Quantifying the Uncertainty of Nutrient Load Estimates in the Shepparton Irrigation Region

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EXTENDED ABSTRACT

This paper presents the identification and quantification of uncertainty in nutrient load estimates for the Goulburn-Broken catchment from irrigation drains. The reliable estimation of pollutant loads is a difficult task since, typically, water quality data is relatively sparse. The sparse nature of the data means that some estimation technique must be applied, based on assumptions about the behaviour of pollutant concentrations instream in the times when water quality was not sampled. Twenty two methods of estimating annual nutrient loads have been identified and compared in this study. The results vary significantly and show that the choice of estimation method contributes to the overall uncertainty of load estimation.

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 sampling and estimation techniques in future. In particular, it is recommended that the framework provided in this paper (or similar logic) is applied to select appropriate techniques. Furthermore, any estimation of loads should be accompanied by clear documentation of the techniques used and a justification of the technique selected. Additionally, when assessing changes in loads over time, it is important that the same estimation technique is applied to determine all annual estimates for comparative purposes.

There is a large body of research investigating load estimation techniques, however, little attention has been given to quantifying the uncertainty surrounding estimated loads. In this paper, three main sources of uncertainty in the estimation of nutrient loads are identified: knowledge uncertainty (arising from the choice of estimation technique), stochastic uncertainty (arising from the variability of data) and data uncertainty (arising from measurement, scaling and sampling errors).

A quantification of uncertainty has been performed for Total Phosphorous for thirteen sites in the Shepparton Irrigation Region for all available years, examples of which are provided in this paper. 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 and it is recommended that this methodology be applied wherever robust estimates are required which consider the potential effects of uncertainty.

1. INTRODUCTION

This paper presents the identification and quantification of the uncertainty in annual nutrient load estimates for the Goulburn-Broken catchment from irrigation drains. The reliable estimation of pollutant loads is a difficult task since, typically, water quality data is relatively sparse. The sparse nature of the data means the uncertainty in load estimates is significant and should be considered in any analysis of pollutant loads.

The quantification of uncertainty presented here is focussed on the interpretation of historical data, and provides a range of load estimates which could have occurred. Future research will focus on the design of sampling protocols to reduce the uncertainty associated with load estimation.

This paper is structured into four sections. Firstly, in Section 2, background is given into the available techniques for estimating loads, a framework is presented for selecting an appropriate technique and a summary is given of the sampling regime in the Shepparton Irrigation Region (SIR). In Section 3, a range of equally valid estimates are presented for Total Phosphorous (TP) loads from thirteen drain sites in the SIR in the years 1993/94, 1998/99 and 2003/04. Then, in Section 4, the main sources of uncertainty of load estimates are explained and this uncertainty is quantified and analysed for the same thirteen sites. Finally, some recommendations are made for the estimation of nutrient loads using historical data.

2. ESTIMATING LOADS FROM SPARSE WATER QUALITY DATA

Estimation of nutrient loads in the drains of the Goulburn irrigation region by Goulburn-Murray Water is predominantly based on daily flow data and fortnightly concentration data. Whilst fortnightly water quality sampling is not unusual (given the high cost of sampling), this relative scarcity of data has the potential to create significant uncertainties in load estimates and also presents major limitations in quantifying the error of load estimates.

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 instream in the times when water quality was not sampled. Three main types of estimation techniques can be used:

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. For the SIR, 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 and lagged flows. 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.

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 and Ratio Techniques and a comparison is given in Section 3.

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 variance of concentrations with relation to time or flow.

There are many potential methods for estimating the quantity of nutrients discharged from a stream. In the first instance, Fox (2004) distinguishes direct estimation methods (using actual concentration and flow data) from indirect methods (using catchment models which simulate load arising from catchment processes), 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 Fox (*ibid.*) notes, the problem of obtaining 'representative' load is difficult since data is sparse relative to the estimation of continuous flow-concentration flux. There are many potential approximation techniques with varying level of performance with regard to precision and bias. 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 Donohu (2002), Mukhopadhyay and Smith (2000)). These studies have usually concluded that there is no single method which universally provides precise (i.e. minimum variance) and unbiased estimates. However, these reviews have typically been limited to specific datasets and situations, and usually, have 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 1). This matrix provides broad guidance on the categories of techniques to be considered, however, there are many specific variations of these techniques. Additionally, guidance on the sampling regime should be adjusted depending on the characteristics of the catchment in question and this issue will be investigated in future research.

Table 1 Typology of annual nutrient load estimation methods

Nutrient Sampling Regime	No significant relationship[1]	Significant relationship present
Sparse sampling (> monthly)	Averaging or Ratio	Regression
Regular sampling (e.g. fortnightly) · Limited event data	Averaging or Ratio · Seasonally stratified	Regression or Averaging or Ratio · Seasonally stratified
· Repre-sentative event data	Averaging or Ratio · Seasonally stratified · Flow-weighted stratified	Regression or Averaging or Ratio · Seasonally stratified · Flow-weighted stratified
Continuous sampling (e.g. daily)	Linear interpolation	Linear interpolation

The typology presented in Table 1 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 (an example is given in Figure 1 for Rodney Main Drain, site 405720). Therefore, unless a significant relationship is established for a particular site in SIR, regression techniques are of limited use (and are therefore not included in the following analyses).

