The Quantification of Prediction Uncertainty associated with Water Quality Models using Monte Carlo Simulation

by
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Declaration

By submitting this thesis electronically, I declare that the entirety of the work contained therein is my own, original work, that I am the authorship owner thereof (unless to the extent explicitly otherwise stated) and that I have not previously in its entirety or in part submitted it for obtaining any qualification.

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Abstract

Water Quality Models are mathematical representations of ecological systems and they play a major role in the planning and management of water resources and aquatic environments. Important decisions concerning capital investment and environmental consequences often rely on the results of Water Quality Models and it is therefore very important that decision makers are aware and understand the uncertainty associated with these models. The focus of this study was on the use of Monte Carlo Simulation for the quantification of prediction uncertainty associated with Water Quality Models.

Two types of uncertainty exist: Epistemic Uncertainty and Aleatory Uncertainty. Epistemic uncertainty is a result of a lack of knowledge and aleatory uncertainty is due to the natural variability of an environmental system. It is very important to distinguish between these two types of uncertainty because the analysis of a model's uncertainty depends on it. Three different configurations of Monte Carlo Simulation in the analysis of uncertainty were discussed and illustrated: Single Phase Monte Carlo Simulation (SPMCS), Two Phase Monte Carlo Simulation (TPMCS) and Parameter Monte Carlo Simulation (PMCS). Each configuration of Monte Carlo Simulation has its own objective in the analysis of a model's uncertainty and depends on the distinction between the types of uncertainty.

As an experiment, a hypothetical river was modelled using the Streeter-Phelps model and synthetic data was generated for the system. The generation of the synthetic data allowed for the experiment to be performed under controlled conditions. The modelling protocol followed in the experiment included two uncertainty analyses. All three types of Monte Carlo Simulations were used in these uncertainty analyses to quantify the model's prediction uncertainty in fulfilment of their different objectives.

The first uncertainty analysis, known as the preliminary uncertainty analysis, was performed to take stock of the model's situation concerning uncertainty before any effort was made to reduce the model's prediction uncertainty. The idea behind the preliminary uncertainty analysis was that it would help in further modelling decisions with regards to calibration and parameter estimation experiments. Parameter uncertainty was reduced by the calibration of the model. Once parameter uncertainty was reduced, the second uncertainty analysis, known as the confirmatory uncertainty analysis, was performed to confirm that the uncertainty associated with the model was indeed reduced. The two uncertainty analyses were conducted in exactly the same way.

In conclusion to the experiment, it was illustrated how the quantification of the model's prediction uncertainty aided in the calculation of a Total Maximum Daily Load (TMDL). The Margin of Safety (MOS) included in the TMDL could be determined based on scientific information provided by the

uncertainty analysis. The total MOS assigned to the TMDL was -35% of the mean load allocation for the point source. For the sake of simplicity load allocations from non-point sources were disregarded.

Opsomming

Watergehalte modelle is wiskundige voorstellings van ekologiese sisteme en speel ’n belangrike rol in die beplanning en bestuur van waterhulpbronne en wateromgewings. Belangrike besluite rakende finansiële beleggings en besluite rakende die omgewing maak dikwels staat op die resultate van watergehalte modelle. Dit is dus baie belangrik dat besluitnemers bewus is van die onsekerhede verbonde met die modelle en dit verstaan. Die fokus van hierdie studie het berus op die gebruik van die Monte Carlo Simulasie om die voorspellingsonsekerhede van watergehalte modelle te kwantifiseer.

Twee tipes onsekerhede bestaan: Epistemologiese onsekerheid en toeval afhangende onsekerheid. Epistemologiese onsekerheid is die oorsaak van ‘n gebrek aan kennis terwyl toeval afhangende onsekerheid die natuurlike wisselvalligheid in ’n natuurlike omgewing behels. Dit is belangrik om te onderskei tussen hierdie twee tipes onsekerhede aangesien die analise van ’n model se onsekerheid hiervan afhang. Drie verskillende rangskikkings van Monte Carlo Simulasies in die analise van die onsekerhede word bespreek en geïllustreer: Enkel Fase Monte Carlo Simulasie (SPMCS), Dubbel Fase Monte Carlo Simulasie (TPMCS) en Parameter Monte Carlo Simulasie (PMCS). Elke rangskikking van Monte Carlo Simulasie het sy eie doelwit in die analise van ’n model se onsekerheid en hang af van die onderskeiding tussen die twee tipes onsekerhede.

As eksperiment is ’n hipotetiese rivier gemodelleer deur gebruik te maak van die Streeter-Phelps teorie en sintetiese data is vir die rivier gegenereer. Die sintetiese data het gesorg dat die eksperiment onder beheerde toestande kon plaasvind. Die protokol in die eksperiment het twee onsekerheids analises ingesluit. Al drie die rangskikkings van die Monte Carlo Simulasie is gebruik in hierdie analises om die voorspellingsonsekerheid van die model te kwantifiseer en hul doelwitte te bereik.

Die eerste analise, die voorlopige onsekerheidsanalise, is uitgevoer om die model se situasie met betrekking tot die onsekerheid op te som voor enige stappe geneem is om die model se voorspellings onsekerheid te probeer verminder. Die idee agter die voorlopige onsekerheidsanalise was dat dit sou help in verdere modelleringsbesluite ten opsigte van kalibrasie en die skatting van parameters. Onsekerhede binne die parameters is verminder deur die model te kalibreer, waarna die tweede onsekerheidsanalise uitgevoer is. Hierdie analise word die bevestigingsonsekerheidsanalise genoem en word uitgevoer met die doel om vas te stel of die onsekerheid geassosieer met die model wel verminder is. Die twee tipes analises word op presies dieselfde manier toegepas.

In die afloop tot die eksperiment, is gewys hoe die resultate van ’n onsekerheidsanalise gebruik is in die berekening van ’n totale maksimum daaglikse belading (TMDL) vir die rivier. Die veiligheidgrens (MOS) ingesluit in die TMDL kon vasgestel word deur die gebruik van wetenskaplike

kennis wat voorsien is deur die onsekerheidsanalise. Die MOS het bestaan uit -35% van die gemiddelde toegekende lading vir puntbelasting van besoedeling in die rivier. Om die eksperiment eenvoudig te hou is verspreide laste van besoedeling nie gemodelleer nie.

Acknowledgements

I want to thank my supervisor, Mr. Wageed Kamish, for all the assistance he gave me in the past two years. His office door was always open to me for questions and he always treated me with friendliness and a great sense of humor.

Dedicated to my parents, Kobus and Martie Smit.

Table of Contents

List of Figures

List of Tables

List of Symbols

B = model bias

BOD = Biochemical Oxygen Demand (mg/L)

c = concentration

C = concentration of the constituent simulated in the WQM

CCDF = Complement of the Cumulative Distribution Function

CDF = Cumulative Distribution Function

$C_{j,0}$ = base prediction j when all parameters are kept constant at their means

$c_{m,i} = i$th measured concentration

COD = Chemical Oxygen Demand

COV = Coefficient of Variation

$c_{p,i} = i$th model prediction of concentration

D = dissolved oxygen deficit (mg/L)

D_c = critical oxygen deficit (mg/L)

DO = Dissolved Oxygen (mg/L)

DO_{act} = actual dissolved oxygen concentration in the stream (mg/L)

DO_c = critical Dissolved Oxygen concentration (mg/L)

DO_{sat} = dissolved oxygen saturation concentration in the stream (mg/L)

D_0 = initial dissolved oxygen deficit (mg/L)

F = relative dominance of the variability of the predictions over the observations

$F(x)$ = probability of exceedence

$F'(x)$ = probability of non-exceedence (1- $F(x)$)

FOA = First-Order Approximation Method

FOAMs = First-Order Approach Methods

FOE = First-Order Error Method

FORA = First-Order Reliability Analysis

FOVP = First-Order Variance Propagation

$g(\,)$ = functional representation of the procedures simulating constituent C in the WQM

GIS = Geographical Information Systems

H/WQ modelling = Hydrological and Water Quality modelling

k_a = reaeration rate (d^{-1})

$(k_a)_T$ = reaeration rate (d^{-1}) at a specific temperature T (˚C)

$(k_a)_{20}$ = reaeration rate (d^{-1}) at 20˚C

k_d= decomposition rate of BOD in the stream (d^{-1})

$(k_d)_T$ = decomposition rate (d^{-1}) of BOD at a specific temperature T (˚C)

$(k_d)_{20}$ = decomposition rate (d^{-1}) of BOD at 20˚C

k_r = total removal rate of BOD (d^{-1})

k_s = settling removal rate of BOD in the stream (d^{-1})

L = Biochemical Oxygen Demand (BOD) concentration (mg/L)

LHS = Latin Hypercube Sampling

L_0= initial Biochemical Oxygen Demand (BOD) concentration (mg/L)

MCS = Monte Carlo Simulation

MOS = Margin of Safety

MSE = Mean Squared Error

n = sample size (number of model runs in MCS)

n = Manning's n

OHO = Ordinary Heterotrophic Organisms

p = number of basic variables

PDF = Probability Density Function

p_F = probability of exceedence (as a fraction)

PMCS = Parameter Monte Carlo Simulation

Q = discharge or flow (m^3/s)

RMSE = Root Mean Squared Error

SD = Standard Deviation

$SN_{j,i}$ = normalized sensitivity coefficient

S_o = standard deviation of the system observations

S_p = standard deviation of the model predictions

SPMCS = Single Phase Monte Carlo Simulation

S_r = sum of squares of the residuals

S_0 = slope (m/m)

T = water temperature (˚C)

t_c = critical travel time (days)

TMDL = Total Maximum Daily Load

TPMCS = Two Phase Monte Carlo Simulation

U = velocity (m/day)

W = loading

WQM (s) = Water Quality Model(s)

x = position (point) in space along the river length (m)

X_e = vector of basic variables (input) at the expansion point

x_i = basic variables

x_{ie} = vector value of basic variable

$x_{i,0}$ = original value of parameter i, which in this case is equal to the parameter mean

X_o = mean observed value

X_p = mean predicted value

$\frac{\partial g}{\partial x_i}$ = rate of change of the model output with respect to a unit change in each basic variable

ΔC_j = change in prediction j as a result of change Δx_i in parameter i with all other parameters kept constant at their means

Δx_i = change in parameter i

$\sum LA$ = load allocation (non-point sources)

$\sum WLA$ = waste load allocation (point sources)

1. Introduction

1.1. Uncertainty placed into Context

Water quality modelling plays a major role in the planning and management of water resources and aquatic environments. Water quality models (WQMs) help us to understand how an environment works as a unit, thus they are of great value in both research and management contexts.

WQMs are mathematical by nature. They are idealized formulations of the diverse physical, chemical and biological information that constitutes a complex environmental system. They are formulated to simulate observed conditions and to predict the potential effect of planned scenarios on the system.

Decisions concerning huge capital investment and dire environmental consequences often rely on the results of WQMs. It is thus very important that models are realistic and reliable. Uncertainty concerning various facets of WQMs usually contributes to models being inaccurate representations of environmental systems. Poor data or a lack of knowledge forces water quality modellers to make weakly supported assumptions regarding model parameters and structure. This leads to an increased model prediction uncertainty and greatly affects decision making for environmental and water resources management.

1.2. Problem Statement

To make important decisions based on the results of a model, one must have confidence in the model's predictions. The model must be a reliable, transparent and realistic representation of the real system being modelled. The decision maker also needs insights into the shortcomings of the model and must also understand the important assumptions made by the modeller. It is thus very important that the decision maker has a proper understanding of the uncertainty associated with the model's predictions and its parameters.

Environmental systems can have multiple sources of uncertainty, all contributing to the total uncertainty of the model's predictions. The problem now faced is: How do we quantify the uncertainty associated with the model's predictions to instill a sense of confidence in the model? Once the prediction uncertainty has been quantified, how does one go about making decisions with the newly acquired knowledge concerning the uncertainty associated with the model?

1.3. Study Objective

Monte Carlo Simulation (MCS) can be successfully applied for the purpose of analyzing the prediction uncertainty associated with a WQM. MCS is a full distribution probabilistic technique that uses random sampling of the model's inputs to generate sufficient model output for statistical analysis. Basic statistical analysis is then applied to the model's output to quantify the prediction uncertainties associated with the WQM. The focus of this study is on investigating MCS and how it is used in the specific context of analyzing the prediction uncertainty associated with WQMs.

1.4. Chapter Overviews

Chapter 2 is the Literature Review. Water Quality Models (WQMs) are introduced and the uncertainty associated with them explained. The importance of being aware of uncertainty is then explained followed by an introduction to uncertainty analysis. Monte Carlo Simulation (MCS) and the quantification of prediction uncertainty are then explained. Finally some considerations in uncertainty analysis are explained and the literature review concluded.

Chapter 3 is the Methodology and starts by introducing the Streeter-Phelps model and why it was chosen as model to be analyzed for uncertainty in this study. The fundamentals of the Streeter-Phelps model are explained and a hypothetical environment is created along with system characteristics, which will serve as an ecosystem to be modelled. The methodology then continues by explaining the whole modelling protocol along with all the steps of the uncertainty analysis applied to the model.

Chapter 4 is the Results and Discussion and is structured in relatively the same way as the modelling and uncertainty analysis protocol presented in the methodology. A number of graphs and results associated with each of the Methodology's steps are shown and discussed. Finally these results are used in a Management Application where it is shown how the results from an uncertainty analysis can be used to make decisions in terms of designing intervention actions and testing their performance.

In Chapter 5 and Chapter 6 the study comes to a Conclusion and some General –and Future Research Recommendations are made.

2. Literature Review

2.1. Introduction

Water Quality Models (WQMs) are important tools for water resources and environmental management. They help environmental regulatory agencies to organize, understand and utilize available information for the purpose of making decisions (Summers et al., 1992:161). As an alternative to, or in addition to field monitoring, WQMs are used for analysing and predicting water quality in response to loads on the environment (Hession et al., 1996:1309).

WQMs can be either empirical or mechanistic. Empirical WQMs are based on statistical summaries of observed data. Empirical modellers use observational data to guide the selection of model specification and estimates of parameters (Reckhow, 1994:3). Mechanistic WQMs are theoretical descriptions of hydrological and ecological processes (Reckhow, 1994:8; Chapra, 2008:12). The reason for the existence of mechanistic WQMs was due to the constraints of limited available data and the limited resources to collect additional data to support the empirical models. In addition to that, there was also the general belief that the theory around environmental systems was well understood and that it could be expressed mathematically (Reckhow, 1994:9).

Scientific uncertainty is present in all ecological modelling and risk assessments (Reckhow, 1994:2). Mechanistic WQMs depend on parameters to describe the natural processes of the environment being modelled and to accommodate the spatial and temporal variability of the system. Due to limited data, modellers' choices of parameters are often determined by guesswork to a large degree and it is very difficult to replicate the natural complexity of an environmental system without a degree of prediction uncertainty in the model output (Shirmohammadi et al., 2006:1034; Reckhow, 1994:9).

According to Shirmohammadi et al. (2006:1034) the uncertainty of mathematical model simulation results is a major concern due to the important policy, regulatory and management implications it may have. However, the quantification of uncertainty's magnitude and its impact on model performance has not been well studied. In addition to the aforementioned, the accounting for uncertainty in management processes has not been well studied or implemented. Summers et al. (1993:162) also mention that uncertainty is a major aspect of environmental risk assessment and modelling but is poorly understood.

The purpose of this literature review is to gain a better understanding of uncertainty associated with WQMs and to investigate some of the methods used in the analysis of uncertainty associated with WQMs. Section 2.2 is devoted to the definition of uncertainty associated with WQMs. It discusses and integrates the types and sources of uncertainty associated with WQMs. Section 2.3 explains the

importance of being aware of the uncertainty associated with WQMs and why uncertainty must be analysed. In addition to that it also defines the objectives of an uncertainty analysis.

Section 2.4 introduces uncertainty analysis and explains some terms and methods associated with uncertainty analysis. It clarifies the difference between actual prediction error propagation and the quantification of prediction uncertainty. Additionally, the section introduces the two dominant methods of prediction error propagation: (1) First Order Approach Methods (FOAMs) and (2) Monte Carlo Simulation (MCS) and further discusses FOAMs. It also explains the difference between a sensitivity analysis and an uncertainty analysis. Section 2.5 discusses MCS in depth. It explains the general procedure of MCS; how Monte Carlo sampling works; some advantages and disadvantages; and finally looks at the accuracy with which MCS predicts. Section 2.6 explains all of the basic statistical tools used in the quantification of prediction uncertainty and how their results are interpreted. Section 2.7 discusses some considerations and configurations of MCS in an uncertainty analysis to achieve the main objectives of a WQM's uncertainty analysis.

2.2. Definition of Uncertainty associated with Water Quality Models

To understand model uncertainty in the context of WQMs, it is important to formulate a good definition of uncertainty associated with WQMs. What are we talking about when talking about uncertainty associated with WQMs? Furthermore, how do we define uncertainty so that it becomes quantifiable?

Hession et al. (1996:1310) define uncertainty as "the condition of being in doubt" and state that the only thing we are sure about in hydrological and water quality modelling (H/WQ modelling) is the fact that we are uncertain. According to Shirmohammadi et al. (2006:1033) uncertainty is the estimated amount by which an observed or calculated value may depart from the true value. Summers et al. (1993:162) defines model uncertainty by bluntly asking the question; once a model result is determined, how good is it? Uncertainty reflects the mistaken impression that an assessment is precise (Reckhow, 1994:1).

The definition of uncertainty is a difficult subject and is complicated further by the fact that there are different types of uncertainty and various sources of uncertainty within WQMs. This continuously changes the definition of uncertainty and a structure needs to be laid out that will help to better understand and define uncertainty. The rest of this section continues with the division of uncertainty into two types of uncertainty and an explanation of both types of uncertainty. Then the sources of uncertainty in WQMs are discussed by looking at various problem areas within water quality modelling. Finally, the two types of uncertainty and the various sources of uncertainty in WQMs are integrated and presented in **Figure 2.1**, which summarizes the relation between the two types of uncertainty and the various sources of uncertainty.

2.2.1. Types of Uncertainty

There are two types of uncertainty (Vose, 2008:47):

1. **Aleatory uncertainty**.
2. **Epistemic uncertainty**.

Aleatory uncertainty is also known as stochastic variability and is due to the random variability of the natural environment and is a property of the natural system. Aleatory uncertainty can be quantified but rarely can it be reduced (Hession et al., 1996:1311). **Epistemic uncertainty**, on the other hand, is uncertainty due to a lack of knowledge by the modeller. The modeller usually has an incomplete understanding of the system or has inadequate measurements of the system properties. Epistemic uncertainty is a property of the analyst and available data, and it can be reduced by additional measurements (Hession et al., 1996:1311), expert elicitation (Vose, 2008:48), proper calibration of parameters (Mishra, 2011:25), and improved scientific experiments (Beck, 1987:1394).

Vose (2008:48) also mentions a third type of uncertainty: total uncertainty. **Total uncertainty** is the combination of aleatory- and epistemic uncertainty. Together these two components of uncertainty hamper the ability of the modeller to create a model that will give perfect predictions.

2.2.2. Sources of Uncertainty in Water Quality Models

To further define uncertainty, the sources of uncertainty in WQMs have to be identified and related to the two types of uncertainty. According to Beck (1987:1394) there are four problem areas of uncertainty in WQMs:

1. Uncertainty about the relationships among the variables characterizing the dynamic behaviour of systems, i.e. uncertainty about model structure.
2. Uncertainty about the values of the parameters appearing in the identified structure of the dynamic model for a system's behaviour, i.e. parameter uncertainty.
3. Uncertainty associated with predictions of the future behaviour of the system, i.e. prediction uncertainty.
4. The design of experiments, or monitoring programs, for the specific purpose of reducing the critical uncertainties associated with the model.

The fourth problem area mentioned above is not relevant to this study and the problem areas of uncertainties that will be considered in the rest of this section are as follows:

- Uncertainty in **model structure**.
- Uncertainty in **model parameters**.
- Uncertainty in **model predictions**.

Model structure uncertainty refers to any doubt or confidence associated with the choice of model structure. Model structure includes the equations and algorithms used to describe an environmental system (Lindenschmidt et al., 2007:290). Error in terms of model structure is unavoidable because environmental systems are just too complex to be numerically represented without some arising flaws (McIntyre, 2004:29). In some cases model structure can outweigh all other sources of uncertainty (Lindenschmidt et al., 2007:299).

There can be a number of algorithms used in different approaches to the same problem and uncertainty due to the algorithms and different approaches used can greatly affect a model's predictions (Shirmohammadi et al., 2006:1036). Empirical algorithms are regression equations developed for a specific system using observed data. These empirical equations cannot necessarily be applied to any other system because they would give erroneous results. Theoretical algorithms are based on physical laws that can be applied to diverse climatic and physiographic regions given proper input values for the parameters of interest. These laws are almost always a simplification of the real

world and are based on a number of assumptions which leads to uncertainty. Theoretical algorithms also need proper calibration and validation. To complicate matters further, models are rarely purely empirical or theoretical. Empirical models usually have an element of theory in them and the opposite is true for theoretical models. This means that models are subjected to uncertainty of both theoretical and empirical nature.

Different methods of numerical solving might also cause a slight difference in model output which can contribute to uncertainty. Truncation errors, rounding errors and typographical mistakes in the numerical implementation of a solution cause uncertainty in the model output (McIntyre, 2004:24).

In addition to algorithms, the model structure also includes model resolution. Model resolution refers to the degree to which space, time and matter is segmented in the model (Chapra, 2008:339). Naturally, the level of model resolution will have effects on the model output which could also lead to uncertainty in the model output. Each environment being modelled is unique and requires appropriate time- and space scales (Chapra, 2008:341). For example, the respective horizontal space scale and time scale for bacteria can vary from 100m to 10km and 0 days to 20 days. On the other hand, the respective horizontal space scale and time scale of nutrients can vary from 1km to 300km and 10 days to 10 000 days (Chapra, 2008:340).

