 'true' load of 5517.10kg, $\hat{L}_1$ is seen to *underestimate* the true load by 33%. This overestimation is a consequence of the high (positive) correlation between log-concentration and log-flow. A bias correction factor (Fox 2004) can be applied in attempt to reduce this effect. In this case an improved estimate is obtained by multiplying $\hat{L}_1$ by $\exp\left\{Cov\left[\ln C,\ln Q\right]\right\}=\exp\left(\rho\sigma_c\sigma_q\right)=1.2954$. This gives a modified total load of 4830.5kg which has reduced the bias to 13%.

From equation (8) we have

$$Var\left[\hat{L}_1\right]=\frac{279^2}{(29)(29)}Var\left[L\right]=350220.28$$

and hence $SE\left[\hat{L}_1\right]=\sqrt{Var\left[\hat{L}_1\right]}=591.8$.

Method#2

From equation (9)

$$\hat{L}_2=K'\sum_{i=1}^{29}c_i\,q_i$$

$$=\frac{279}{29}(434.410)=4179.32\,\text{kg}.$$

Compared to the 'true' load of 5517.10kg, $\hat{L}_2$ is seen to *underestimate* the true load by 24%. From equation (10) we have

$$Var\left[\hat{L}_2\right] = \frac{279^2 Var\left[L\right]}{(29)\left(\sum_{i=1}^{29} q_i\right)^2} \sum_{i=1}^{29} q_i^2$$

$$= \frac{279^2}{29} \frac{(4553.11)(3132.863)}{330.643^2} = 350220.28$$

and hence $SE\left[\hat{L}_2\right] = \sqrt{Var\left[\hat{L}_2\right]} = 591.8$.

Method#3

From equation (11)

$$\hat{L}_3 = K \frac{\sum_{i=1}^{29} q_i^2}{\left(\sum_{i=1}^{29} q_i\right)^2} Var\left[L\right]$$

$$= \frac{279(4553.11)(3132.863)}{330.643^2} = 36402.82 \text{ kg.}$$

Compared to the 'true' load of 5517.10kg, $\hat{L}_2$ is seen to *underestimate* the true load by 24%. From equation (10) we have

$$Var\left[\hat{L}_2\right] = \frac{279^2 Var\left[L\right]}{(29)\left(\sum_{i=1}^{29} q_i\right)^2} \sum_{i=1}^{29} q_i^2$$

$$= \frac{279^2}{29} \frac{(4553.11)(3132.863)}{330.643^2} = 36402.82$$

and hence $SE\left[\hat{L}_3\right] = \sqrt{Var\left[\hat{L}_3\right]} = 190.8$.

Appendix A – Derivation of Equation 6

Equation (1) can be written in matrix notation as $\hat{L} = K\left(1^{\mathbf{T}}Wc\right)\left(1^{\mathbf{T}}Vq\right)$. Observe that the term inside each bracket is a scalar and hence $\hat{L}^T = \hat{L}$. Thus

$$\begin{aligned}\hat{L} &= K\left(c^T W^T 1\right)\left(1^T Vq\right)\\ &= Kc^T\left(W^T 11^T V\right)q\\ &= Kc^T Aq\end{aligned}$$

where $A = W^T 11^T V$. Since the trace of a scalar is the scalar itself, we have

$$c^T Aq = tr\left(c^T Aq\right) = tr\left(Aqc^T\right) = tr\left(AB\right)$$

where $B = qc^T$.

Now *A* can be written as the product of two vectors, $A = wv^T$ where the vectors *w* and *v* are each of length n and are zero except for the sampled days, (for concentration and flow respectively), when they contain the respective weights for those sampled days. So the (i, j) element of *A* is the product of the sample weights when i is in I and j is in J, and 0 otherwise. The matrix *B* is also the product of two vectors, so $B_{i,j} = q_i c_j$.

Now, $tr\left(AB\right) = \sum_{i=1}^{n}\sum_{j=1}^{n} a_{ij}\, b_{ji}$ and so $tr\left(AB\right) = \sum_{i\in I}\sum_{j\in J} w_i v_j c_i q_j$ hence

$$Var\left[tr\left(AB\right)\right] = \sum_{i\in I}\sum_{j\in J}\left(w_i v_j\right)^2 Var\left[c_i q_j\right] + 2\sum_{i\in I}\sum_{j\in J}\sum_{i'\in I}\sum_{j'\in J} Cov\left[c_i q_j, c_{i'} q_{j'}\right]$$

Equation (6) is obtained by assuming the covariances in the expression above are zero. While this is not unreasonable for daily loads well separated in time, it is unlikely to be true on short time scales, in which case equation (6) will most likely underestimate the true variance (since loads will tend to be positively correlated).

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