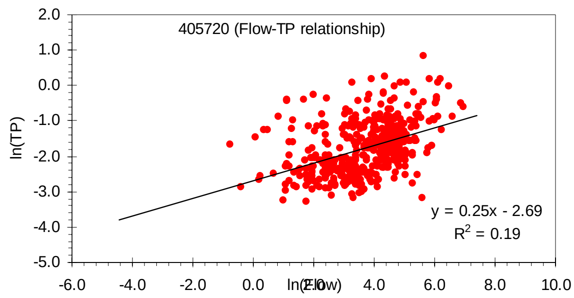

Figure 1 Correlation between flow and TP concentration for site 405720

In order to apply linear interpolation techniques, the assumption that concentrations vary linearly between fortnightly samples would need to be validated. Two brief experiments were undertaken by Etchells et al. (2005) to investigate this issue and it was demonstrated that this assumption is not supported by the data. Consequently, unless there is evidence to the contrary, the use of averaging or ratio estimators is a valid approach for load estimation.

The sampling regimes in SIR have so far all been systematic but sampling has not been designed specifically to capture a proportionate share of high-flow events. These events have a very large impact on overall loads since the concentration during those events is multiplied by large volumes, and also, the variation in high-flow concentration tends to be significantly higher than that in low-flow periods. This issue will be analysed more thoroughly in future research.

Twenty two methods of estimating annual nutrient loads have been identified and calculated for this study. These methods and details about the sources

[1] Between flow and nutrient concentration

of these methods are provided in Appendix A. These methods can broadly be grouped into three categories: with Methods 1-8 representing unstratified calculations, Methods 9-15 representing seasonally stratified versions of Methods 2-7 and Methods 16-22 representing flow-stratified versions of Methods 2-7.

A model, GUMLEAF v0.1alpha (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).

Using the twenty two methods described in Appendix A, many separate estimates of annual load were calculated for each of the thirteen sites in the SIR 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 in 2003 at Rodney Main Drain (405720) are shown in Figure 2. Not surprisingly, estimates vary considerably across the twenty-two methods, although some discernible pattern exists depending on the type of stratification (seasonal, flow or none). These results demonstrate that the 'true' load cannot be estimated.

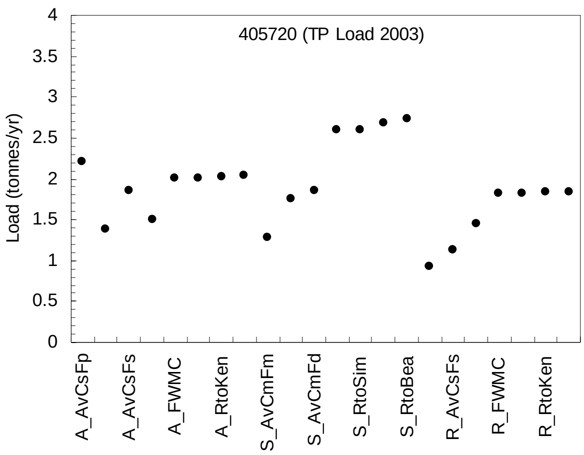

Figure 2 TP Load Estimates for Rodney Main Drain in 2003 using 22 estimation techniques

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 (without significant increases in the number 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 load is generated during these events, and frequently, higher than average concentrations occur then.

Using each estimate of annual load for each site in 1993, 1998 and 2003, five year and ten year percentage reductions were calculated (Figure). On the basis of these calculations, there can be some confidence in concluding that, despite significant uncertainty, most sites have had load reductions of over 50% in the past decade. Furthermore, the standard deviation of some reductions is quite low giving a reasonable degree of certainty at particular sites (e.g. Rodney and Deakin Main Drains). 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.

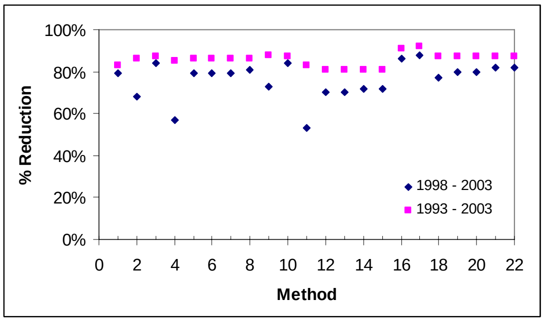

Figure 3 5 year and 10 year load reductions at site 405720 for 22 load estimation methods

3. SOURCES OF UNCERTAINTY IN LOAD ESTIMATION

Overall, three sources of uncertainty contribute significantly to overall uncertainty in nutrient load estimation. Those three sources are knowledge uncertainty, stochastic uncertainty and measurement uncertainty (Figure 4).

[2] Not all twenty two methods could be applied for all sites in all years due to insufficient data.