In the case of the resolution of matter, it is often aggregated to prevent the complexity it will cause if its diversity was included in models. For instance, instead of defining each of the compounds of sewage or defining each of the heterotrophic organism species in a reactor, the compounds and different organisms are aggregated and referred to as Chemical Oxygen Demand (COD) and Ordinary Heterotrophic Organisms (OHO). There is a fine balance between model complexity and the effects it has on prediction uncertainty. Increasing a model's complexity can improve its predictions but it also opens up more degrees of freedom which could result in increased uncertainty (Lindenschmidt, 2006:73).

Computing technology and information management have made complex numerical solving fast and easy and it also made spatial data and Geographic Information Systems (GIS) integrated modelling frameworks very accessible. In the excitement of the new technology and its convenience, it is easy to overlook the factors that might contribute to the uncertainty in a model.

Model parameter uncertainty refers to both erroneous parameter values and variance in parameter values. Both erroneous parameter values and erroneous variance in parameter values can be due to inadequate data used to describe model parameters and coefficients. In addition to that, the variance in parameter values can also be due to the stochastic variability of the natural system.

The collection of data used for water quality modelling is expensive. Normally, the data used to calibrate and verify a model is collected during basin-wide surveys designed to check whether water quality regulations are complied with. This is inadequate data collection for modelling purposes. The frequency of the data collection is usually insufficient and some water quality constituents are sometimes sampled because they are easy to sample, not because they increase knowledge of key water quality processes. As a result, this inadequate data causes modellers to make weakly supported assumptions regarding model parameters and input (Melching et al., 1996:105).

Shirmohammadi et al. (2006:1033) say that measurement errors in input parameter values, initial- and boundary conditions are also great sources of uncertainty in models. Measurement errors in the sampling of input data can partly be seen as a property of experimental design (Beck, 1987:1394). Experiments or processes for the estimation of input data could have faulty designs resulting in inaccurate results for measured input data. In addition to that, human reliability and error during sampling in the field or laboratory also contributes to parameter uncertainty.

Natural variability in the environmental system causes uncertainty in the estimates of model parameters. Stochastic variability of the natural system can for example refer to seasonal variance as in variance in rainfall, temperature, sunlight etc. It also refers to the continuous change in the physical properties of an environment being modelled (i.e. depth, width and flow of a river). It can also refer to the variation in the genetic properties of organisms like for instance growth rate of bacteria or algae etc. (Beck, 1987:1423). This natural variability is an important consideration in model setup if one wishes to have a realistic description of the environmental system (Shirmohammadi et al., 2006:1035).

Model prediction uncertainty is the error and variance in model output (predictions) as a result of the aggregation of model structure uncertainty and model parameter uncertainty (Mailhot et al., 2003:491). Uncertainty in predictions arises when data that do not accurately characterize the system are used to describe highly stochastic and heterogeneous problems. In addition to that, uncertainty in model predictions also exists due to an environmental system being characterized by a variety of model algorithms, scale, spatial heterogeneity etc. (Shirmohammadi et al., 2006:1033). Prediction uncertainty is the product of all the other uncertainty associated with the model. Prediction uncertainty can be seen as the modeller's inability to know exactly what the future value of an environmental constituent will be. Model predictions in this sense can only be seen as calculated guesswork. Prediction uncertainty is often characterized by probability distributions of the water quality constituents that models are supposed to predict (Chin, 2009:1315).

Figure 2.1 is a simplified summary and integration of the types of uncertainty and sources of uncertainty in WQMs. As shown, uncertainty associated with WQMs is divided into two types of uncertainty: (1) aleatory uncertainty and (2) epistemic uncertainty. Aleatory uncertainty is known as

the environmental system's natural stochastic variability. Epistemic uncertainty is due to the modeller's lack of knowledge. Within WQMs there are three problem areas of uncertainty: (1) model parameter uncertainty and (2) model structure uncertainty, which together, lead to (3) model prediction uncertainty. One part of model parameter uncertainty is aleatory uncertainty which includes natural environmental variability and genetic variability. The other part is epistemic uncertainty due to parameter estimation errors, lack of sufficient sampling and faulty experimental designs. Model structure uncertainty is epistemic uncertainty due to the modeller's inability to know exactly how to accurately characterize the natural system. This includes different model algorithms representing the environmental theory, model resolution and methods of numerical solving. As a result of the combination of model parameter uncertainty and model structure uncertainty, model prediction uncertainty is both aleatory and epistemic. Model prediction uncertainty is characterized by the variation in model predictions, and the predictions' departure from the true observed values.

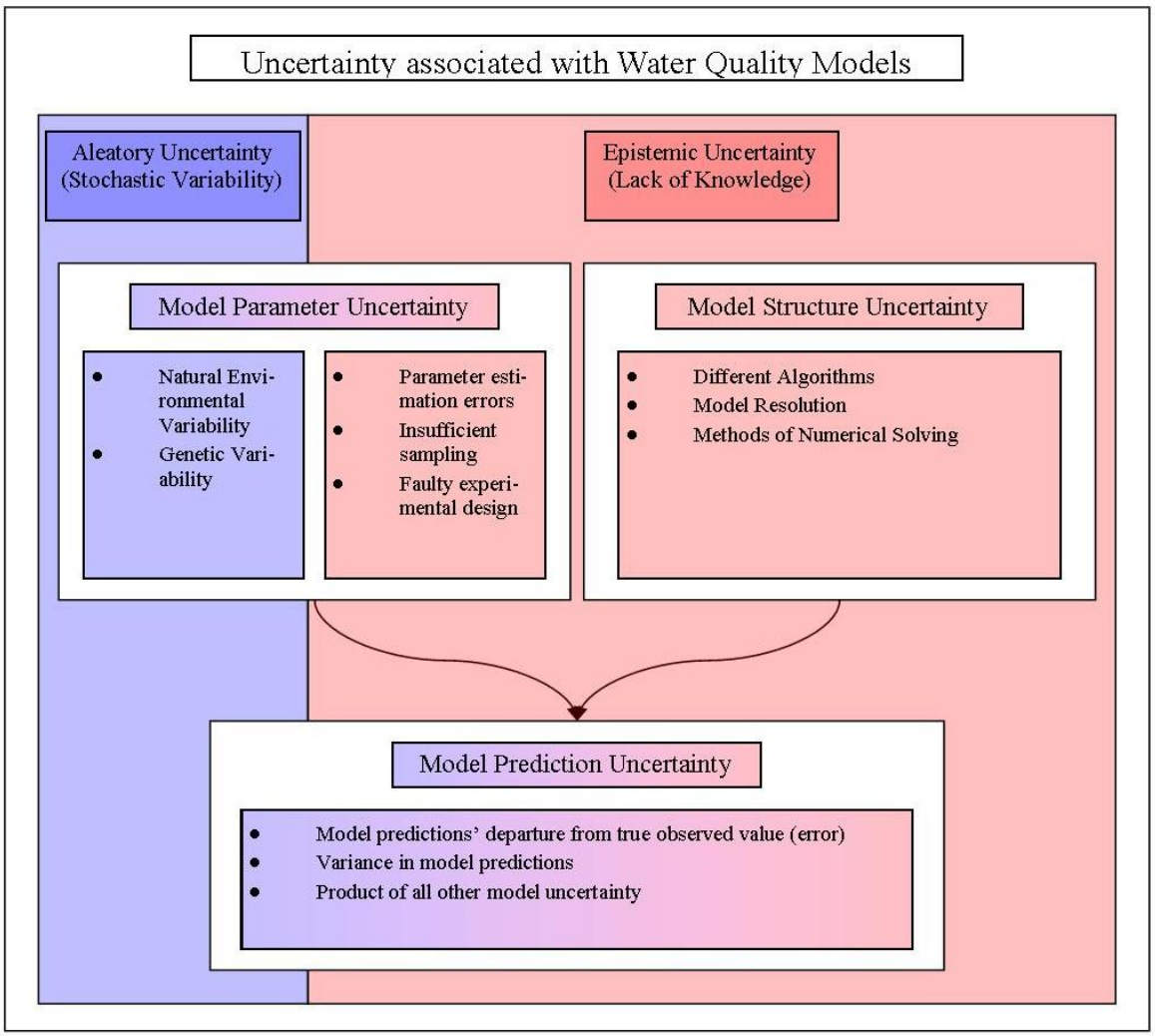

Figure 2.1 Summary of the types and sources of uncertainty in WQMs.

2.3. The Importance of Uncertainty Awareness and Analysis

Uncertainty associated with WQMs is defined in section 2.2. This section explains the importance of being aware of model uncertainty and why it must be analysed. Why is it important for a water quality modeller to be aware of the uncertainty associated with a model? What are the implications of uncertainty on the decisions being made? How does an analysis of uncertainty help to make decisions with regards to further modelling, sampling and environmental management?

2.3.1. Determine Quality of Model Predictions

According to Beck (1987:1395) the main concerns of environmental managers are to:

- Guide decisions to restore damaged aquatic systems.
- Prevent damage to environments as a result of development.
- Maintain acceptable environmental quality in the face of seasonal variability, accidents, failures and extreme events.

In light of the objectives above, it is expected that models used as tools by environmental regulatory agencies must be realistic and reliable. Uncertainty undermines the credibility of a model and therefore environmental managers need to know the expected uncertainty associated with model predictions. They need to know whether model predictions are meaningful and useful (Beck, 1987:1394). Models thus need to be rated in terms of the quality of their predictions. This is important so that decision makers may decide on other more precisely assessed models, may consider the value of additional, more refined experimentation and monitoring and/or to hedge decisions away from large losses (Reckhow, 1994:2).

2.3.2. Identify Uncertain Parameters

It is important for stakeholders (regulatory agencies, government and public) to be aware of scientific uncertainties in environmental assessments to obtain and properly focus research funding (Reckhow, 1994:2). Time and resources are often limited for the purpose of data sampling and modelling. Uncertainty analysis makes it possible for stakeholders to identify the parameters that affect the output of the model the most and by focussing time and resources on those parameters, both model parameter- and model prediction uncertainty can be reduced (Shirmohammadi et al., 2006:1045). Quantifying the uncertainty associated with models can also indicate to what extent parameter uncertainty should be reduced, providing a basis for cost effective field data collection (Shirmohammadi et al., 2006:1046).

An uncertainty analysis also gives the type of the uncertainty associated with a model. Determining the dominance of either aleatory or epistemic uncertainty in prediction uncertainty is very important. Separating these two types of uncertainty allows modellers to understand how to reduce the prediction uncertainty of a model (Vose, 2008:53). Knowing which type of uncertainty dominates the model

also leads to a more confident feeling for the system, which is of more value to system intervention decision making (Reckhow, 1994:2).

2.3.3. System Management

Uncertainty analysis greatly improves management decisions by presenting model output in association with respective probabilities of occurrence. For instance, the probabilities of meeting or violating water quality standards in environmental systems can be determined. This benefits the development of Total Maximum Daily Load (TMDL) implementations plans in which management scenarios are presented with the associated costs and probabilities of meeting water quality standards (Shirmohammadi et al., 2006:1046). In addition to that, Mishra (2011:1) explains that an uncertainty analysis gives an estimate of the margin of safety (MOS) that needs to be incorporated into TMDL calculations to account for the inherent uncertainty present in both natural systems and models.

An example of the consequences, that a lack of uncertainty awareness resulted in, is given by Melching et al. (1996:105): Billions of dollars were spent on the upgrading of wastewater treatment plants on North American rivers. The designs were based on WQMs assessing the allowable maximum loads of point sources and non-point sources, to comply with certain water quality standards in the rivers. However, after the implementation of the new wastewater treatment designs, some rivers' water quality still did not improve. After massive investments, results were still unsatisfactory. The reason was that uncertainty in the WQMs caused the wrong estimation of the rivers' assimilative capacities, which greatly contributed to the poor results from the use of the water pollution control plans.

A proper analysis of model limitations and uncertainties can be interpreted as modelling honesty (Hession et al., 1996:1309). It is important that simplifications and assumptions are presented in association with results to instill a proper level of confidence in the model (Vose, 2008:65). A model must be transparent and have nothing to hide. For an uncertainty analysis to be truly advantageous it must be complete. All scientific uncertainties in a model used for ecological risk assessment must be accounted for. Failure to do so may result in decisions that are not optimal or satisfactory (Reckhow, 1994:2). Decision makers may not be under any false impressions regarding the environmental systems subjected to their management. The consequences of poor decisions can be dire in both environmental- and capital investment terms.

2.4. Analysis of Uncertainty

Model uncertainty is defined in section 2.2 and the importance of its analysis emphasised in section 2.3. This section introduces uncertainty analysis by looking at some important uncertainty analysis terms and methods.

An uncertainty analysis is the means of calculating and representing the certainty with which a model's results represents reality (McIntyre, 2004:24). Generally it consists of two steps: (1) prediction error propagation and (2) quantification of prediction uncertainty, but it does not consist of only performing these two steps in a straight forward manner. According to Melching et al. (2001:403), an uncertainty analysis also relates the uncertainty in the basic variables of the model to the uncertainty in the model predictions. This is achieved by different configurations of prediction error propagation and then analysing the results to quantify prediction uncertainty.

2.4.1. Prediction Error Propagation

In the literature, the terms 'prediction error propagation' and 'quantification of prediction uncertainty' are often used interchangeably. According to Helton et al. (2004:64) there are three aspects of prediction error propagation that need considering:

1. The characterization of the uncertainty in model inputs.
2. The actual propagation of uncertainty through the model.
3. The representation of uncertainty in model predictions.

There is a difference between actual prediction error propagation and the quantification of prediction uncertainty. According to Beck (1987:1422), given the model structure and parameter estimates, subject to uncertainty, **prediction error propagation** determines the model's future behaviour under different input conditions. In other words, Beck (1987:1422) refers to the characterization of model input uncertainty and actual prediction error propagation. The two dominant methods of prediction error propagation are (Beck, 1987:1424; Shirmohammadi et al., 2006:1038):

1. First-Order Approach Methods (FOAMs).
2. Monte Carlo Simulation (MCS).

Once the future behaviour of a system has been determined, basic statistical analysis tools are applied to the model predictions to quantify the extent and nature of the uncertainty associated with the model (Helton et al., 2004:66). This, on the other hand, referred to as the third aspect of propagation of prediction error by Helton et al. (2004:64), is known as the **quantification of prediction uncertainty.** Once the quantification of prediction uncertainty has been completed, valuable information will be available for the purpose of making decisions. The quantification of prediction uncertainty is explained in section 2.6.

2.4.2. First Order Approach Methods

The term 'First Order Approach Methods (FOAMs)' will be used as the aggregate term for all the propagation methods derived as refinements of (and include) the first-order error method (FOE method). Some other names for the FOE method are:

- The first-order approximation (FOA) method (Shirmohammadi et al., 2006:1038);
- The first-order variance propagation (FOVP) method (Summers et al., 1993:163);
- The first-order sensitivity analysis (Beck, 1987:1424; Chapra, 2008:327);
- The first-order reliability analysis (FORA) (Melching et al., 1996:106).

FOAMs of prediction error propagation involves computing a nominal (mean) reference trajectory for the future state of the system and then to assess the effects of various small-amplitude sources of uncertainty in the parameters on the uncertainty of the trajectory (Beck, 1987:1424).

According to Summers et al. (1993:163), the general procedure is as follows:

1. Identification of one or many points in time along the output trajectory.
2. Linearization of the model about each of these points by using the first two terms of the Taylor series expansion of the model equations.
3. Computation of the first and second moments (means and variances) of the estimated output distributions at these points.

The Taylor series expansion, truncated after the first term, is given by the following equation (Melching et al., 1996:106; Shirmohammadi et al., 2006:1039):

$$C = g(X_e) + \sum_{i=1}^{p} (x_i - x_{ie})\left(\frac{\partial g}{\partial x_i}\right)_{X_e}$$

C = concentration of the constituent simulated in the WQM.

$g(\,)$ = functional representation of the procedures simulating constituent C in the WQM.

X_e = vector of basic variables (input) at the expansion point.

p = number of basic variables.

x_i = basic variables.

x_{ie} = vector value of basic variable.

$\frac{\partial g}{\partial x_i}$ = represents the rate of change of the model output with respect to a unit change in each basic variable, usually referred to as the sensitivity coefficient.

X_e = indicates that the partial derivative is taken at the expansion point.

In H/WQ engineering the expansion point is usually taken to be the mean value of the variables.

The third term in the Taylor series can also be included to permit the examination of uncertainty over larger regions of parameter space. The focus of this study, however, is not on the propagation of prediction error by using FOAMs, thus, only the advantages and disadvantages of FOAMs will now be briefly discussed.

Melching et al. (2001:404) claim that the advantage of FOAMs lies in their simplicity. They require only the first two statistical moments of the basic variables of models when applying the Taylor series expansion to assess model uncertainty.

The main problem with FOAMs is that they assume a single linearization of the model output function at the central values (means) of the basic variables. This is to represent the statistical properties of model output over the complete range of basic variable values. For non-linear systems this assumption becomes more inaccurate as the basic variables depart from the central values (Melching et al., 1996:106). Hession et al. (1996:1309) also mentions that FOAMs are restricted by their assumptions of linearity and the magnitudes of input variances. First-order approximations deteriorate if the coefficient of variation (COV) of model parameters is larger than 10 to 20%.

Another shortcoming is their assumption of normal parameter distributions (Melching et al., 1996:106). If parameter distributions have skewed tails, the propagation of the output mean and variance will not describe the likelihood of extreme values. This can be an issue for the examination of environmental problems that may depend more on extreme conditions than on mean conditions (Summers et al., 1993:164).

Finally, Summers et al. (1993:164) claimed that the set-up of variance propagation must be hand programmed for each model, greatly increasing labour costs in terms of time and money.

Despite all the shortcomings of FOAMs, they have been successfully applied to H/WQ models (Melching et al., 2001:404). Although an earlier attempt in this study was made to distinguish between prediction error propagation and the quantification of prediction uncertainty, FOAMs can partly be seen as methods that accomplish both tasks within one method. Their simplicity can be attributed to this in the sense that they propagate the means and variances of the basic variables, and the results obtained immediately quantify prediction uncertainty (Melching et al., 1996:106).

2.4.3. Sensitivity Analysis

Beck (1987:1422) explains that there is a lot of confusion about different methods associated with uncertainty analysis due to the overlapping use of terms associated with uncertainty.

A major distinction needs to be made between sensitivity analysis and uncertainty analysis. A **sensitivity analysis** is not an uncertainty analysis. Models often have a very large number of parameter inputs, sometimes numbering in the hundreds (Helton et al., 2004:40). Sensitivity analysis

uses the propagation of error to identify the parameters to which the system is most sensitive, or to explore the behaviour of a model to better understand the model (Wallach et al., 1998:338).

A sensitivity analysis makes no use of information concerning the sources or ranges of uncertainty in model input data i.e. no use of parameter distributions or variances etc. (Summers et al., 1993:162). The only purpose of the conventional sensitivity analysis is to determine effects on the model's output response due to changes in the model input parameters, given the model structure (Beck, 1987:1422; Wallach et al., 1998:338), thus the results of a sensitivity analysis do not depend on the true uncertainty in the input data (Wallach et al., 1998:338).

An **uncertainty analysis,** on the other hand, can be partly similar to sensitivity analysis (Wallach et al., 1998:338), but it considers the inherent uncertainty in model input data and the subsequent effects this uncertainty has on model output (Summers et al., 1993:162).

Sensitivity analysis is described by Wu et al. (2006:352) as a "one-variable-at-a-time" approach although it can also be used to examine interactions between parameters (Wallach et al., 1998:338). The parameters are evaluated with respect to the model output of interest. A sensitivity analysis is conducted by increasing the value of the investigated parameter in increments of, say 5%, 10% or 20% while keeping the other parameters constant, and calculating the normalized sensitivity coefficients (SN) of the parameter in the model (Melching et al., 1996:109).

$$SN_{j,i} = (\Delta C_j / C_{j,0}) / (\Delta x_i / x_{i,0})$$

$SN_{j,i}$ = normalized sensitivity coefficient.

ΔC_j = change in prediction j as a result of change Δx_i in parameter i with all other parameters kept constant at their means.

$C_{j,0}$ = base prediction j when all parameters are kept constant at their means.

$x_{i,0}$ = original value of parameter i, which in this case is equal to the parameter mean.

Δx_i = change in parameter i.

Melching et al. (1996:109) describes how the sensitivity coefficients of parameters must be ranked to identify the key parameters that cause sensitive behaviour from the model. Once the key parameters have been identified, their influence on the model can be confirmed by conducting an uncertainty analysis that relates the uncertainty in model predictions with the uncertainty in the key parameters (Melching, 1996:110).

The quality of a model's predictions are not explicitly related to a sensitivity analysis (Wallach et al., 1996:338) and research has shown that the conventional sensitivity analysis is not appropriate for determining the sources of uncertainty that significantly affect model output (Melching et al.,

2001:403). For instance, it can happen that the uncertainty in a key parameter, identified with sensitivity analysis, is so little that it does not affect the prediction uncertainty. The inverse can also happen, where great uncertainty associated with a parameter, where the model sensitivity to that parameter was perceived to be unimportant, can have notable effects on the prediction uncertainty.

However, sensitivity analysis definitely has a role to play along with uncertainty analysis, especially when models have a large number of input parameters. It is often conducted on complex models, before the commencement of the uncertainty analysis, to identify the key sensitive parameters in the model. The contribution of the key parameter uncertainty to prediction uncertainty can then be assessed in the uncertainty analysis (Rigosi et al., 2012:204; Melching et al., 1996:110).

2.5. Monte Carlo Simulation

2.5.1. Introduction to Monte Carlo Simulation

The other dominant method of prediction error propagation is Monte Carlo Simulation (MCS). The use of MCS for prediction error propagation is the focus of this study and the exact procedure of MCS for the propagation of prediction error is explained in this section.

According to Chin (2009:1315), MCS uses the model parameters' probability distributions and combines them with a deterministic model to calculate the probability distributions of water quality constituent concentrations, thus characterizing the prediction uncertainty of the model. Hession et al. (1996:1309) describe MCS as a method for numerically operating a complex system that has random components.

MCS involves the repeated sampling of the probability distributions and multivariate distributions of model parameters, driving variables, boundary conditions and initial conditions and then to use each sample set in a model run (Summers et al. 1993:163). The result should be a sample of solutions for the model, each solution corresponding to a set of input parameters. A MCS will consist of an *n* number of model runs, using an *n* number of sample sets, resulting in an *n* number of model predictions.

According to Ang & Tang (1984:274), a sample of Monte Carlo solutions is similar to a sample of experimental observations; therefore the results from a MCS may be treated statistically. The ensemble of *n* model predictions can therefore be used to derive a probability distribution of the model's behaviour and basic statistical analysis and comparisons with observed data can then be applied to quantify the prediction uncertainty associated with the model. If different model structures are to be compared, each model's ensemble of predictions will be compared with the other model's ensemble of predictions (Summers et al., 1993:174). The application of the statistical analysis will be explained in section 2.6.

2.5.2. Monte Carlo Sampling

MCS samples the probability distribution of a parameter by considering the parameter's cumulative distribution function (CDF) (see **Figure 2.2**). The parameter's probability density function (PDF) represents plots of frequency of occurrence $f(x)$ versus the parameter values (x). The area under the PDF is equal to one, provided that they encompass the total probability of occurrence (Chapra, 2008:333). On the other hand, the CDF of a parameter represents the integral of the parameter's PDF (Chapra, 2008:334).

$$F(x) = \int_{-\infty}^{x} f(x)dx$$

The CDF specifies the probability $F(x)$ that the parameter will be less than a value of x. The range of a CDF's y-axis is always between 0 and 1. By using a uniform random number generator, a computer can uniformly generate any amount of random numbers between 0 and 1. Then by propagating the numbers through the CDF, the computer obtains values for the input parameter. This method considers the probability of occurrence of all values of the input parameter. It is robust in the sense that it can effectively sample distributions that are off-centred or "skewed" (Chapra, 2008:333; 334).

Figure 2.2 shows the PDF and its associate CDF for a normally distributed parameter. Say for instance the computer randomly generated 0.5. This would propagate through the CDF to the parameter value (x) of 1.

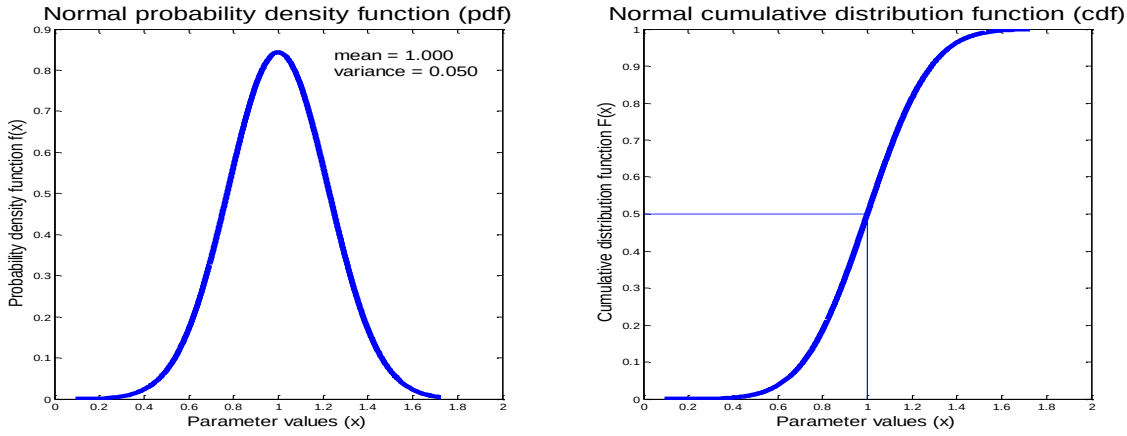

Figure 2.2. The Normal Probability Density Function (left) and the Normal Cumulative Distribution Function (right).

It is important to be aware that the accuracy of the prediction estimates from a MCS depends on the adequacy of the parameter probability distributions assigned to the parameters. The distributions of many parameters in WQMs are often unknown. If the model's parameters are correlated, multivariate sampling of the parameters must be used in the model simulations.

2.5.3. Monte Carlo Simulation applied to a Water Quality Model

WQMs predict water quality in response to loads on the environment. Mathematical equations are used to describe the cause-effect relationship between loading (W) and concentration (c) and the relationship depends on the physical, chemical and biological characteristics of the receiving water. A WQM can be represented by the following equation (Chapra, 2008:11):

$$c = f(W; physics, chemistry, biology)$$

A WQM consists of a model structure and model input to produce model output (predictions). The model structure consists of the mathematical algorithms and model resolution that describe the environmental system and relates the physical, chemical and biological characteristics of the system. The model input consists of values for model parameters such as boundary conditions, initial conditions, forcing functions, reaction kinetics, and other basic variables that are all inserted into the model structure to produce model output.

$$model\ structure\ (input) = output$$

As mentioned in section 2.2.2, both model structure and model parameters are subjected to uncertainty. Model parameters are in the position to be assigned probability distributions either by scientific experiments or making assumptions. Additionally, interdependent model parameters can be identified and multivariate distributions assigned to them. As shown in **Figure 2.3**, if a MCS performs only one model run, each parameter's distribution will only be sampled once. Together the values sampled from the different parameters' distributions and multivariate distributions are known as one parameter set. This one parameter set is inserted into the model to produce one model prediction. This one model prediction is a single solution of the model across space or time or both (depends on whether the model is steady state or time variable). This means that for every step in time and space, the model predicts a single value for the water quality constituent being modelled.

As shown in **Figure 2.4**, if a MCS performs 1000 model runs, each parameter's distribution will be sampled 1000 times. The samples from the various input parameters will be grouped into 1000 parameter sets. Each parameter set will contain a value for each model parameter. All 1000 parameter sets will be inserted into the model, one at a time, to produce an ensemble of 1000 model predictions. It is on ***this ensemble*** of model predictions that statistics are applied for the purpose of quantifying the prediction uncertainty.

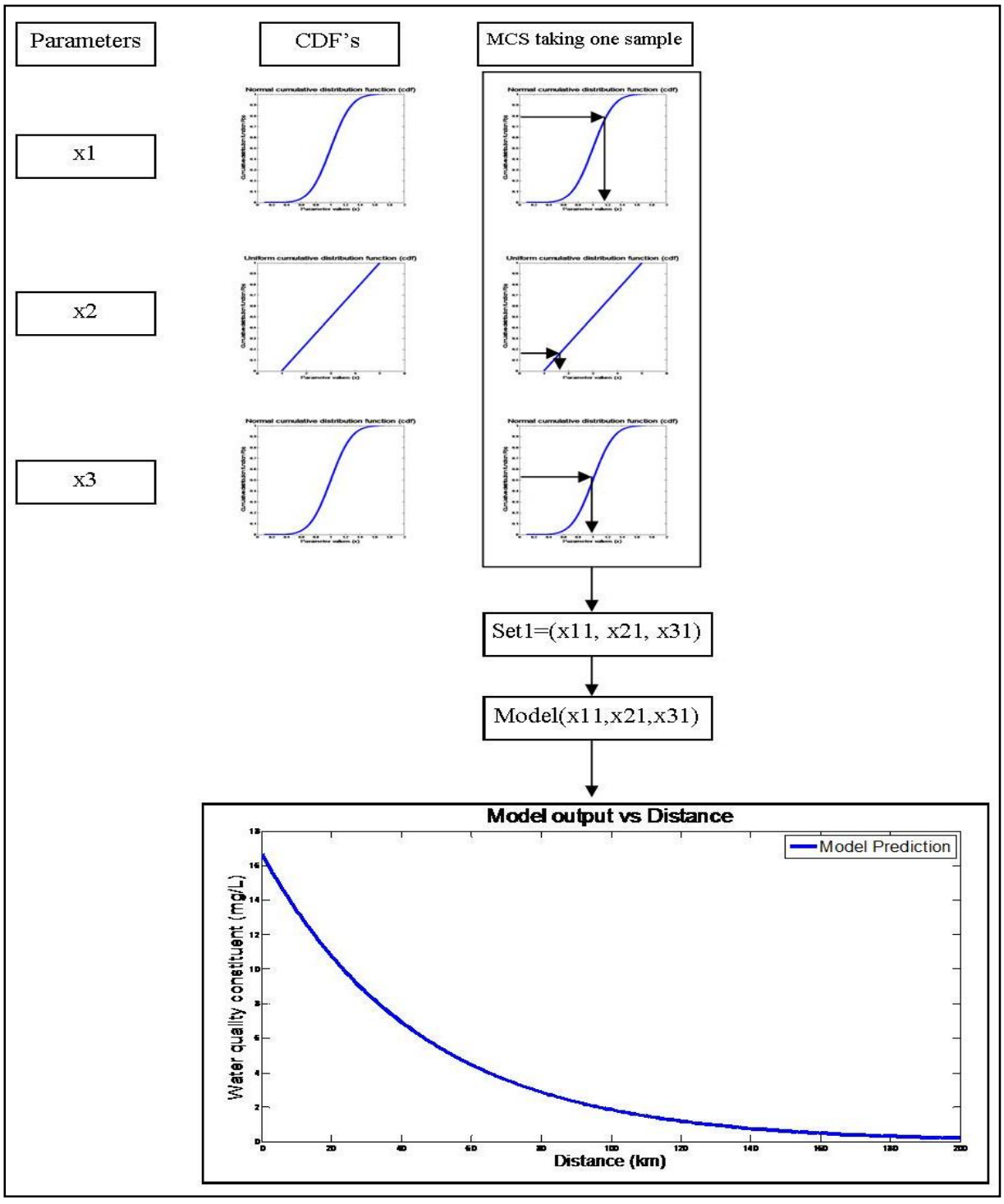

Figure 2.3. Monte Carlo Simulation performing only a single model run.

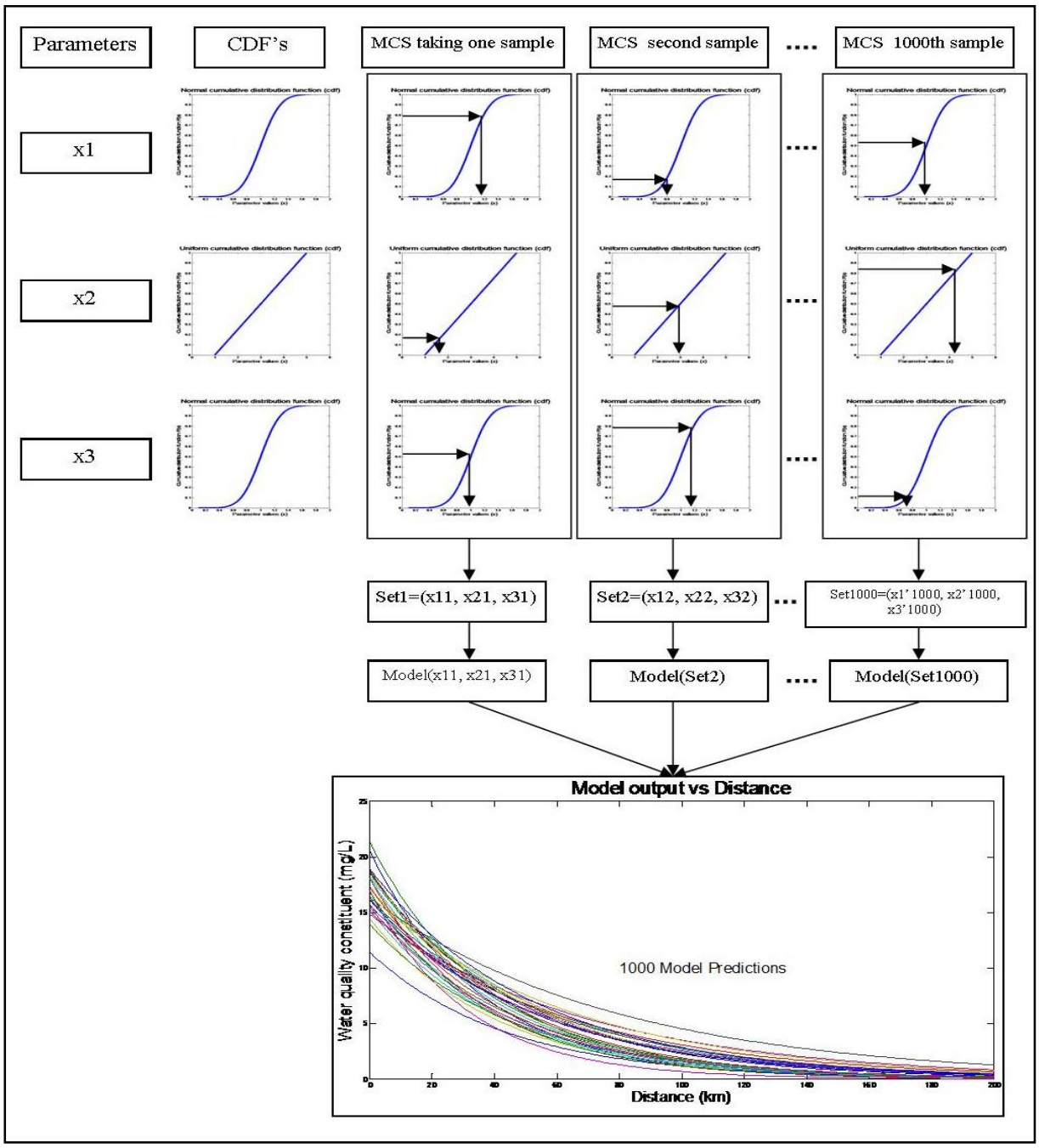

Figure 2.4. Monte Carlo Simulation performing 1000 model runs.

2.5.4. Advantages and Disadvantages of Monte Carlo Simulations

MCS is the most robust method of prediction error propagation for estimating prediction uncertainty and is commonly selected as the standard against which all other methods are compared (Shirmohammadi et al. 2006:1039). The first advantage of MCS is that it is a full distribution technique that can effectively sample the extremes of non-normal input distributions.

Secondly, MCS does not require reformulation of model code in contrast with FOAMs that need variance propagation algorithms to be hand-programmed for each model (Summers et al., 1993:164). For effective MCS, efficient and general pre-and post-processors can be coded to sample inputs, to run the model a sufficient number of times and to compute output statistics (**Figure 2.5**). These processors can be used with a number of models (Summers et al., 1993:164).

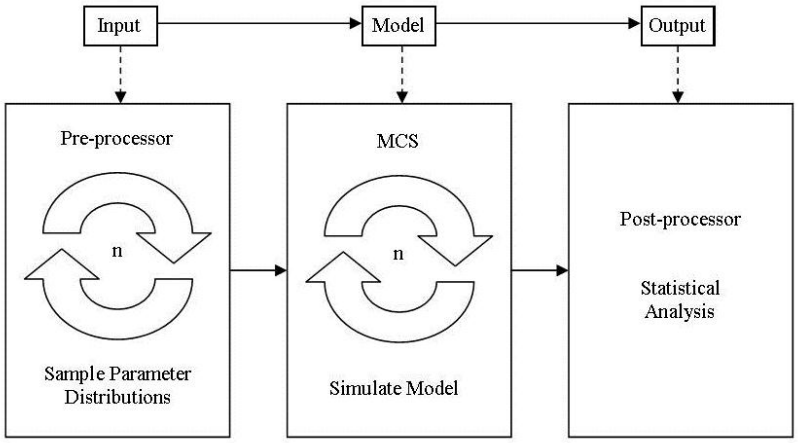

Figure 2.5 Model relationship to Monte Carlo Simulation pre -and post-processors.

Furthermore, the cumulative distribution function (CDF) and the complement of the cumulative distribution function (CCDF) are two statistical functions that are applied in the quantification of prediction uncertainty to produce very valuable information for decision making. CDFs and CCDFs require relatively large amounts of data to be constructed. MCS is ideal for the construction of CDFs and CCDFs because the purpose of MCS is to generate large amounts of data (Summers et al., 1993:171).

In the past, MCS' major disadvantage was the method's cost of computer calculations and was limited by constraints of computer capability (Ang & Tang, 1984:274). Some WQMs can be very complex and a large number of model simulations may result in the computer providing inefficient and time consuming computations (Summers et al., 1993:164). However, advancing computer technology will soon render this disadvantage almost obsolete except for the most complex models.

2.5.5. Monte Carlo Convergence

A very important aspect about MCS that needs to be mentioned is the following (Shirmohammadi et al., 2006:1039): The accuracy of prediction uncertainty estimates is going to depend on the number of model simulation runs performed in the MCS. Because Monte Carlo is similar to a sample of experimental observations, it shares the same problems as sampling theory, namely sampling errors. Therefore, Monte Carlo solutions from finite samples are never exact unless the sampling size is infinitely large (Ang & Tang, 1984:274). The amount of model simulation runs must be sufficient to reliably estimate the probability distribution of the model predictions. Ang & Tang (1984:291) say that it is important to know the error underlying an estimated probability of an occurrence or to know how many model runs are required to obtain certain accuracy from a MCS.

Wu et al. (2006:357) describe a way to determine the sufficient amount of simulation runs. By conducting an initial MCS with few model simulations and then by increasing the amount of model simulation runs in increments, the change in the prediction uncertainty results can be recorded. Once the prediction uncertainty results between increments start to converge, the sufficient amount of model simulation runs in the MCS has been determined. This will, however, lead to the use of more computer resources. Wu et al. (2006:352) explain that there is a trade-off between the desired accuracy of the prediction uncertainty estimate and the affordable computation burden.

Ang & Tang (1984:292) proposed an equation that could be used to calculate the expected error of a MCS' results, or for determining the sample size required to produce results subject to a percent of error:

$$\%\ error = 200\sqrt{\frac{1-p_F}{np_F}}$$

p_F = probability of exceedence (as a fraction).
n = sample size (number of model runs in MCS).

According to this equation, there is a 95% chance that the percent error in the estimated probability will be less than the %error given by the equation. This equation was derived by approximating a binomial distribution with a normal distribution and the 95% probability of %error originates from this derivation. Ang & Tang (1984:292) also gave the following example: If 10 000 model simulations were performed, with an estimated 0.01 probability of exceedence, the equation would give an error of less than 20%. That means there is a 95% chance that the actual probability will be within 0.01 ± 0.002. The same example can be applied to determine MCS sampling size and reads as follows; 10 000 model simulations are required to produce a Monte Carlo solution with a probability of exceedence of 0.01 ± 0.002.

There are a number of methods for the sampling of the parameter distributions. These include random sampling methods and non-random sampling methods such as Latin Hypercube Sampling (LHS). To produce an accurate MCS of a WQM, random methods can require several hundred or thousand model runs while, on the other hand, LHS might require less than a hundred model runs, saving computer resources such as computing time and memory (Summers et al., 1993:163).

Vose (2008:59) explains that LHS uses a technique that is known as "stratified sampling without replacement". It splits each probability distribution into intervals equal to the number of model iterations required in the MCS. With each model run each probability distribution is sampled and as a specific sample falls in an interval, the interval is crossed out for any further sampling during the rest of the MCS. Because the number of intervals is equal to the number of model runs in the MCS, each interval will be sampled only once and each probability distribution will be properly and uniformly covered in the MCS. The benefit of LHS is eroded if the number of model runs nominated in the beginning of the MCS is not completed.

2.6. The Quantification of Prediction Uncertainty

2.6.1. Introduction to the Quantification of Prediction Uncertainty

MCS as a method of prediction error propagation is discussed in section 2.5. This section focuses on the quantification of prediction uncertainty. This involves calculating the certainty with which a model's predictions represents reality. Once an ensemble of model predictions has been obtained through MCS, statistical analysis is applied to the ensemble to characterize the uncertainty associated with the model. The rest of this section discusses the statistical tools applied in the quantification of prediction uncertainty and how to interpret the results.

2.6.2. Statistical Tools

Summers et al. (1993:170) explains that there are two components to model prediction uncertainty:

1. **Accuracy**.
2. **Precision**.

Accuracy refers to the closeness between the model's average predictions and the observations made in the real system. Model predictions should be close to the true observed value of the water quality constituent of interest (usually observed). If the model prediction is equal to the true observed value, the model prediction is said to be unbiased (Montgomery & Runger, 2006:237). For the assessment of accuracy, the model output's **bias** is determined. The bias of the model output is the difference between the mean benchmark data value and the mean of the model output. The mean is a measure of the center or middle of a probability distribution (Montgomery & Runger, 2006:74). This difference is calculated at the specific point in time and space that is of interest. The bias indicates whether the model predicts well on the average (Summers et al., 1993:170). The bias is defined as:

$$B = X_p - X_o$$

B = model bias.

X_p = mean predicted value.

X_o = mean observed value.

The bias is equal to zero if the prediction mean and observation mean are equal (Summers et al., 1993:172).

Precision refers to the amount of variation inherent in the model output. Even though a model's mean prediction is equal to the mean observed value, the variance of the two distributions may be different. When the point estimate of a prediction is reported, it is usually desirable to give some idea of the precision of estimation (Montgomery & Runger, 2006:239). If a MCS of a WQM produces predictions that do not vary substantially from each other, then the model has a high level of

precision. On the other hand, if the MCS produces predictions that do vary by a notable amount, the model has a low level of precision. Wallach et al. (1998:344) claim that variance in model output is the direct consequence of uncertainty in model parameters.

Model precision is estimated by the **variance or standard deviation** of the model predictions. Variance is a measure of the dispersion or variability in a distribution. Standard deviation (SD) is the positive square root of the variance and is probably the more widely used measure of variability (Montgomery & Runger, 2006:74; 239; 760). Variance and standard deviation are often used as measures of risk in the financial sector because they represent uncertainty (Vose, 2008:96). In investment management, risk is generally proxied by volatility of returns and volatility is measured by the standard deviation of returns (Busetti, 2009:163).