The annual load estimates of TP given in Figure 2 show significant variation due to the estimation technique selected. Unless other overriding factors are considered to be relevant, any of the values in Figure 2 are equally legitimate as estimates of the 'true' load. However, the 'true' load is not known, and therefore, the selection of estimation technique is one source of uncertainty in load estimation. For the purposes of this research, this source of uncertainty has been labelled 'knowledge' uncertainty.

Knowledge uncertainty can be reduced through an increased understanding of the pollutant wash-off and transport processes. In general, for sites with limited high flow samples, methods that do not account for flow stratification will tend to underestimate the 'true' load.

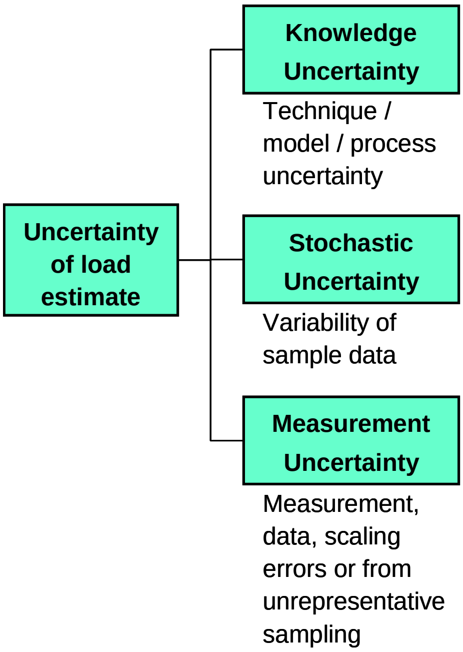

Figure 4 Sources of uncertainty in load estimates

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 represented in this study by estimates of variance. The standard deviations used in the analysis are based on the work of Fox (2005).

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 miscalibration in equipment, infilling missing data, poor sampling techniques or inaccurate scaling assumptions. Additionally, data and sampling uncertainty will arise from unrepresentative sampling, for instance, where few high-flow samples are available. However, since no information is known about the magnitude of these errors, they will be ignored for the purposes of this analysis. Since one source of uncertainty is being ignored, the remaining quantification is likely to be relatively more conservative.

4. 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:
5. $L_k = \mu_j + t_k.\sigma_j$
6. Repeat for $k = 1 \ldots 1000$
7. Present histogram of L for each site in each year.

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

Example output showing the uncertainty of estimated loads for site 405720 is presented for three years in Figures 5 – 7.

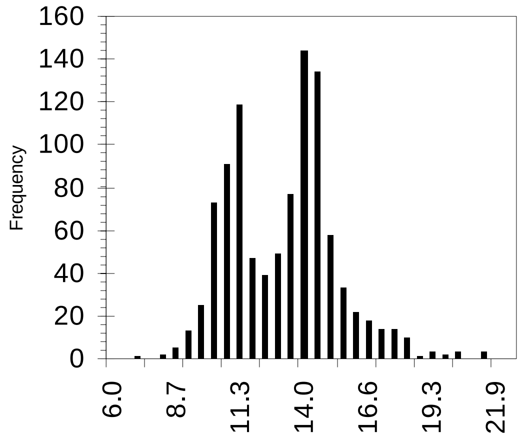

Figure 5 Histogram of simulated annual loads for site 405720 in 1993

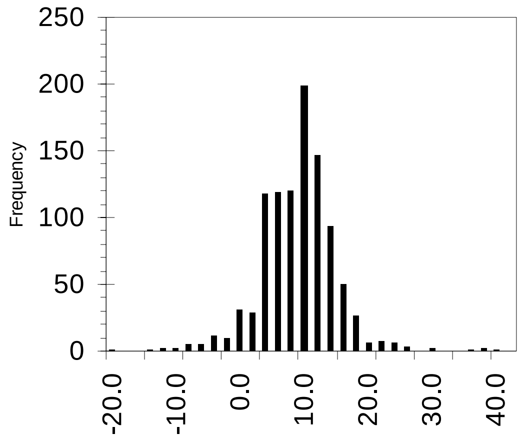

Figure 6 Histogram of simulated annual loads for site 405720 in 1998

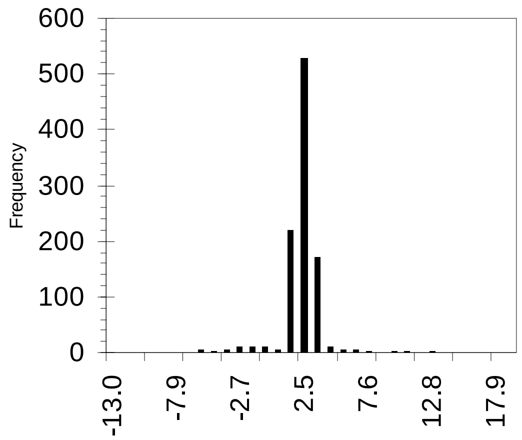

Figure 7 Histogram of simulated annual loads for site 405720 in 2003

5. CONCLUSIONS

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 1 (or similar logic) be 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 undertaken for Total Phosphorous for thirteen sites in the Shepparton Irrigation Region 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.

6. ACKNOWLEDGMENTS

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Appendix A Load estimation methods considered

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