It is often convenient to describe the relative amount of variation in parameters or predictions, especially if their uncertainty needs to be compared. The relative amount of variation is given by the parameter or prediction's **Coefficient of Variation (COV)** (McBean & Rovers, 1998:32). COV is calculated as follows:

$$COV = \frac{SD}{Mean}$$

COV is dimensionless and effective at describing the relative variability of a distribution and good for comparing the uncertainty between different predictions or parameters.

A measure of the relative precision with which a model predicts system observations can be provided by comparing the standard deviation of the benchmark data with the standard deviation of the model predictions at a specific point in time and space (Summers et al., 1993:170). This comparison is defined as follows:

$$F = S_p/S_o$$

F = relative dominance of the variability of the predictions over the observations.
S_p = standard deviation of the model predictions.
S_o = standard deviation of the system observations.

Relative dominance is equal to one if the standard deviations of the predictions and observations are equal (Summers et al., 1993:172).

Model precision is related to the level of confidence in the model. Usually **confidence intervals** use historical information for the construction of one or more lines or limits to characterize the uncertainty associated with a particular parameter such as the mean. They are constructed from sample data and are thus random quantities (McBean & Rovers, 1998:107). In section 2.5 it is explained that Monte

Carlo solutions are similar to sampled data, so confidence intervals can definitely be applied to the results from a MCS.

A confidence interval is interpreted as the values between which the model prediction is likely to occur. A 90% confidence interval will give the values between which a model prediction is 90% likely to occur. The length of a confidence interval is a measure of the precision of model estimation. It is desirable to obtain a confidence interval that is short enough for decision making purposes, but which also has adequate confidence. Confidence intervals are very convenient for defining exceedence probabilities of model predictions in space. This will be demonstrated in Chapter 4.

In addition to accuracy and precision, Summers et al. (1993:171) also suggest two other statistical measures used for the characterizing of uncertainty in model predictions:

1. **Mean Squared Error (MSE) or Root Mean Squared Error (RMSE).**
2. **The Complement of the Cumulative Distribution Function (CCDF).**

These two statistics provide a great deal of information about the uncertainties associated with the model predictions. Together they adequately characterize prediction uncertainty without the need and expense of rigorous hypothesis testing (Summers et al., 1993:172).

MSE combines both accuracy and precision as an estimate of total uncertainty. The square root of the MSE **(RMSE)** is in fact a better measure of total uncertainty because it has the same units as the original observed data.

The RMSE focuses on the correspondence of point-by-point comparisons of predicted and observed values, by concentrating on the means and standard deviations of the model output and the system observations. It estimates the total uncertainty of the model predictions at a specific point of interest in time and space (Summers et al., 1993:171; 172). Wallach et al. (1998:339;340) mention that the RMSE is the natural measure of model quality and that it is of interest to compare the effects of parameter uncertainty on the RMSE of the model predictions during an uncertainty analysis. The effect of each parameter's uncertainty on prediction uncertainty can be examined by calculating the change in RMSE of the model predictions as each parameter's uncertainty is investigated in turn. RMSE is the square root of the sum of the squared bias and the squared standard deviation (variance) of model predictions. RMSE is defined by the following equation:

$$RMSE = \sqrt{B^2 + S_p^2}$$

The model bias (B) is only affected by non-linearity in the model, whereas uncertainty (variation) in model input always contributes to the model standard deviation (S_p) in RMSE. The usefulness of additional measurements to reduce parameter uncertainties largely depends on the RMSE of a model's

predictions. If the contribution from parameter uncertainty to the RMSE of the model's predictions is small, then additional measurements of model parameters might not be worthwhile (Wallach et al., 1998:344).

The **CCDF** provides a detailed examination of the extremes of the model prediction distribution at a specific point in time and space, and is very useful in exposure assessments in the sense that they can be used to determine the probability of meeting or violating any water quality standard (Shirmohammadi et al., 2006:1046). Hession et al. (1996:1313) also mentions that a single average value for a model prediction is not good enough for detailed management decisions because it contains very little information. A CCDF on the other hand allows management decisions to be based on probability of occurrence and acceptable risk, which is defined in this case as the occurrence probability of an undesired event.

The cumulative distribution function (CDF) of a set of model predictions plots the likelihood $F(x)$ of the predictions being below a selected value (x). On the other hand the CCDF estimates the likelihood $F'(x)$ that the predictions would exceed a given value (x) (Summers et al., 1993:168). The values of the CCDF are provided by the following equation (Montgomery et al., 2006:35):

$$F'(x) = 1 - F(x) \; or \; CCDF = 1 - CDF$$

In the example in **Figure 2.6**, the likelihood $F'(x)$ of exceeding a prediction value of 1.2 is 0.1855.

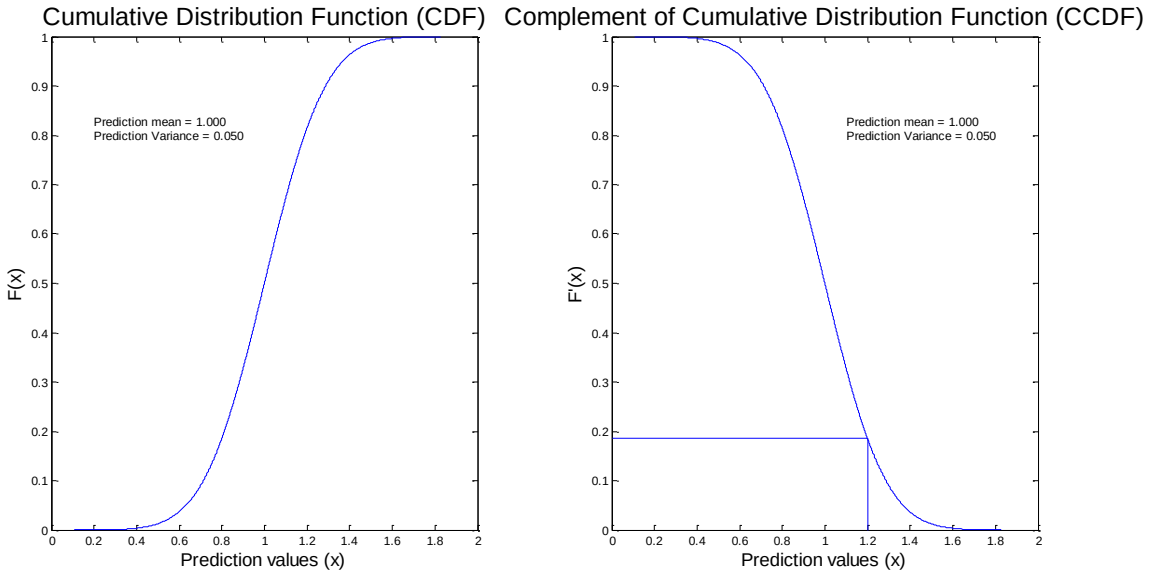

Figure 2.6. The Cumulative Distribution Function (left) and the Complement of the Cumulative Distribution Function (right).

A very important point about CDFs and CCDFs must be remembered. Before computing either the CDF or CCDF of a model's predictions, the type of probability distribution of the model predictions must be determined. Model predictions could, for instance, have a normal or lognormal distribution. This must be determined beforehand; otherwise the calculation of the CCDF will be approached with the wrong distribution equation. One of the most effective ways of determining the type of a model's output distribution is by plotting the output in a histogram. The shape of the histogram will quickly give the character of the model output distribution (McBean & Rovers, 1998:17). **Figure 2.7** is an example of a histogram plotting the predictions obtained from a MCS that completed 10000 model runs. The frequency of the prediction values are shown on the y-axis while the values of the predictions are shown on the x-axis. From the histogram it can clearly be seen that the probability of the model predictions tend to be normally distributed. Thus, a CDF or CCDF equation applicable to normally distributed solutions would be the correct type of distribution equation to represent the model output. If the histogram proved that the model solutions were NOT normally distributed, for instance if it were log-normally distributed, the CDF or CCDF equations applicable to log-normally distributed data would have been the correct type of distribution equations to represent the model output.

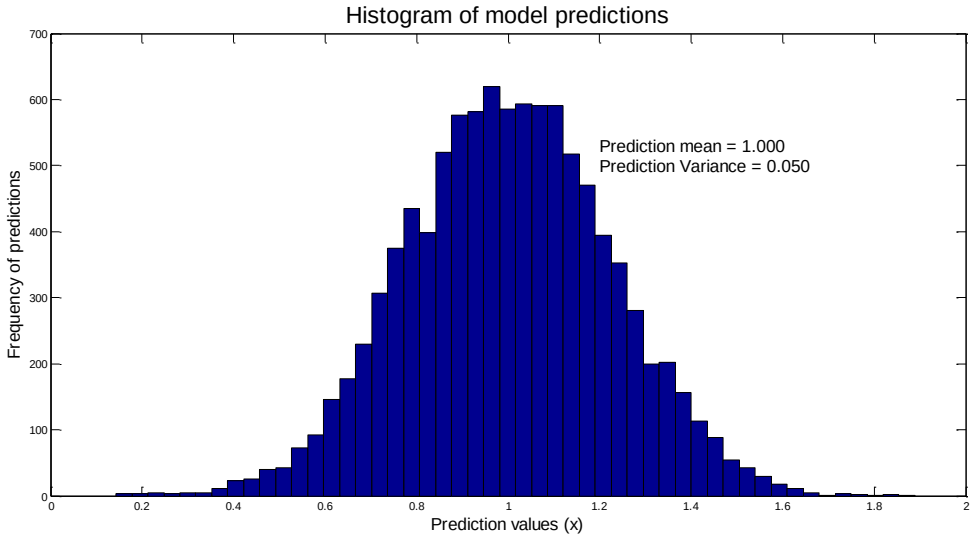

Figure 2.7. Histogram of model output showing the output's probability to be normally distributed.

2.6.3. Interpretation of Statistical Results

This subsection describes different model prediction interpretations with hypothetical CCDF graphs, along with the corresponding model and observation statistics, as was done by Summers et al. (1993:173).

In **Figure 2.8** the model predictions closely resemble the actual observations in terms of both accuracy and precision. The bias is almost zero and the standard deviations of the actual data and model predictions are almost the same. In this case the uncertainty associated with the model predictions is basically equivalent to the uncertainty inherent in the actual data. There will be no need for the reduction of parameter uncertainty in this case (Summers et al., 1993:172).

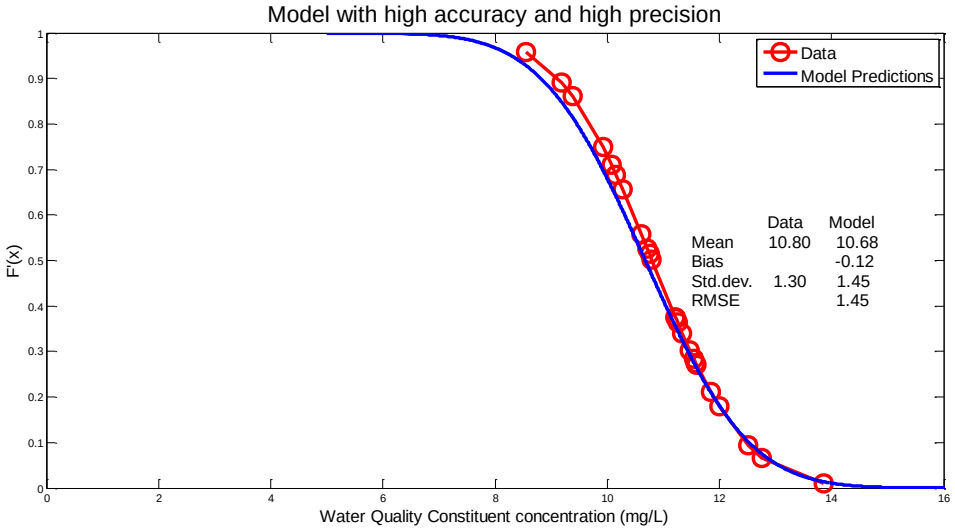

Figure 2.8 Model predictions with high accuracy and high precision (adapted from Summers et al., 1993:173).

In **Figure 2.9** a model that predicts with high accuracy, but with a lower degree of precision is demonstrated. The model's bias is almost zero. However, the variation in the model's predictions is almost five times higher than the variation in the actual data; thus, this model predicts the average concentration well but with less precision (Summers et al., 1993:173).

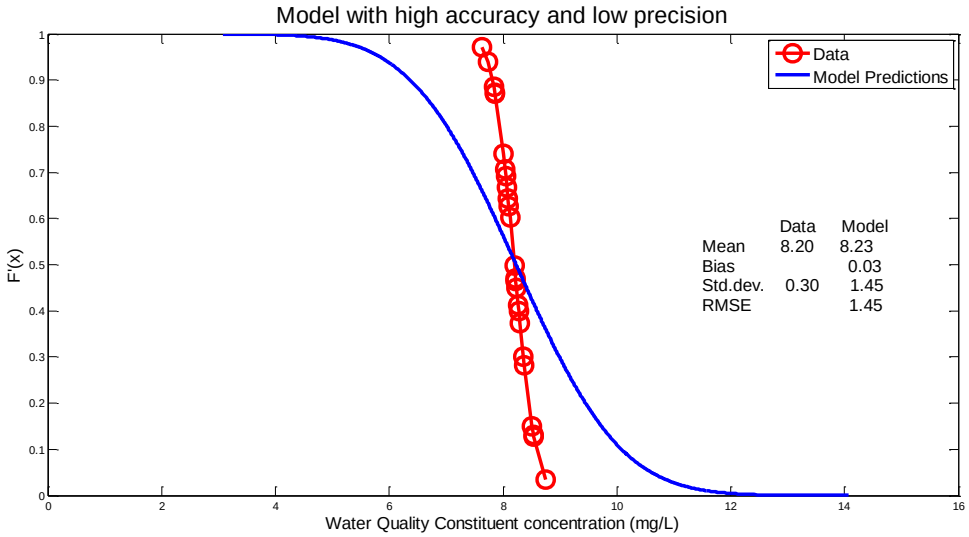

Figure 2.9 Model predictions with high accuracy and low precision (adapted from Summers et al., 1993:173).

In **Figure 2.10**, as shown by the little difference in their standard deviations, the model predictions show the same level of precision as the actual data. However, the model's accuracy is low as shown by the model's bias. The model underestimates the actual data by almost 3mg/L.

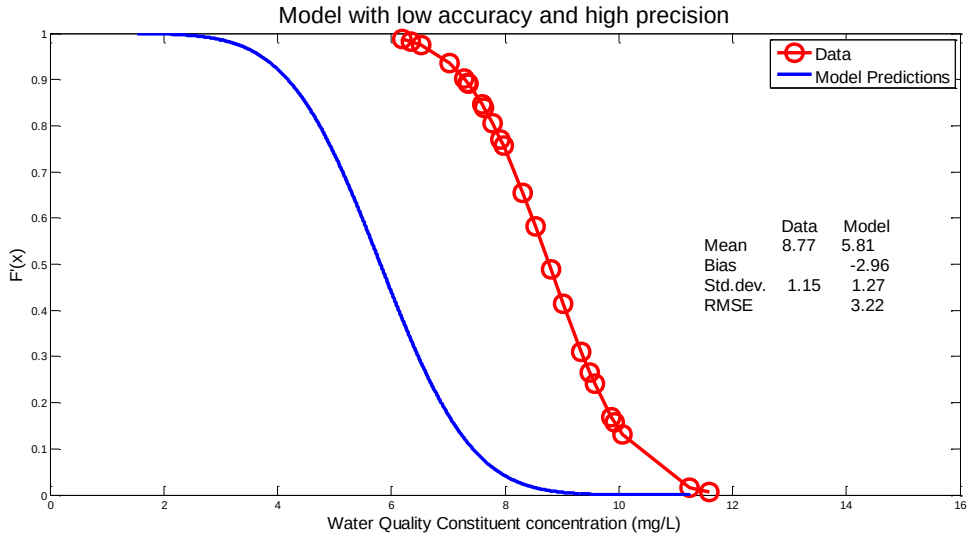

Figure 2.10 Model predictions with low accuracy and high precision (adapted from Summers et al., 1993:173).

In **Figure 2.11** the model predicts with neither accuracy nor precision. In this case, the model underestimates the actual data and is also generating predictions that are varying much more than the actual data.

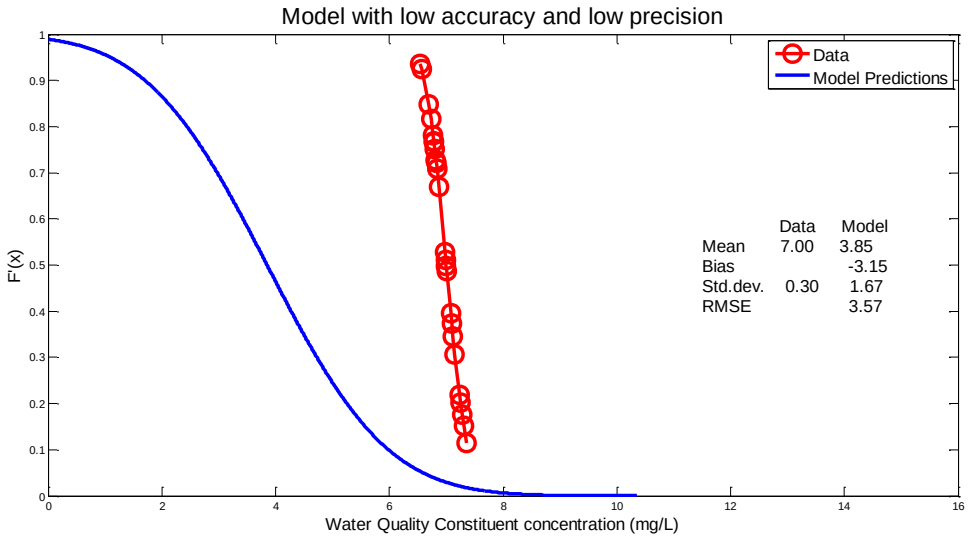

Figure 2.11 Model predictions with low accuracy and low precision (adapted from Summers et al., 1993:173).

To summarize prediction error propagation and the quantification of prediction uncertainty, the following example and **Figure 2.12** and **Figure 2.13** should help to clear any misunderstandings or

confusion about MCS and the quantification tools. Say for instance a MCS performing 1000 model runs has produced an ensemble of 1000 predictions (see **Figure 2.12**). The mean prediction as well as standard deviation of all 1000 model simulation runs can be depicted at all points in space. In the case of **Figure 2.12**, 21 points in space have been identified in steps of 10km.

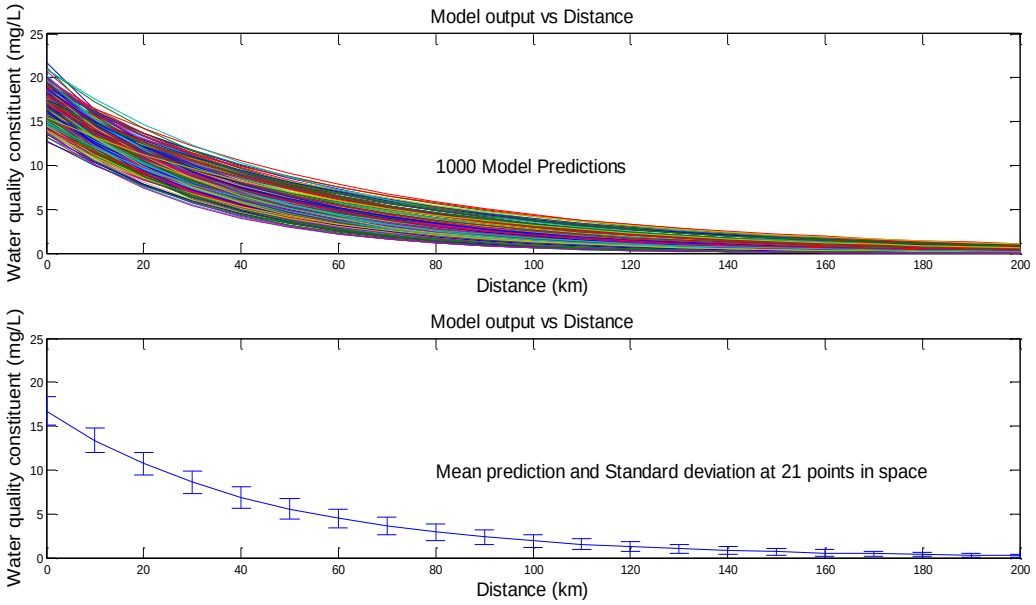

Figure 2.12 MCS with 1000 predictions as well as the associated mean prediction and standard deviation of all 1000 model simulation runs, at specific points in space.

Additionally, at any point in space, one should be able to compute a CCDF and quantify the uncertainty in terms of precision and accuracy as shown in **Figure 2.13**. If a water quality standard was set for a river at a distance of 40km downstream, the probability of violating the standard can be read from **Figure 2.13**. If the maximum allowable concentration of the water quality constituent was 8mg/L, the likelihood of exceeding the limit of 8mg/L is 0.19 or 19%.

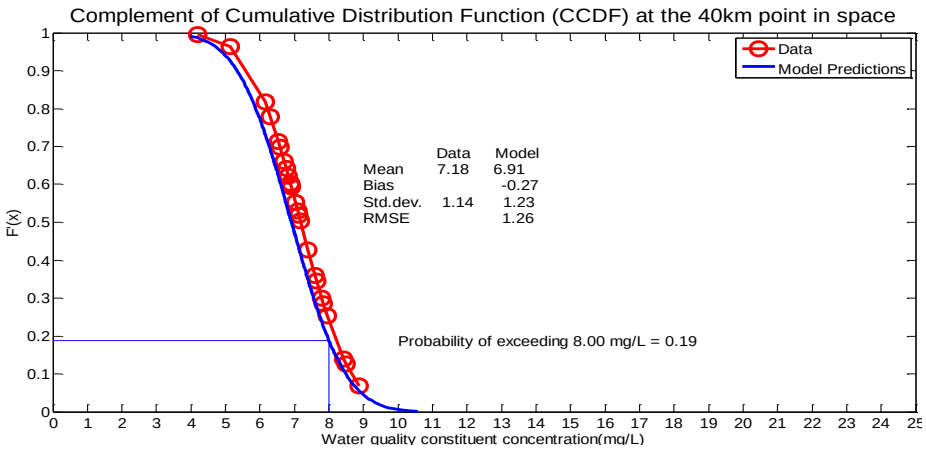

Figure 2.13 CCDF of model predictions drawn at a distance of 40 km downstream. Note that real data is also depicted and compared with the model predictions.

2.7. Uncertainty Analysis Considerations

This section introduces a protocol for uncertainty analysis in water quality modelling. It continues by making some important comments on the calibration of WQMs and the effect that it may have on the analysis of a model's uncertainty. Furthermore, some uncertainty analysis objectives and configurations on how to achieve those objectives are discussed. Finally, some views on quantifying model structure uncertainty are shared.

2.7.1. Uncertainty Analysis Protocol

Figure 2.14, adapted from Summers et al. (1993:165), describes the proposed protocol for quantifying and comparing model prediction uncertainties. The protocol is divided into two sequences. The first deals with the identification and selection of the uncertainty analysis' prediction error propagation method, for example, MCS. The second sequence involves six application steps of which the first four are usually encountered in the general protocol for water quality modelling (Chapra, 2008:319). As shown in this protocol, the analysis of uncertainty is performed after the calibration (2c) and verification (2d) of the model.

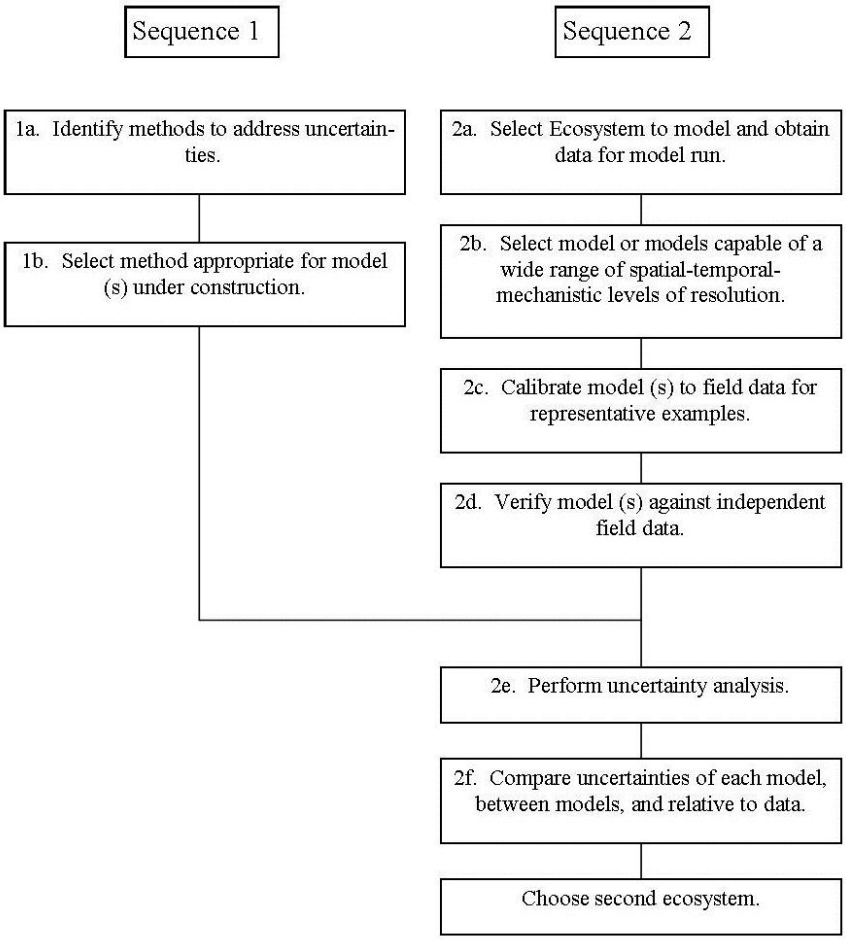

Figure 2.14 Proposed protocol for quantifying and comparing model prediction uncertainties (Summers et al., 1993:165).

A very important step in the calibration of the model is worth mentioning now. Sometimes the results of a model are simultaneously affected by two or more parameters that are interdependent. The distribution of a parameter that is interdependent on other parameters must be regarded as conditional on the value of all the other interdependent parameters. It is therefore necessary to refer to a joint parameter distribution which is defined by a continuous function of all the parameters. Parameters are then sampled as parameter sets rather than individual parameters (McIntyre, 2004:25). For example, the BOD rate of removal due to settling (k_s) and the reaeration rate (k_a) of a body of water can be interdependent because both coefficients are functions of water depth (H) (Chapra, 2008:359; 377) , thus they could be sampled from a joint parameter distribution.

Summers et al. (1993:167) describes a method of calibrating a model's interdependent parameters by using MCS to produce a vector of mean values for the parameters as well as a variance-covariance structure of the parameters that would lead to acceptable model predictions. This variance-covariance matrix contains information concerning the interrelationships among the parameters that are used in the assessment of prediction uncertainty. With the mean vector and variance-covariance matrix, acceptable parameter sets can be generated in a MCS from multivariate normal or log-normal distributions that would result in acceptable model behaviour. So, during the uncertainty analysis, the sampling of parameters' distributions does not necessarily have to be separate from each other. Interdependent parameters can be sampled together by sampling their multivariate distributions.

Hession et al. (1996:1311) and Reckhow (1994:6) both mention the importance of including the correlations among input parameters during error propagation. Their reason for this is that individual parameters may be highly uncertain but specific pairs of parameters may vary in a predictable way, thus collectively lessening uncertainty.

2.7.2. Total Prediction Uncertainty

The total prediction uncertainty, resulting from all the parameters' uncertainties together, can be large and must be assessed to determine the cumulative result on the total uncertainty of the model's predictions (Wallach et al., 1998:344). This is done by performing a Single Phase Monte Carlo Simulation (SPMCS) that considers both epistemic and aleatory uncertain parameters simultaneously. This type of uncertainty analysis calculates the overall quality of a model's predictions.

2.7.3. Separating Epistemic and Aleatory Uncertainty

A very important consideration in an uncertainty analysis is the separation of the two types of uncertainty in WQMs: (1) aleatory uncertainty and (2) epistemic uncertainty. Helton et al. (2004:61) mention that the separation of the two types of uncertainty can become so important that in many cases it dominates the design and computational cost of many analyses for complex systems.

If these two types of uncertainty are not separated in the uncertainty analysis, their effects on prediction uncertainty become commingled, making it difficult to draw useful insight. By separating the two types of uncertainty, one is able to determine which of the two types is dominating the predictions of the model. The separation determines whether additional measurements might help to reduce prediction uncertainty or whether the prediction uncertainty is not reducible and needs to be taken into account when designing system intervention options (Hession et al., 1996:1315; Vose, 2008:53).

Hession et al. (1996:1312) describes a method to separate aleatory- and epistemic uncertainty by performing a Two Phase Monte Carlo Simulation (TPMCS). This method basically consists of nesting the MCS of aleatory parameters within the MCS of epistemic parameters. The result should be an ensemble of CCDFs on one set of axes. The multiple CCDFs should result from the epistemic parameters, while each individual CCDF arises from the aleatory parameters (Helton et al., 2004:60). Thus, the use of each epistemic set of parameters should contain the entire MCS of the aleatory parameters. The variation within each of the CCDFs characterizes the aleatory uncertainty of the model predictions while the variation in the collective distribution of the CCDFs characterizes the effects of epistemic uncertainty on the model predictions.

2.7.4. Identifying Key Uncertain Parameters

Once it is known that a model is dominantly subjected to epistemic uncertainty, the key parameters responsible for contributing to the uncertainty must be identified. The contribution of each parameter's uncertainty on the model's prediction uncertainty is assessed one at a time, just as the model's sensitivity to key parameters is assessed in the sensitivity analysis. This uncertainty analysis is very similar to a sensitivity analysis (Wallach et al., 1998:338), but considers the inherent uncertainty in model input data and the subsequent effects this uncertainty has on model output (Summers et al., 1993:162). It also consists of an entire MCS for each individual parameter under investigation. This can increase the computational costs of identifying the key uncertain parameters immensely.

If it is determined that a parameter's uncertainty significantly affect the prediction uncertainty of the model, that parameter's uncertainty will need to be reduced. Once the parameter uncertainties have been reduced, the uncertainty analysis must be performed again to confirm that the reduction in parameter uncertainties did result in a reduction of model prediction uncertainty, as was done by Melching et al. (1996:112).

2.7.5. Model Structure Uncertainty

As depicted in step 2b of the uncertainty analysis protocol (**Figure 2.14**), a number of models can be used to describe the same system. These models can differ in terms of levels of resolution and complexity. The different levels of resolution and complexity will be propagated to the model

predictions. When the different models have been calibrated to the same data set, the relative prediction uncertainties of the models are analysed (step 2e) and compared statistically (step 2f) (Summers et al., 1993:166).

The comparison of different models' uncertainty analyses will describe the uncertainty (doubt) associated with the choice of model structure (Summers et al., 1993:174). By doing this, Summers et al., (1993:174) appear to make a suggestion on how to quantify the uncertainty associated with model structure, but the quantification of model structure uncertainty is very difficult and only a few attempts are found in literature (Lindenschmidt et al., 2007:290). Model building is subjective (Vose, 2008:65) and McIntyre's (2004:30) opinion is that even though one tries to improve on model structure, the "correct" model will never be found.

The argument is that by confronting structural error, there is generally a large number of improvements one can make that would result in a better model fit. But do these improvements lead to a better, more realistic model or do they adjust the model output in a black box manner just to give a better fit to system observations? Wallach et al. (1998:341) mentioned the example of model equations that could be incorrect but that it is possible to improve the model predictions by using incorrect parameter values rather than correct parameter values. Furthermore, McIntyre (2004:30) also mentions of the errors inherent to data that make it difficult to distinguish between prediction uncertainty due to uncertain parameter data, and prediction uncertainty due to uncertain model structure. Finally, it is mentioned that model structures can perform well during calibration but might be flawed in the sense that their behaviour change as boundary conditions of the system shifts. This might make models inappropriate for studying the intervention options that they are meant to investigate (McIntyre, 2004:29).

In light of McIntyre's (2004:30) thoughts on model structure uncertainty, it is concluded that model structure uncertainty is a very complex subject on its own and will not be investigated any further in this study. The suggestion by Summers et al., (1993:174), of comparing different models' uncertainty analyses results, for the purpose of quantifying structure uncertainty, will have to suffice as the only method for now.

2.8. Conclusion

WQMs are tools for water resources and environmental management. Decisions are based on the results of these models and it is therefore very important that the models are realistic and reliable and that all uncertainties associated with the models are identified and properly managed. An uncertainty analysis plays the crucial role of determining the quality of a model's predictions, identifying the key sources of uncertainty in WQMs and characterizing their effects on the model predictions.

Without a basic understanding and good definition of uncertainty associated with WQMs, the analysis of uncertainty will probably be a futile attempt. Uncertainty is a difficult subject and its definition changes the whole time. The two types of uncertainty are; (1) aleatory uncertainty and (2) epistemic uncertainty. The problem areas of uncertainty in WQMs are; (1) model structure uncertainty, (2) model parameter uncertainty and (3) model prediction uncertainty. By integrating the types of uncertainty with the problem areas of uncertainty in WQMs, it is possible to define different uncertainties associated with WQMs.

Due to the important role that WQMs have to play in the management of environments and resources, model simplifications and scientific uncertainties need to be analysed to help make decisions with regards to further modelling, data collection and system management.

There is some confusion around the different methods and terms associated with uncertainty analysis and an explanation is summarized in **Figure 2.15**. Although similar in some aspects, uncertainty analysis and sensitivity analysis are two different methods associated with WQMs. Sensitivity analysis is only concerned with the propagation of error through the model and assessing the effect it has on model output. Uncertainty analysis also includes the propagation of error but considers the inherent sources and ranges of uncertainties associated with the WQM.

The two dominant methods of prediction error propagation for the purpose of uncertainty analysis are; (1) Monte Carlo Simulation (MCS) and (2) First Order Approach Methods (FOAMs). Although MCS can be expensive in terms of computer calculations, it is the most robust and effective method of prediction error propagation. MCS involves the repeated simulation of a model, using in each model run, a particular set of values for the model variables. These model variables are generated in accordance with their corresponding probability distributions. By repeatedly running the model, a sample of solutions is obtained, each solution corresponding to a different set of values for the model variables.

The results from a MCS are similar to a sample of experimental observations, therefore they may be treated statistically and statistical methods can be applied to them. Basic statistical tools are used for the quantification of prediction uncertainty in the analysis of uncertainty. Model prediction uncertainty is measured by taking into account both the accuracy and precision of the model. For the

purpose of measuring uncertainty, the Bias and Standard deviation of model predictions are calculated. As a measure of model quality, the RMSE of the model predictions can be calculated to assess the effects of parameter uncertainty on prediction uncertainty. A CCDF provides a detailed examination of the extremes of the model prediction distribution and the probability of exceeding any water quality standard can be easily obtained from the CCDF. A CCDF allows management decisions to be based on probability of occurrence and acceptable risk.

The analysis of a WQM's uncertainty has a few individual objectives. Firstly, the overall quality of the model's predictions must be determined. Secondly, the dominance of either aleatory or epistemic uncertainty in the model must be determined to make decisions with regards to further data collection or to instill confidence in system intervention management. Thirdly, the key parameters contributing the most to model prediction uncertainty must be identified so that they can be reduced.

Achieving all of the objectives consists of various configurations or sequences of MCSs, to produce output in such a way that the analysis of the results would fulfil in the objectives. Determining the overall quality of the model's predictions is achieved by a SPMCS. Separating the two types of uncertainty in the model is achieved by a TPMCS which consists of two MCSs, the one nested within the other. Identifying the key uncertain parameters is achieved by a PMCS, which is similar to a sensitivity analysis, but instead of considering small errors in the model parameters and recording the change in model output, the PMCS considers the uncertainty of each model parameter and the effect it might have on model predictions. This means that each model parameter's uncertainty is related to the uncertainty in the model predictions.

Analysing the contribution of model structure uncertainty to model prediction uncertainty is a very complex task. It is very difficult because the uncertainty in model input parameters can quickly mar the identification of model structure uncertainty and the effect it might have on model predictions.

In final conclusion to the literature review it must be mentioned that the successful communication of an uncertainty analysis' results is very important. It doesn't matter how good an analysis' results are if they are misunderstood. Knowledgeable decision making depends on both the incorporation of a thorough uncertainty analysis as well as the correct interpretation of the analysis' results.

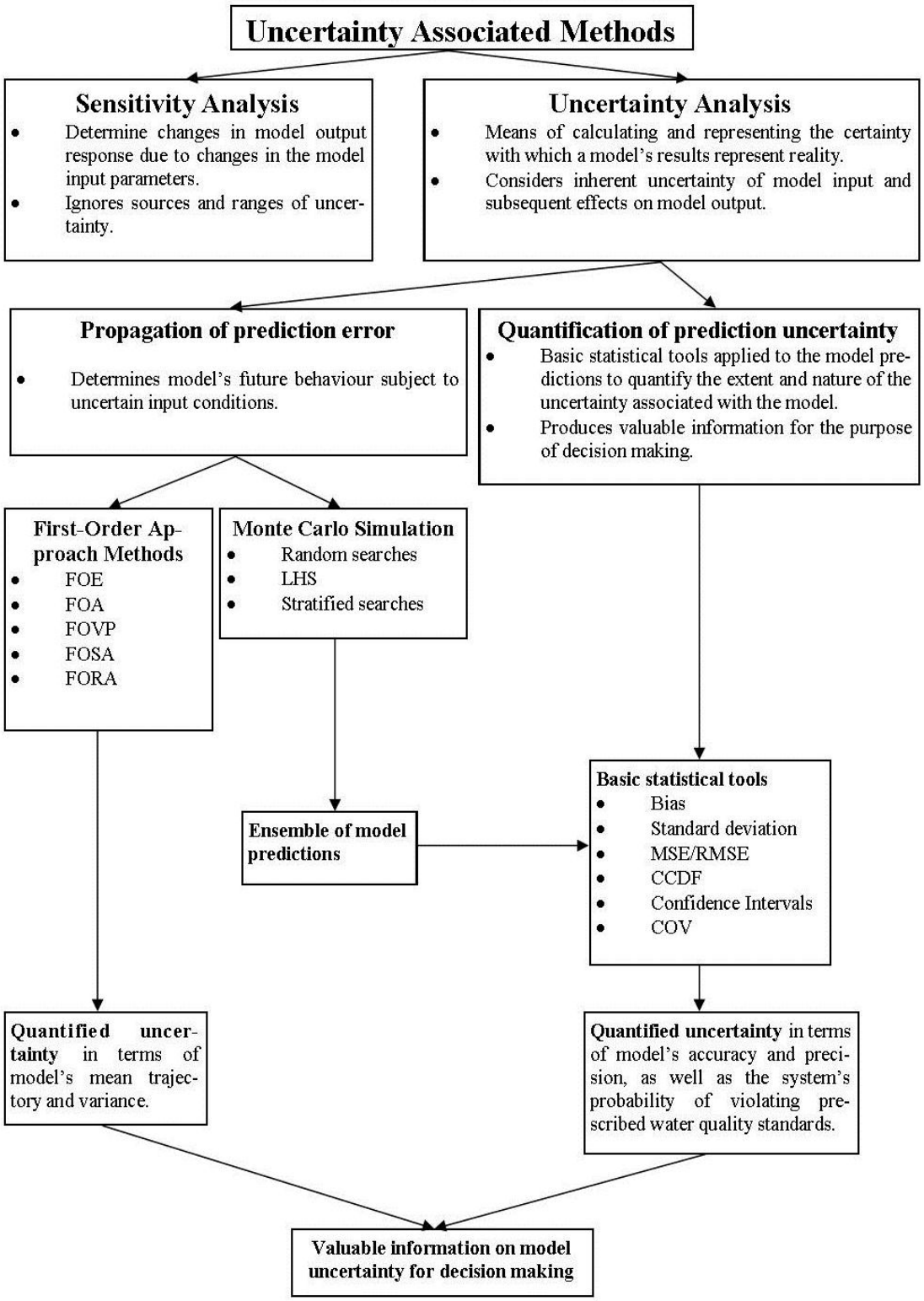

Figure 2.15 Summary of the different methods and tools associated with uncertainty analysis.

3. Methodology

3.1. Introduction

The purpose of this study was to investigate Monte Carlo Simulation (MCS) as a method of prediction error propagation and to demonstrate its use in an uncertainty analysis. This uncertainty analysis was to be applied in the context of a water quality model (WQM), thus the research primarily had to focus on model simulations and the analysis of the model results. To understand MCS properly, it was decided to write a model and uncertainty analysis from first principles with a basic understanding of the fundamental theory of WQMs and uncertainty analyses. This was done with the use of MATLAB which proved to be very powerful and effective. MATLAB is briefly introduced as a tool in Appendix A.

The WQM chosen for this study was the classic Streeter-Phelps equations for the calculation of dissolved oxygen (DO) and critical oxygen deficit (D_c) in a stream or river. A single point source of carbonaceous biochemical oxygen demand (BOD) was considered in this case. Although our knowledge of DO modelling in rivers is far more advanced and complex today than the Streeter-Phelps equations suggest, the Streeter-Phelps theory still remains the cornerstone of stream WQMs. The equations are widely accepted and still used today (Hamed et al., 2004:233; Liu et al., 2011:1348; Stow et al., 2007:1503).

Complex models are very expensive to evaluate in terms of calculations and their uncertainty analyses become increasingly more difficult to conduct (Mishra, 2011:9). It was therefore desirable to choose a model with low dimensionality in terms of the number of parameters, to easier depict the process of uncertainty analysis. The Streeter-Phelps equations have few parameters but they are balanced in the sense that they could be successfully divided into aleatory and epistemic uncertain parameters. It was therefore the combination of simplicity, low but balanced dimensionality, and universal acceptance that made the Streeter-Phelps equations very appealing as the model to be used in this study. The Streeter-Phelps theory is explained in section 3.2.

To complete this study's experimental model, a combination of the multistep water quality modelling process by Chapra (2008:319), and the uncertainty analysis protocol by Summers et al. (1993:165) was followed. The entire design of the model and uncertainty analysis was based on the integration of MCS within uncertainty analysis processes. MCS was also used in the model calibration which served as the mechanism for reducing parameter uncertainty. Synthetic data was also generated in a Monte Carlo fashion for the purpose of serving as system observations in the calibration and confirmation of the model. Thus the whole experiment took place under controlled conditions.

A very important facet of the study was to illustrate the reduction in model prediction uncertainty once model parameter uncertainty was reduced, thus, to confirm the reduction in model prediction uncertainty, the uncertainty analysis processes were repeated once parameter uncertainty was reduced.

Three uncertainty analysis processes were conducted and their results analysed:

1. **Single Phase Monte Carlo Simulation (SPMCS).** This analysis quantifies the model's total prediction uncertainty by considering all the parameter uncertainty at once in a single MCS. Analysing total prediction uncertainty determines the overall quality of the model's predictions and this analysis also contributes the most towards managerial decision making with regards to violating water quality standards.
2. **Two Phase Monte Carlo Simulation (TPMCS).** This analysis is designed to separate the two types of uncertainty in the model; epistemic and aleatory uncertainty. It illustrates the dominance of the one type of uncertainty in the model over the other type of uncertainty and provides information on whether a further reduction in parameter uncertainty will improve model predictions.
3. **Parameter Monte Carlo Simulation (PMCS).** This analysis is similar to a conventional sensitivity analysis. It is designed to relate the model's prediction uncertainty to individual parameters' uncertainty. By considering each model parameter's uncertainty one at a time, this analysis identifies the key parameters whose uncertainty contributes the most to the model's prediction uncertainty. Once identified, the reduction of parameter uncertainty should be focussed on the key parameters.

The application of SPMCS, TPMCS and PMCS is explained in section 3.3. It is important to make a brief comment now, on the statistical methods used for the quantification of the uncertainty. Although only the most basic statistical methods were used in this study, the robustness of MCS ensures that the statistical methods used for the analysis of model results are effective enough for providing valuable information with regards to the uncertainty of model output and for decision making.

The whole exercise of the experiment should be of great value to any interested person who would like to design their own simple, robust and effective method of uncertainty analysis. This will increase their knowledge and decision making capability with regards to water quality modelling and the management of environmental systems.

3.2. Streeter-Phelps

Before the rest of the methodology is explained, the environmental model used in this study must be explained first. The Streeter-Phelps model is a representation of the self purification capacity of a stream/river and ties together the two primary mechanisms governing DO in a stream receiving sewage. These two mechanisms are: (1) the decomposition of organic matter in the stream and (2) the oxygen reaeration of the stream (Melching et al., 1992:797; Chapra, 2008:389). The Streeter-Phelps model provides an analytical framework for predicting the effect of both point and nonpoint sources of organic wastewater on stream and estuary DO (Chapra, 2008:389).

Chapra (2008:348) presents a detailed explanation of the natural process that an environment in a stream or river experiences just below a point source of untreated sewage (refer to **Figure 3.1**): If the stream is unpolluted upstream of the point source, the DO concentration in the stream should be near oxygen saturation concentration. The untreated sewage introduced to the stream at the point source will elevate the levels of both dissolved and solid oxidizable organic matter, measured as Biochemical Oxygen Demand (BOD). The solid matter makes the water turbid, which means that light cannot penetrate the water and plant growth is suppressed as a result. Some of the organic solid matter settle downstream and form sludge beds that can emit noxious odours. The organic matter also provides food for heterotrophic organisms and decomposition of the organic matter takes place.

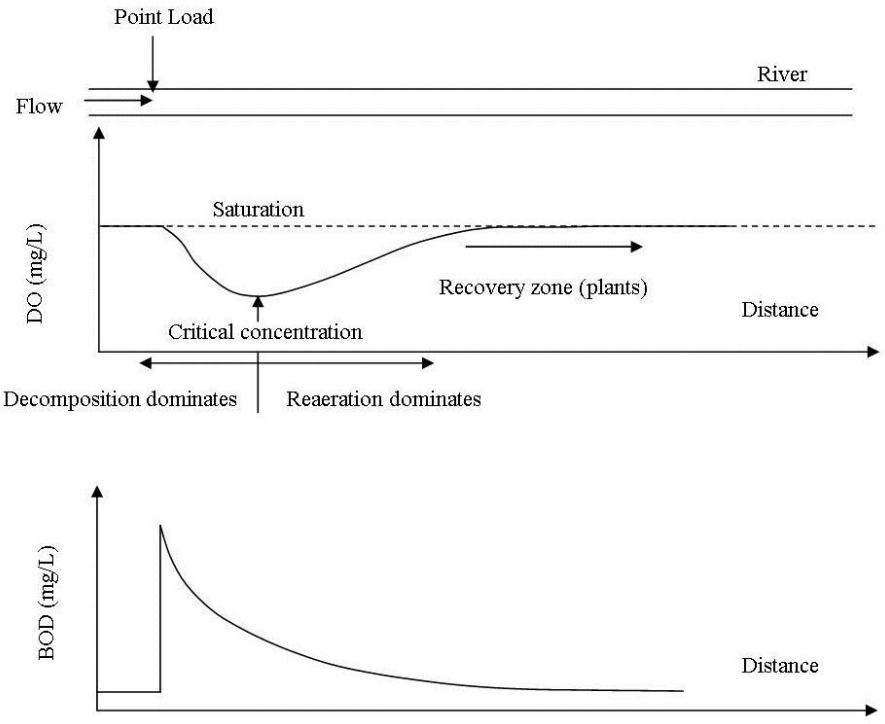

Figure 3.1 DO "sag" and decomposition of the oxidizable organic matter (BOD) that occurs below sewage discharges into streams (adapted from Chapra, 2008:349; 390).

The decomposition of the organic matter by the large populations of organisms causes a depletion of the DO in the stream. As the oxygen in the stream is depleted, atmospheric oxygen enters the stream to compensate for the oxygen deficit. At first the depletion of the oxygen is greater than the reaeration of the oxygen, but then a point is reached where the depletion and reaeration will be in balance. At this point the lowest level of DO concentration is reached and it is known as the critical concentration of DO. From this point the reaeration of the stream dominates the decomposition in the stream and the oxygen concentration in the stream starts to rise. The water will start to clear up and inorganic nutrients released during decomposition will stimulate the growth of plants.

The following equations are the classic Streeter-Phelps model for a stream with a single source of BOD and are the representation of the oxygen "sag" and BOD decomposition in **Figure 3.1**. They are steady-state solutions for the stream and are characterized by plug flow with constant hydrology and geometry (Chapra, 2008:390,391; Mihelcic & Zimmerman, 2010:315).

$$DO_{act} = DO_{sat} - \left[D_0 e^{\frac{-k_a}{U}x} + \frac{k_d L_0}{k_a - k_r}(e^{\frac{-k_r}{U}x} - e^{\frac{-k_a}{U}x})\right]$$

$$D = DO_{sat} - DO_{act}$$

$$L = L_0 e^{\frac{-k_r}{U}x}$$

$$k_r = k_d + k_s$$

DO_{act} = actual dissolved oxygen concentration in the stream (mg/L).

DO_{sat} = dissolved oxygen saturation concentration in the stream (mg/L).

D = dissolved oxygen deficit (mg/L).

D_0 = initial dissolved oxygen deficit (mg/L).

L = Biochemical Oxygen Demand (BOD) concentration (mg/L).

L_0= initial Biochemical Oxygen Demand (BOD) concentration (mg/L).

U = velocity (m/day).

x = position (point) in space along the river length (m).

k_a = reaeration rate (d^{-1}).

k_r = total removal rate of BOD (d^{-1}).

k_d= decomposition rate of BOD in the stream (d^{-1}).

k_s = settling removal rate of BOD in the stream (d^{-1}).

According to Melching et al. (1992:798) the water temperature of freshwater systems is the primary forcing function of the DO saturation concentration and the following equation describes its relation to temperature:

$$DO_{sat} = 14.652 - 0.41022T + 0.0079910T^2 - 0.000077774T^3$$

T = water temperature (˚C).

Melching et al. (1992:798) also mentions that the reaction rate coefficients k_a and k_d are also temperature dependent and need to be corrected for different temperatures as follows:

$$(k_a)_T = (k_a)_{20}(1.024)^{(T-20)}$$

$$(k_d)_T = (k_d)_{20}(1.024)^{(T-20)}$$

$(k_a)_T$ = reaeration rate (d^{-1}) at a specific temperature T (˚C).
$(k_d)_T$ = decomposition rate (d^{-1}) of BOD at a specific temperature T (˚C).
$(k_a)_{20}$ = reaeration rate (d^{-1}) at 20˚C.
$(k_d)_{20}$ = decomposition rate (d^{-1}) of BOD at 20˚C.

The critical travel time and critical oxygen deficit can be calculated with the following equations (Chapra, 2008:397):

$$t_c = \frac{1}{k_a - k_r} ln\left\{\frac{k_a}{k_r}\left[1 - \frac{D_0(k_a - k_r)}{k_d L_0}\right]\right\}$$

$$D_c = \frac{k_d L_0}{k_a}\left\{\frac{k_a}{k_r}\left[1 - \frac{D_0(k_a - k_r)}{k_d L_0}\right]\right\}^{\frac{-k_r}{k_a - k_r}}$$

t_c = critical travel time (days).
D_c = critical oxygen deficit (mg/L).

The equations that were used as models to be analysed in terms of uncertainty were the ones that calculate DO and D_c in a stream. Both DO and D_c are important water quality constituents and the former could be modelled all along the reach of the river while the latter lends itself very well as a point estimate and is very convenient for the plotting of CCDFs.

3.3. Water Quality Model and Uncertainty Analysis

This section explains the multistep process (**Figure 3.2**) that was followed to set up the water quality model and to analyse its uncertainty. It introduces various tasks performed in the process and is a modification and combination of the water quality modelling process introduced by Chapra (2008:319) and the uncertainty analysis protocol introduced by Summers et al. (1993:165).

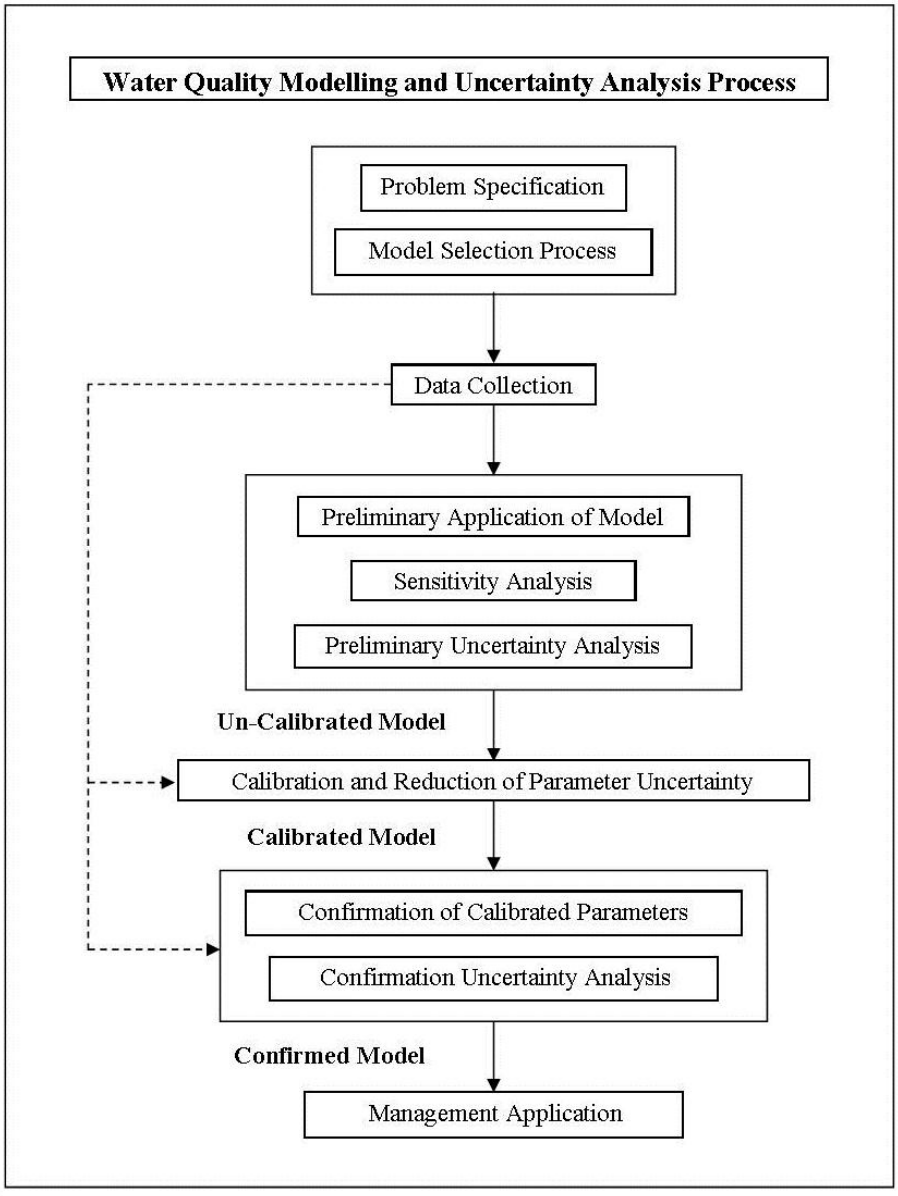

Figure 3.2 The water quality modelling process combined with uncertainty analysis.

Each of the tasks depicted in **Figure 3.2** is explained in depth under their own sub headings and has their own flow chart that summarizes the task. **Figure 3.2** serves as an overview or summary of all the tasks and how they fit together. To better understand each task, it is suggested to simultaneously follow the flow charts as the paragraphs in each subsection are read.

3.3.1. Problem Specification and Model Selection Process

The hypothetical environment that serves as the problem to be modelled is a river with a single point source of BOD. It is acceptable to approach the river's cross section as a trapezoid, with constant properties throughout the entire reach (**Figure 3.3**). The reach starts at the point source and continues downstream for 200km while meandering at a slope (S_0) of 0.001 and with a Manning's n of 0.05. The river's flow varies between the summer and winter months. The mean summer flow is 3m^3/s and the mean winter flow is 15m^3/s. The water temperature also varies between seasons. The mean temperature is 20˚C in summer and 10˚C in winter. The mean BOD concentration at the start of the reach is 60 mg/L in the summer with a standard deviation of 6 mg/L. During winter the mean BOD concentration is lower at 40mg/L but with a larger standard deviation of 8mg/L. The river is assumed to be unpolluted upstream of the point source. The river's properties and parameters are summarized in **Table 3.1**.

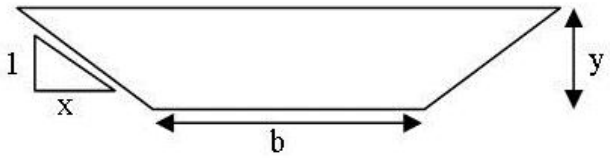

Figure 3.3 River cross-section.

Table 3.1 Summary of river properties and parameters.

Property/Parameter	Units	Mean Value	Standard Deviation
b	m	15	-
x	-	3	-
y	m	$f(Manning)$	-
S_0	m/m	0.001	-
Reach Length	km	200	-
Manning's n	-	0.05	-
Q_{summer}	m^3/s	3	0.3
Q_{winter}	m^3/s	15	1.5
T_{summer}	$°C$	20	1
T_{winter}	$°C$	10	1
$L_{0\ summer}$	mg/L	60	6
$L_{0\ winter}$	mg/L	40	8

The objective of the model is to assess the impact that the BOD point source has on the DO levels of the river. The DO is required to maintain a balanced community of organisms in the river. The water quality standard set for this system is a minimum limit of 4.5 mg/L DO throughout the entire reach. The introduction of BOD to the water body leads to the depletion of DO levels and if the concentration of DO drops below 4.5 mg/L, the reproduction by fish and macroinvertebrates will be impaired. If the depletion of DO gets severe, anaerobic conditions can develop that could lead to the

loss of biodiversity and poor aesthetics due to turbidity and odour problems (Mihelcic & Zimmerman, 2010:311). If the concentration of DO drops below 4.5mg/L, the water quality standard is said to have been violated.

The environmental system is expected to function exactly as the theory of the Streeter-Phelps model suggests. The horizontal space scale of the problem is in meters and the time scale is in days. The length of the river is segmented in increments of 1000m and the kinetic scale of the model is equal to the time scale of the model.

The model of the river must be subjected to an uncertainty analysis with the ultimate goal of reducing parameter uncertainty and quantifying model prediction uncertainty, thereby increasing confidence in the model predictions. The uncertainty analysis will help improve management decisions by presenting model predictions in association with probabilities of occurrence. This should aid in determining whether water quality standards are in danger of being violated.

Finally, once the model's parameter uncertainty has been reduced and its prediction uncertainty quantified, the model is to be applied in a management context and used in the determination of intervention strategies to manage the system in such a way that water quality standards are adhered to.

3.3.2. Data Collection

Due to the fact that the environment being modelled is a hypothetical one, real data for the system does not exist. Synthetic data for DO concentrations in the river had to be generated in order to calibrate and confirm the model. To avoid confusion, the reader must understand that the data generated for the system is treated as real data. In reality, this kind of data is collected from a river and not synthetically generated. The synthetic data was generated in a Monte Carlo fashion by using the Streeter-Phelps equation for DO:

$$DO_{act} = DO_{sat} - \left[D_0 e^{\frac{-k_a x}{U}} + \frac{k_d L_0}{k_a - k_r}\left(e^{\frac{-k_r x}{U}} - e^{\frac{-k_a x}{U}}\right)\right]$$

Means and standard deviations were assigned to all of the equations' parameters. The distributions assigned to the parameters were all normal distributions and these were randomly sampled to provide input for the DO equation. Two sets of data were generated. The first set corresponds to the river's summer flow and the second set corresponds to the river's winter flow. The parameter characteristics (means, standard deviations and distributions) for both summer and winter are provided in **Table 3.2** and **Table 3.3**.

Note that the initial DO concentration for the 200km reach is equal to the DO saturation concentration in the stream. This is because the stream is unpolluted upstream of the BOD point source.

$$DO_0 = DO_{sat}$$

Note also that the river's velocity (U) is a function of flow and geometric properties (Manning's n and S_0 etc.) and changes between summer and winter. The velocity is calculated with the Manning equation.

Table 3.2 Parameter characteristics for the generation of synthetic Summer DO data.

Parameter	Units	Mean	Standard Deviation	Coefficient of Variation	Probability Distribution
L_0	mg/L	60	6	0.1	Normal
DO_0	mg/L	River initially unpolluted. $DO_0 = DO_{sat}$.			
DO_{sat}	mg/L	$DO_{sat} = f(Temperature)$			
Q	m^3/s	3	0.3	0.1	Normal
T	$°C$	20	1	0.05	Normal
$(k_d)_{20}$	d^{-1}	0.9	0.12	0.1333	Normal
k_s	d^{-1}	0.3	0.03	0.1	Normal
$(k_a)_{20}$	d^{-1}	5	0.25	0.05	Normal

Table 3.3 Parameter characteristics for the generation of synthetic Winter DO data.

Parameter	Units	Mean	Standard Deviation	Coefficient of Variation	Probability Distribution
L_0	mg/L	40	8	0.2	Normal
DO_0	mg/L	River initially unpolluted. $DO_0 = DO_{sat}$.			
DO_{sat}	mg/L	$DO_{sat} = f(Temperature)$			
Q	m^3/s	15	1.5	0.1	Normal
T	$°C$	10	1	0.1	Normal
$(k_d)_{20}$	d^{-1}	0.9	0.12	0.1333	Normal
k_s	d^{-1}	0.3	0.03	0.1	Normal
$(k_a)_{20}$	d^{-1}	5	0.25	0.05	Normal

Temperature serves as the primary forcing function in the calculation of DO_{sat} (Melching et al., 1992:798):

$$DO_{sat} = 14.652 - 0.41022T + 0.0079910T^2 - 0.000077774T^3$$

Because the initial DO concentration is equal to the DO saturation concentration, the initial dissolved oxygen deficit (D_0) is equal to zero:

$$D_0 = DO_{sat} - DO_0 = 0$$

The first set of data is used in the calibration of the model and the second set is used in the confirmation of the model. For each set, the reach was segmented in increments of 5000m and 10

values for DO were calculated at each of the increments. The increments of 5000m are analogous to sampling stations every 5km along the reach and the 10 values for DO are analogous to 10 years of data for the river. **Figure 3.4** and **Figure 3.5** are graphical representations of the 'sampled' values for DO that served as the real data in this model.

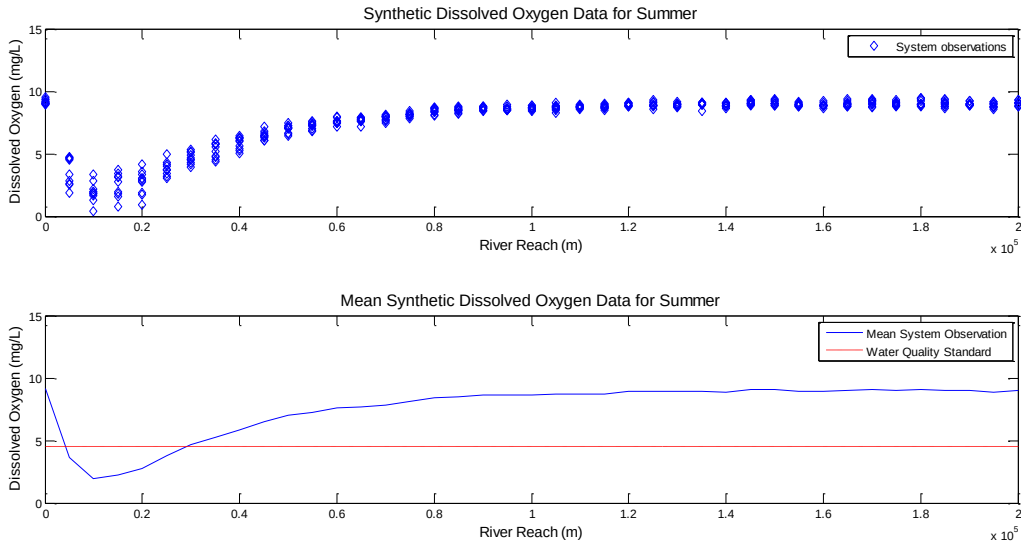

Figure 3.4 Synthetic DO summer data that serves as 'real summer data collected from the river'.

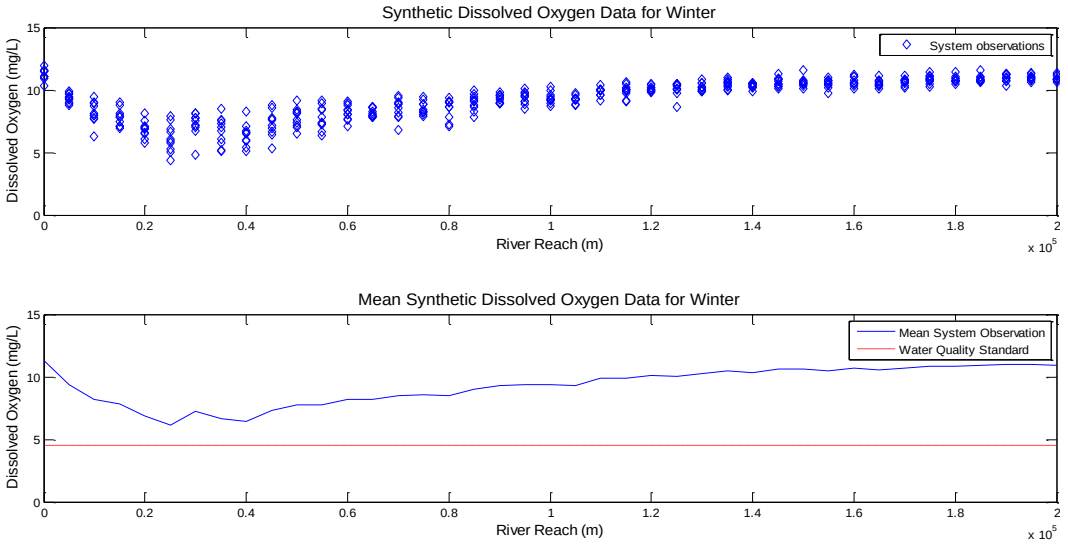

Figure 3.5 Synthetic DO winter data that serves as 'real winter data collected from the river'.

Notice in **Figure 3.4** and **Figure 3.5** how the DO saturation changes from being below 10 mg/L in the summer to being above 10 mg/L in the winter. This is because the temperature of the river serves as the forcing function in the calculation of DO_{sat}. Temperature also has an effect on the kinetic

coefficients k_d and k_a. The DO concentration in the winter is also generally higher than in the summer and it changes much more gradually along the reach. Whether the increased flow during winter has an effect on the DO levels of the river will have to be tested in the management application of the model. This could give some insight in how to manage the system later on. **Figure 3.4** and **Figure 3.5** also show that the water quality standard of a minimum 4.5 mg/L DO was violated on various occasions, especially in summer.

The use of synthetic data in this study might not seem completely objective, but it does have some advantages. Using synthetic data in the calibration of the model allowed the calibrated parameters to be compared with the 'true' parameter values used to generate the synthetic data. **Table 3.2** and **Table 3.3** contain the true values of the system's parameters. Thus, once the kinetic parameters were calibrated, one could confirm that calibration was in fact correct and that the parameter uncertainty was realistically reduced. This means that one is able to determine whether the whole exercise of uncertainty analysis worked as the theory explained it would. If it did not work under controlled conditions, there would have been no way that it could have worked in the real world with a real environmental system. In the real world, data would obviously have to be obtained from the system. It is important to remind the reader now that the whole purpose of this exercise was to investigate MCS as a method of uncertainty analysis and a very effective way of determining how MCS worked was by testing it under controlled conditions.

3.3.3. Preliminary Application of the Model and Sensitivity Analysis

The preliminary application of the model consists of a single simulation of the system's model. Data used in this step is often lacking or very uncertain so the application is only used to identify theoretical gaps in the model (Chapra, 2008:322).

In this case an application of the DO equation was made. Only mean values for the parameters were used and the graph of the model output only had to resemble the DO data 'collected' from the river. **Table 3.4** gives the mean values assigned to the model parameters. The mean values of the summer parameters were used in this model simulation. Note how L_0, Q and T correspond to the summer data in **Table 3.2**, but the kinetic coefficients are assigned different values. This is because the model is un-calibrated at this stage and there is no way that it could have been known what the values of k_d, k_s and k_a are. At this stage in the modelling process values for these parameters are only assumed or read from literature, or even from manuals provided with the modelling software. A lot of model parameter uncertainty is generally associated with kinetic coefficients.

Table 3.4 Mean parameter values used as input in the preliminary application of the model.

Parameter	L_0	Q	T	k_d	k_s	k_a
Mean	60	3	20	0.7	0.5	7

The preliminary application often goes hand in hand with a sensitivity analysis. A sensitivity analysis is useful for identifying which model parameters affect model output the most. It consists of varying each parameter by a set percentage and observing how the model predictions vary (Chapra, 2008:322).

In this case the D_c equation was tested for being sensitive to the kinetic parameters k_d, k_s and k_a. The same parameter values as in the preliminary application were assigned to the model in the sensitivity analysis and the base prediction was calculated. Then each of the kinetic parameters was varied in turn by increasing and decreasing their values by 20% and the change in the model prediction was calculated.

The kinetic parameters were then ranked accordingly by using the following formula from Melching et al. (1996:110):

$$SN_{j,i} = (\Delta C_j / C_{j,0}) / (\Delta x_i / x_{i,0})$$

$SN_{j,i}$ = normalized sensitivity coefficient.

ΔC_j = change in prediction j as a result of change Δx_i in parameter i with all other parameters kept constant at their means.

$C_{j,0}$ = base prediction j when all parameters are kept constant at their means.

$x_{i,0}$ = original value of parameter i, which in this case is equal to the parameter mean.

Δx_i = change in parameter i.

3.3.4. Preliminary Uncertainty Analysis

In most cases, the literature states that the uncertainty analysis is conducted after the calibration of the model. Why then is an uncertainty analysis conducted before model calibration in this case? WQMs are generally much more complex than the Streeter-Phelps model used in this study. They have hundreds of parameters and many of these parameters will need calibration, field sampling and laboratory experiments. This will take a lot of time and money and projects are often on a tight schedule and budget. It is usually during the preliminary model application that the sensitivity analysis is conducted to see which parameters are the most important to a model. It thus made sense to test the effect of a preliminary uncertainty analysis on the rest of a modelling strategy, especially the effect it might have on the calibration phase.

The preliminary uncertainty analysis takes stock of the models situation concerning uncertainty before any calibrations or additional sampling. It can instil a modeller's satisfaction with his preliminary understanding of the parameters' uncertainty. This means that the preliminary uncertainty analysis will help in making decisions with regards to model calibration and parameter estimation experiments early on in the modelling process. For example, it could determine which coefficients are really worth calibrating and which parameters are worth spending money on to determine experimentally. It can also indicate which parameters' uncertainty are considered acceptable and can be ignored in the calibration and physical experiments. This could save a lot of money and time and the general feeling was that this could be much more effective than a sensitivity analysis because the sensitivity analysis does not take stock of the model's situation concerning uncertainty. The preliminary uncertainty analysis gives a feeling of what the modeller knows thus far, and how much more needs to be learnt before decisions can be made with the model. The preliminary uncertainty analysis of the model consists of the steps summarized in **Figure 3.6**. Each of these steps will now be explained and summarized by their own flow charts.

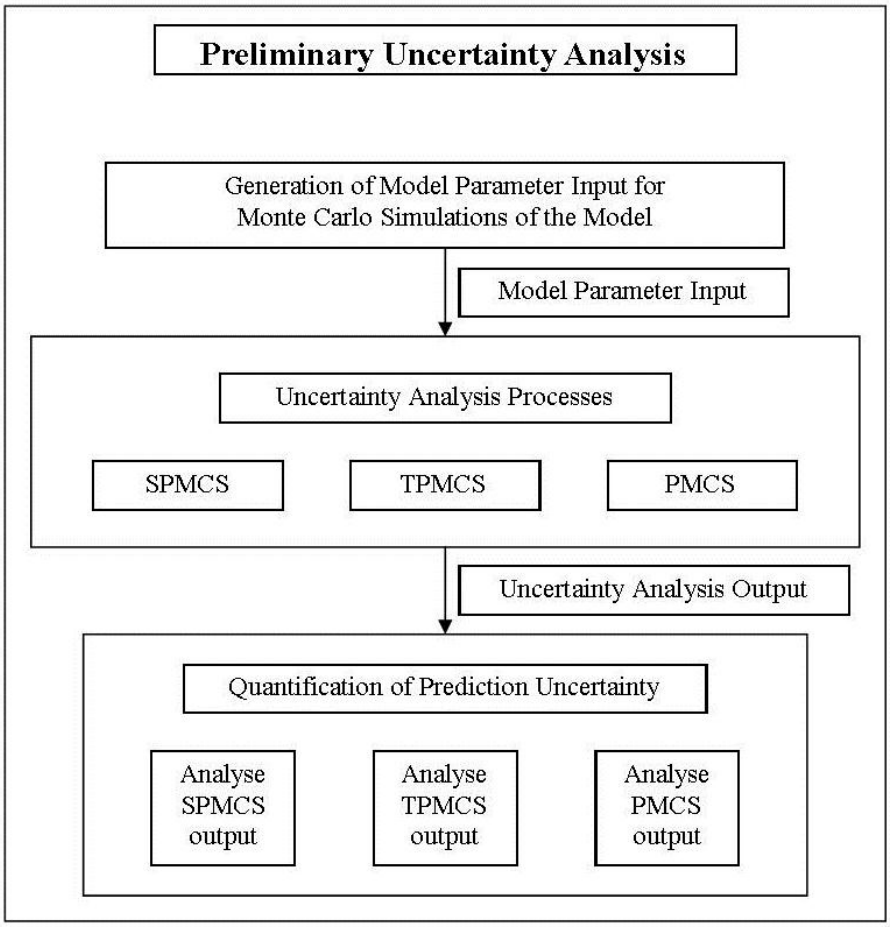

Figure 3.6 Preliminary Uncertainty Analysis flow chart.

Generation of Model Parameter Input

As seen in **Figure 3.6**, before any MCS can be conducted, Model Parameter Input values have to be generated first and **Figure 3.7** summarizes the procedure:

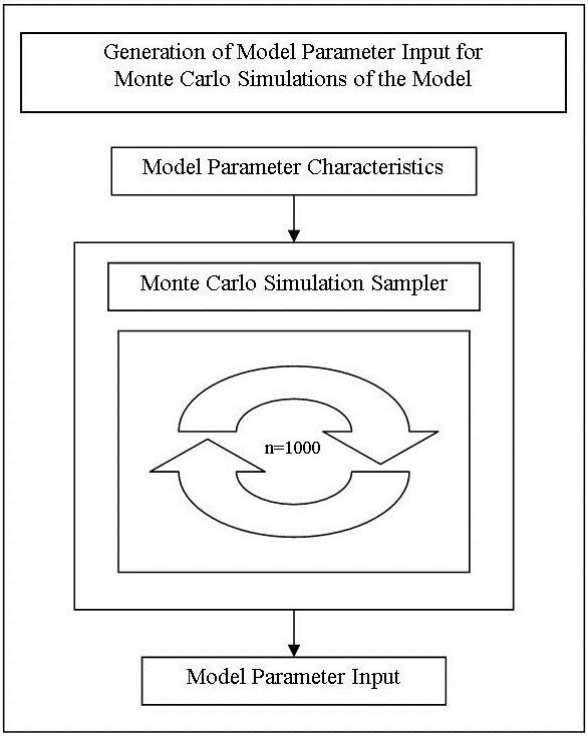

Figure 3.7 Generation of Model Parameter Input for the purpose of conducting Monte Carlo Simulations.

The model parameters were assigned the system's summer parameter characteristics. The parameters were all assumed to be normally distributed. In addition to that, the key parameters' relationship to each other was also defined in a covariance matrix; though the relationship between them was first considered to be non-existent (zero). **Table 3.5** and **Table 3.6** contain the model parameter characteristics and covariance matrix used in the generation of parameter sets for the preliminary uncertainty analysis. Note how the characteristics for the kinetic coefficients are different from their true values in **Table 3.2**. As explained in section 3.3.3, the model is still un-calibrated and significant uncertainty is associated with the kinetic coefficients.

In **Table 3.5** the model parameters are also divided into the two types of uncertainty: **aleatory and epistemic**. This division is an important step in the TPMCS. Note also the relative uncertainty of each model parameter that is defined by the **Coefficient of Variation (COV)**. For the preliminary uncertainty analysis, the epistemic parameters are considered to be highly uncertain.

Table 3.5 Parameter characteristics for the prior distributions used in the generation of model parameter input for the preliminary uncertainty analysis.

Parameter	Units	Mean	Standard Deviation	Coefficient of Variation	Distribution	Type of Uncertainty
L_0	mg/L	60	6	0.1	Normal	Aleatory
Q	m^3/s	3	0.3	0.1	Normal	Aleatory
T	$°C$	20	1	0.05	Normal	Aleatory
k_d	d^{-1}	0.7	0.4	0.57	Normal	Epistemic
k_s	d^{-1}	0.5	0.3	0.6	Normal	Epistemic
k_a	d^{-1}	7	1.5	0.21	Normal	Epistemic

Table 3.6 Covariance matrix that defines the relationship between the key parameters.

	k_d	k_s	k_a
k_d	0.16	0	0
k_s	0	0.09	0
k_a	0	0	2.25

Each of the parameter distributions was randomly sampled 1000 times to create 1000 model parameter sets. Each parameter set contained one value for each of the six input parameters. The number of model runs required in each type of uncertainty analysis determines the number of parameter sets that are generated. To illustrate the use of MCS in this study, 1000 model runs were thought to be sufficient to produce accurate results while also keeping the cost of calculations to a minimum.

All 1000 parameter sets will from now on be collectively known as the Model Parameter Input. The Model Parameter Input was then passed on to each of the three uncertainty analysis processes where the model was subjected to MCS.

Single Phase Monte Carlo Simulation

The first uncertainty analysis process was the **Single Phase Monte Carlo Simulation (SPMCS)** summarized in **Figure 3.8**. This simulation consists of a single MCS where in both aleatory parameter uncertainty and epistemic parameter uncertainty are considered together. It gives an estimate of the overall quality of the model's predictions by quantifying model prediction uncertainty. Both the DO - and D_c equations were used as models in the SPMCS. Each of the equations was solved 1000 times, each solution corresponding to a specific parameter set in the Model Parameter Input.

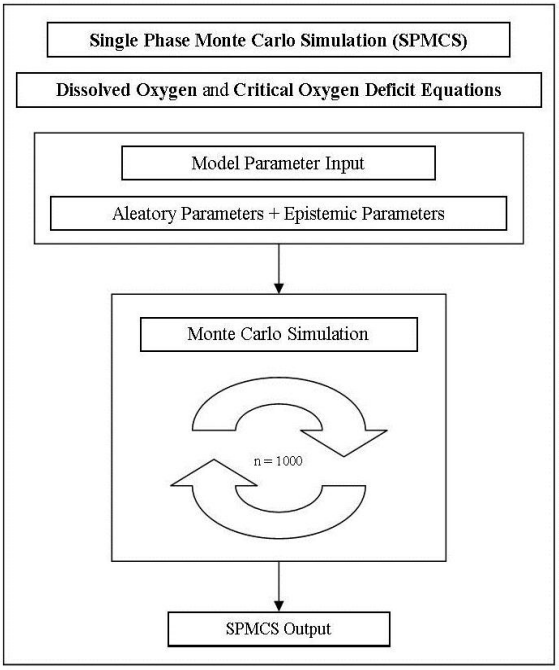

Figure 3.8 The Single Phase Monte Carlo Simulation (SPMCS).

The SPMCS' output consisted of two sets of 1000 model predictions each. The first set consisted of model predictions for DO levels along the reach of the river and the second set consisted of point estimates for the reach's D_c concentration.

The 1000 DO predictions were used to calculate the mean prediction of DO and in addition to that, the 90% confidence bands were also calculated and plotted along with the mean for the entire reach. These results were graphically compared with the summer data for DO. By comparing the model's mean prediction and confidence bands with the system observations, one could get an indication of the accuracy and confidence with which the model predicts.

The SPMCS' output for D_c was used to draw a single CCDF. The mean and standard deviation were also calculated and compared with the mean and standard deviation of the system observations for D_c. The system observations for D_c were calculated by subtracting the DO observations from the expected DO saturation concentration and identifying 10 maximum values for D_c. The expected DO saturation was calculated by the following equation with T = 20˚C (Melching et al., 1992:798):

$$DO_{sat} = 14.652 - 0.41022T + 0.0079910T^2 - 0.000077774T^3$$

Keep in mind that the summer characteristics were used in the preliminary uncertainty analysis and the results had to be compared with summer observations, that is why the temperature in the DO_{sat} equation was set to 20˚C.

The comparison between the model predictions and system observations continued further with the calculation of the model bias and RMSE. The model bias gave an estimate of the accuracy with

which the model predicted D_c and the RMSE gave an indication to the overall quality of the model's predictions. The CCDF of the predictions was also graphically compared to the CCDF of the system observations. One of the major attributes of the CCDF is the fact that it defines the relation between the model's predictions and their probability of occurrence.

Two Phase Monte Carlo Simulation

The second uncertainty analysis process is the **Two Phase Monte Carlo Simulation (TPMCS)** and is summarized in **Figure 3.9**. This type of analysis is designed to separate the two types of uncertainty in the model's predictions and consists of one MCS nested within another. The D_c equation is used as the model in the TPMCS because it gives a point estimate of the critical oxygen deficit and is convenient for the compilation of CCDFs.

In this analysis the Model Parameter Input was divided into aleatory and epistemic uncertain parameters. For the first set of epistemic model parameters a full MCS of the model is conducted using all the sets of aleatory parameters, while keeping the epistemic parameters constant at the first epistemic set's values. Once all the aleatory sets of parameters have been used as model input, the next set of epistemic model parameters is used and the full aleatory simulation is repeated. This process continues until all the epistemic sets of model parameters have been used.

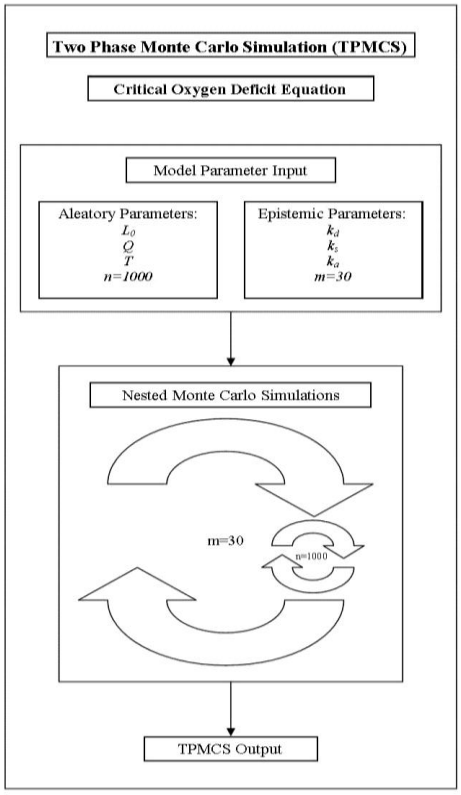

Figure 3.9 The Two Phase Monte Carlo Simulation (TPMCS).

For illustrative purposes this analysis used only 30 sets of epistemic parameters but all 1000 sets of aleatory parameters were used. The nesting of 1000 aleatory model runs within 30 epistemic runs resulted in an uncertainty analysis that completed a total of 30 000 model runs. This gives an idea of how costly a TPMCS can be.

The output from this TPMCS consisted of 30 sets of 1000 predictions each for D_c. The analysis of the TPMCS output for uncertainty consisted of calculating a normal distributed CCDF for each set of 1000 predictions and displaying all of them on a single graph. This means that 30 s-curves would have been drawn on a single set of axes. The distribution of each CCDF showed the effects of aleatory uncertainty on the model predictions while the collective distribution of all the CCDFs together showed the effects of epistemic uncertainty on the model predictions.

The model predictions' mean, standard deviation and minimum and maximum values were also calculated for the 5%, 50% and 95% probabilities of exceedence. These statistics should give an idea of how the predictions vary due to epistemic uncertainty and illustrate the epistemic uncertainty's level of dominance over the aleatory uncertainty in the model's predictions.

Parameter Monte Carlo Simulation

The third uncertainty analysis process is the **Parameter Monte Carlo Simulation (PMCS)** and is summarized in **Figure 3.10**. This method is described by Vose (2008:54). This simulation is designed to determine the contribution of each key parameter's uncertainty to the model's prediction uncertainty and is similar to a conventional sensitivity analysis. Both the DO-and the D_c equations were used as models in this analysis.

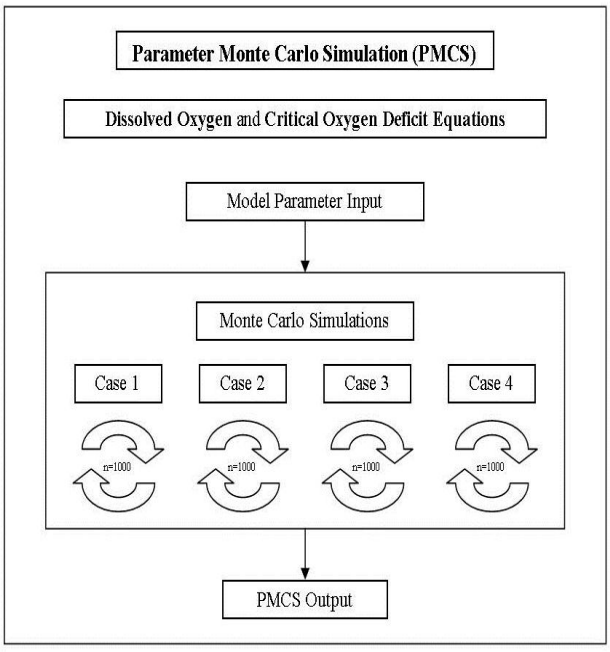

Figure 3.10 The Parameter Monte Carlo Simulation (PMCS).

This analysis consisted of four MCSs. Each of the four MCSs investigated a different case of model parameter uncertainty. The four different cases are presented in **Table 3.7**:

Table 3.7 Cases of model parameter uncertainty analyses.

	Aleatory Parameters considered uncertain	**Epistemic (key) Parameters kept constant at mean**	**Epistemic (key) Parameter considered uncertain**
Case 1	L_0 Q T	k_d k_s k_a	none
Case 2	L_0 Q T	k_s k_a	k_d
Case 3	L_0 Q T	k_d k_a	k_s
Case 4	L_0 Q T	k_d k_s	k_a

The cases are different combinations of Model Parameter Input considered uncertain or constant. A key parameter's contribution to prediction uncertainty is evaluated by using its random sampled input, along with the random sampled input of the aleatory parameters, while the other key parameters are kept constant at their means during the MCS. In Case 1 all the key parameters are held constant at their means and only the aleatory parameters' randomly sampled input is used.

The quantification of the key parameters' contributions to prediction uncertainty consisted of plotting and analysing the PMCS' results for both the DO equation and the D_c equation. The PMCS output for DO is four sets of 1000 predictions each for the entire reach. Each of the four sets of predictions was as a result of one of the four cases in **Table 3.7**. The mean prediction and standard deviation was then calculated from each set of 1000 predictions and plotted along the reach. The anticipated result of the plot was a single mean prediction with associate error bars for the standard deviations. The error bars is supposed to represent the contribution of uncertainty made by the key parameter to prediction uncertainty. The 2nd, 3rd and 4th cases could be graphically compared to the 1st case to determine the key parameters' contributions to prediction uncertainty. The 1st case considered all the key parameters at their means and its result is analogous to the base prediction of a conventional sensitivity analysis. This explanation becomes clear once the results are discussed.

The PMCS output for D_c is also four sets of 1000 point estimates each. Each set of 1000 predictions was as a result of one of the four cases in **Table 3.7**. Being sets of 1000 point estimates, each of the cases lent themselves very well for the calculation of CCDFs. The means and standard deviations of each case's results were also calculated to quantify the uncertainty contributed by the key parameters. Three graphs were plotted, one for each of the 2nd, 3rd and 4th cases' results. In each of the graphs, the results from the 1st case, which served as the base prediction, was compared to the other three cases' results. This explanation will also become clear in the discussion of the results.

3.3.5. Calibration and Reduction of Parameter Uncertainty

Once a model's preliminary prediction uncertainty has been quantified and the relevant model parameters contributing the most to the prediction uncertainty have been identified, ways to reduce uncertainty have to be investigated and applied. Recall that model prediction uncertainty is reduced by the reduction in model parameter uncertainty and that model parameter uncertainty can be reduced by a number of methods which includes calibration, expert elicitation, additional measurements of parameters and improved scientific experiments. This section explains how the calibration of the model's key parameters is performed with a Monte Carlo based method.

Chapra (2008:323) explains that the kinetic parameters of a model should be separated from the rest of the model parameters because they are the parameters in a model to be calibrated. In the case of Streeter-Phelps, the kinetic parameters are the primary source of epistemic uncertainty. Thus, for the purpose of this study it was only appropriate that the calibration of the kinetic parameters (k_d, k_s and k_a) should also serve as the reduction of the model's epistemic uncertainty. As the environment being modelled is a hypothetical one, it also seemed appropriate to use calibration as the method of reducing uncertainty because the other methods would not be objective in this case. In addition to that, MCS could also be tested as a method of model calibration.

According to Chapra (2008:322) the goal of model calibration is to fit the model's predictions to a data set. This is done by varying the model's kinetic parameters until an optimal agreement between model predictions and the data is observed (usually by some "best fit" criteria). The other model parameters (initial conditions, boundary conditions and physics) can be measured with sufficient precision and are kept constant at their nominal values (means) while the kinetic parameters are varied (Summers et al., 1993:168).

An automated technique of calibration was used in this case by using a Monte Carlo method adapted from Summers et al. (1993:167) and is summarized in **Figure 3.11**. The DO equation is used as model for the calibration of the kinetic parameters and observed data for DO was obtained during the 'data collection'.

One thousand model predictions were calculated by a MCS of the model using a thousand parameter sets that were generated as Model Parameter Input by using the parameter distributions summarized in **Table 3.8**. The model runs in this MCS are known as Monte Carlo calibration runs. The initial conditions and forcing functions were kept constant at their means while the kinetic parameters were assigned uniform distributions covering ranges of possible values. The values for the initial conditions and forcing functions correspond to the summer data. Note that the ranges of possible values for the kinetic parameters are not the same characteristics assumed for the kinetic coefficients in the preliminary uncertainty analysis. These ranges in **Table 3.8** are just wide sample spaces for the

coefficients and must be wide enough to contain the true values of the system otherwise the calibration will not work. The kinetic coefficients are also assigned uniform distributions to ensure that the sample spaces are uniformly sampled during the calibration and all values in the sample spaces are equally likely to get sampled for calibration purposes.

The model predictions produced by the Monte Carlo calibration runs were then compared to the summer observed data and ranked in terms of criteria for determining the best model fit to observed data. The criteria used for determining the best fit was based on the minimization of the sum of squares of the residuals:

$$S_r = \sum_{i=1}^{n} (c_{p,i} - c_{m,i})^2$$

S_r = sum of squares of the residuals

$c_{p,i} = i$th model prediction of concentration.

$c_{m,i} = i$th measured concentration.

This term provides a value that should be a minimum when the model predictions and the system's data are in agreement (Chapra, 2008:335).

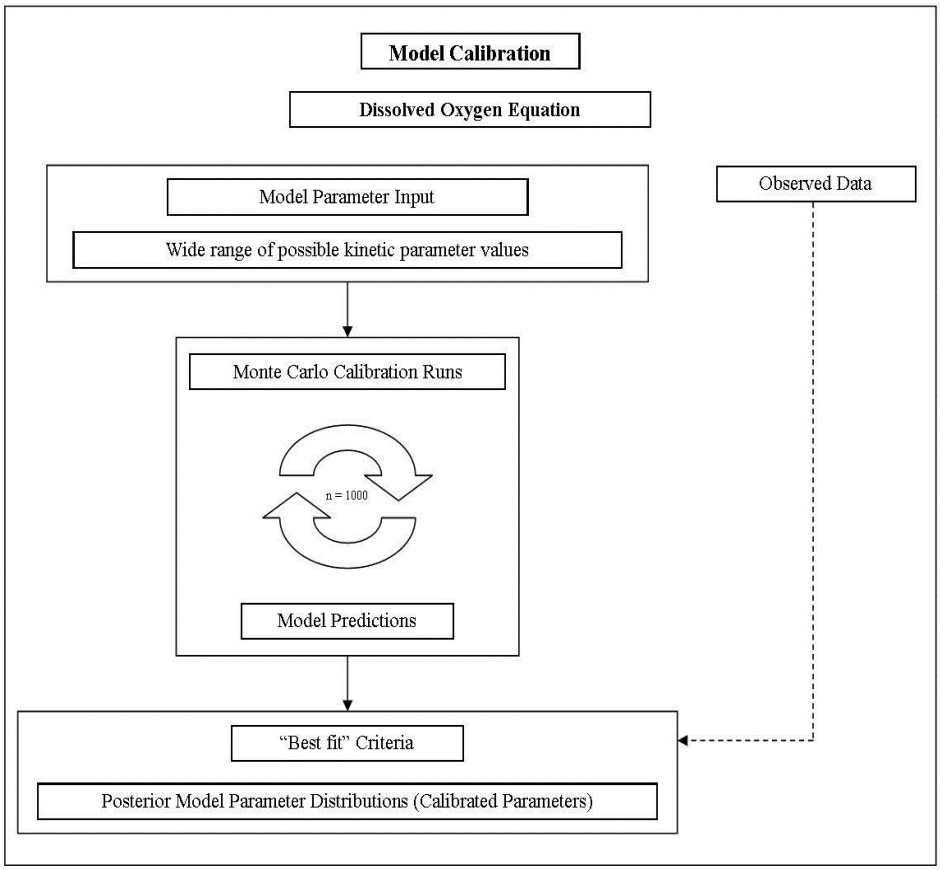

Figure 3.11 Model calibration of the model's kinetic parameters using a MCS of the DO equation.

Table 3.8 Model parameter characteristics assigned to the distributions for the Monte Carlo calibration of the model.

Parameter	Units	Mean	Standard Deviation	Distribution	Range
L_0	mg/L	60	-	-	-
Q	m^3/s	3	-	-	-
T	$°C$	20	-	-	-
k_d	d^{-1}	-	-	Uniform	[0.5 , 1.2]
k_s	d^{-1}	-	-	Uniform	[0.1 , 0.5]
k_a	d^{-1}	-	-	Uniform	[3 , 7]

The ranked model predictions were then mapped back to the parameter sets that produced them and sorted. From all the parameter sets used to produce model predictions in the calibration runs, the top 5% responsible for the best model fit to the observed data were picked for further statistical analysis. From these top parameter sets a parameter space for the kinetic parameters could be determined that would result in acceptable model predictions.

This parameter space was defined by a vector of the improved mean values for the kinetic parameters as well as a covariance matrix that would contain information concerning the interrelationships among the kinetic parameters (if there were any such relationships). The improved parameter characteristics are also known as the posterior distributions of the model parameters and reflect the reduced uncertainty of the model parameters.

3.3.6. Confirmation of Calibrated Parameters

Once the kinetic parameters were calibrated a single model run was conducted with the improved parameters and the initial conditions and forcing functions corresponding to the winter data. The model prediction was then compared to the set of winter data to confirm that the model has been calibrated. This step is exactly the same as the preliminary application of the model except for the fact that improved kinetic coefficients are used, the forcing functions and initial conditions are changed, and a second set of system observations is used to confirm the model (winter data). This is exactly as Chapra (2008:324) explains the confirmation of a calibrated model; a calibrated model should be run for a different data set, with the physical parameters and forcing functions changed to reflect the new conditions, while the kinetic coefficients are kept fixed at their calibrated values. The parameter input is summarized in **Table 3.9**.

Table 3.9 Mean parameter values and calibrated kinetic parameters for the confirmation of the model.

Parameter	L_0	Q	T	k_d	k_s	k_a
Mean	40	15	10	Calibrated	Calibrated	Calibrated

3.3.7. Confirmation Uncertainty Analysis

The confirmation uncertainty analysis is performed to confirm that the quality of the model's predictions has improved and that parameter uncertainty has been reduced. This analysis should indicate whether additional attempts should be made at reducing parameter uncertainty. This step follows the same process as the preliminary uncertainty analysis and is similar to the model's confirmation run in the sense that the winter parameter characteristics and calibrated kinetic parameters were used to generate the Model Parameter Input. The results were also compared with the system's winter data (meaning a second set of data). **Table 3.10** summarizes the characteristics of the posterior parameter distributions used in the confirmation uncertainty analysis. Note that although the distributions in the calibration step were uniformly distributed, the posterior distributions were defined with normal distributions, just as in the prior distributions in the preliminary uncertainty analysis. Note also that the epistemic parameters are supposed to have been reduced by this stage because they were calibrated. **Table 3.11** is the covariance matrix that describes the interrelationships of the kinetic coefficients. It is derived, during calibration, from the parameter sets that produced the best model calibration runs in terms of the minimum criteria for model fit. The calibration's results are discussed in Chapter 4.

Table 3.10 Parameter characteristics for the posterior distributions used in the generation of Model Parameter Input for the confirmation uncertainty analysis.

Parameter	Units	Mean	Standard Deviation	Coefficient of Variation	Distribution	Type of uncertainty
L_0	mg/L	40	8	0.2	Normal	Aleatory
Q	m^3/s	15	1.5	0.1	Normal	Aleatory
T	$°C$	10	1	0.1	Normal	Aleatory
k_d	d^{-1}	Calibrated*	Calibrated*	Calibrated*	Normal	(Reduced) Epistemic
k_s	d^{-1}	Calibrated*	Calibrated*	Calibrated*	Normal	(Reduced) Epistemic
k_a	d^{-1}	Calibrated*	Calibrated*	Calibrated*	Normal	(Reduced) Epistemic

Table 3.11 Covariance matrix that defines the calibrated relationship between the key parameters.

	k_d	k_s	k_a
k_d	Calibrated*	Calibrated*	Calibrated*
k_s	Calibrated*	Calibrated*	Calibrated*
k_a	Calibrated*	Calibrated*	Calibrated*

*To be determined by calibration.

3.3.8. Management Application

Once the model has been confirmed, and its uncertainty reduced, it can be used in management applications. Chapra (2008:324) mentions that many modelling studies result in remedial actions such as the building or upgrading of wastewater treatment plants. However, environmental modifications such as aeration or dredging could also be implemented. The effects that these actions might have on the environment can then be evaluated by modifying the model parameters and forcing functions, and evaluating the results.

An example of a management application to the hypothetical environment will be explained in Chapter 4.

4. Results and Discussion

4.1. Introduction

Chapter 4 reveals all the results from the various steps in the modelling protocol and discusses the knowledge that these results might disclose. The entire chapter is structured in more or less the same way as Chapter 3 (Methodology).

The rest of this chapter starts at the results of the preliminary model application (section 4.2). It continues by discussing the sensitivity analysis' results (section 4.3) and the results from the preliminary uncertainty analysis (section 4.4). The results from the model calibration and reduction of parameter uncertainty are then displayed (section 4.5). The results from the model confirmation (section 4.6) and confirmatory uncertainty analysis (section 4.7) then prove that the model was successfully calibrated and that the reduction in parameter uncertainty did improve on the certainty with which the model predicts.

Finally the improved model is used in the context of managing the hypothetical environment by calculating a TMDL that would improve the ecosystem's water quality (section 4.8). This subsection discusses how the quantification of uncertainty can be used in order to determine a Margin of Safety (MOS) that is based on scientific information rather than just assigning a MOS arbitrarily.

4.2. Results of the Preliminary Model Application

The preliminary application of the model consisted of a single simulation of the DO equation using the mean values from the system's summer characteristics. The result was compared with the system's summer data in **Figure 4.1**. As explained earlier, the system observations were synthetic data, generated with the same model equations as the model equations used to produce the model prediction. It should come as no surprise then, that the shape of the model prediction in **Figure 4.1** is the same as the system observations. This discussion of the preliminary model run's result seems pointless, but it is included to clarify the difference between the model prediction and the synthetic data.

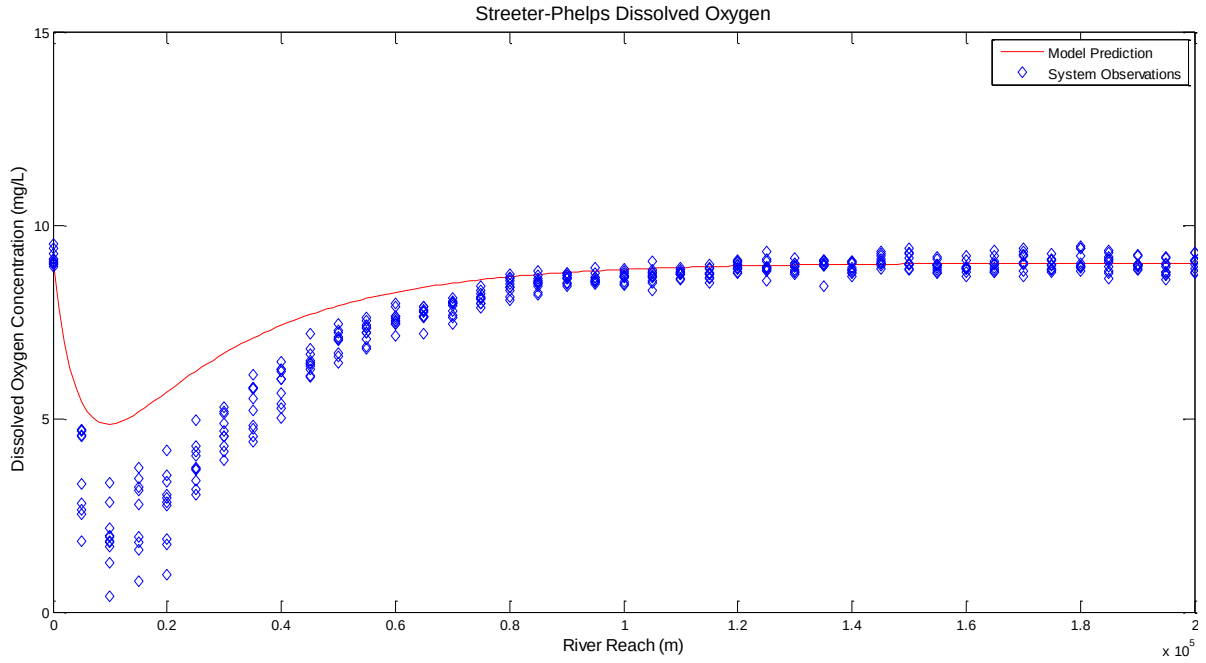

Figure 4.1 Comparison of the results from the preliminary application of the model with the system observations.

Recall that the system's summer observations were generated by using the system's 'true' parameter values for the summer months. This model prediction on the other hand was calculated by using the prior distributions' mean values. The parameter differences are summarized in **Table 4.1**.

Table 4.1 Comparison of true parameter means and prior parameter means.

Parameter	L_0	Q	T	k_d	k_s	k_a
True Mean	60	3	20	0.9	0.3	5
Prior Mean	60	3	20	0.7	0.5	7
%Difference	0	0	0	-22.22	66.67	40

From **Figure 4.1** there is an obvious error visible between the preliminary model prediction and the system observations. This error is due to the difference between the 'true' kinetic parameters and the prior values assumed for the kinetic parameters. Remember that the model still requires calibration at this stage.

Probably the most important thing to make sure of when assessing the results of a preliminary model application, is the general shape of the prediction. This should quickly identify any theoretical gaps in the model. From **Figure 4.1**, the model seems to be predicting the system's behavior very well, although with some error and it can be concluded that theoretical gaps are non-existent in this case.

In reality this is almost completely impossible when modelling real systems, because the complexity of nature is too great to model with 100% accuracy. All models are simplifications of complex systems and have a certain degree of model structure uncertainty. In this hypothetical case, however, it is assumed that the model can predict the system's behavior as precise as the behavior itself. The focus of the study fell on model parameter uncertainty and the quantification of model prediction uncertainty. Differentiating between the effects of parameter uncertainty and structural uncertainty on the prediction uncertainty is very difficult. Structural uncertainty is thus considered to be non-existent in this report.

4.3. Results of the Sensitivity Analysis

Table 4.2 and **Table 4.3** show the results from the sensitivity analysis on the D_c equation. Only the kinetic parameters were tested for sensitivity because they were assumed to be the only epistemic parameters and the sensitivity results will be compared with the uncertainty analysis results. A sensitivity analysis of the aleatory parameters would have been beneficial for the determination of intervention plans because it would show which parameters' alteration would be the most effective at improving the system's water quality.

Table 4.2 Sensitivity Analysis results from a 20% decrease in the kinetic parameter values.

	$x_{i,0}$	Δx_i	$C_{j,0}$	ΔC_j	$SN_{j,i}$
k_d	0.7	-0.14	4.1657	-0.7384	0.8863
k_s	0.5	-0.1	4.1657	0.0835	-0.1003
k_a	7	-1.4	4.1657	0.7616	-0.9141

Table 4.3 Sensitivity Analysis results from a 20% increase in the kinetic parameter values.

	$x_{i,0}$	Δx_i	$C_{j,0}$	ΔC_j	$SN_{j,i}$
k_d	0.7	0.14	4.1657	0.7023	0.8430
k_s	0.5	0.1	4.1657	-0.0788	-0.0945
k_a	7	1.4	4.1657	-0.5506	-0.6609

Table 4.2 shows that a decrease in k_d will result in a decrease in the D_c prediction, while a decrease in k_s and k_a results in an increase in the D_c predictions. In **Table 4.3** the opposite is true for an increase in the parameter values. The system behavior that is identified in this case is that the $D_c$will increase if the decay rate is increased. It will also increase if the reaeration and settling is decreased. This makes sense because when less re-aeration takes place in the river, the DO concentration is less likely to recover; hence the greater D_c. The same holds true for k_s in this case; as less BOD settles out, the demand for DO in the river will increase; hence the greater D_c.

What is noted in the sensitivity analysis is the inverse relationship between k_s and k_a , and the model predictions. This inverse relationship is identified by the negative signs in front of the normalized sensitivity coefficients in **Table 4.2** and **Table 4.3**. It is very interesting to note that for an increase in parameter values, model predictions are more sensitive to k_d than k_a, but when model parameter values are decreased, the model predictions are more sensitive to k_a than k_d, although only slightly.

The sensitivity analysis is very useful for determining system behavior. It lacks, however, in the fact that it does not propagate parameter uncertainty, but only some arbitrary induced parameter error.

4.4. Results of the Preliminary Uncertainty Analysis

The preliminary uncertainty analysis is incorporated into the multistep modelling process as a major modelling activity. This analysis is conducted early in the modelling process to gain an early understanding of the types and sources of uncertainty that affects the model the most. The results of this analysis will determine many decisions made with regards to the rest of the modelling process, especially when it comes to spending resources and time on the collection of data, model calibrations and experiment design.

4.4.1. Single Phase Monte Carlo Simulation Results

The preliminary SPMCS is conducted to obtain an initial measure of the overall quality of the model's predictions. From the result in **Figure 4.2** it can be seen that there is significant uncertainty concerning the predictions and in fact it is so much that decision making for system intervention plans is impossible. At the critical point in the river, the 90% confidence interval for DO ranges from almost saturation point to less than 2 mg/L. Also, the same obvious error as in the preliminary application's result is visible in the mean prediction of the model. The model predicts with a notable bias as well as greater variance than the system observations.

Figure 4.3 shows the SPMCS result for the point estimation of D_c. From the histogram one can confirm that assuming the probability of the MCS output to be normally distributed, is correct. It is however apparent that the quality of the D_c estimate is unsatisfactory. The model under predicts the concentration of D_c by 3.6 mg/L and it predicts with more than 3 times more uncertainty in terms of standard deviation. The standard deviation for the observations is 0.73mg/L versus a standard

deviation of 2.27mg/L for the predictions. The RMSE is 4.23mg/L which, compared with the expected DO saturation level of 9mg/L and the DO water quality standard of 4.5mg/L, is unacceptable.

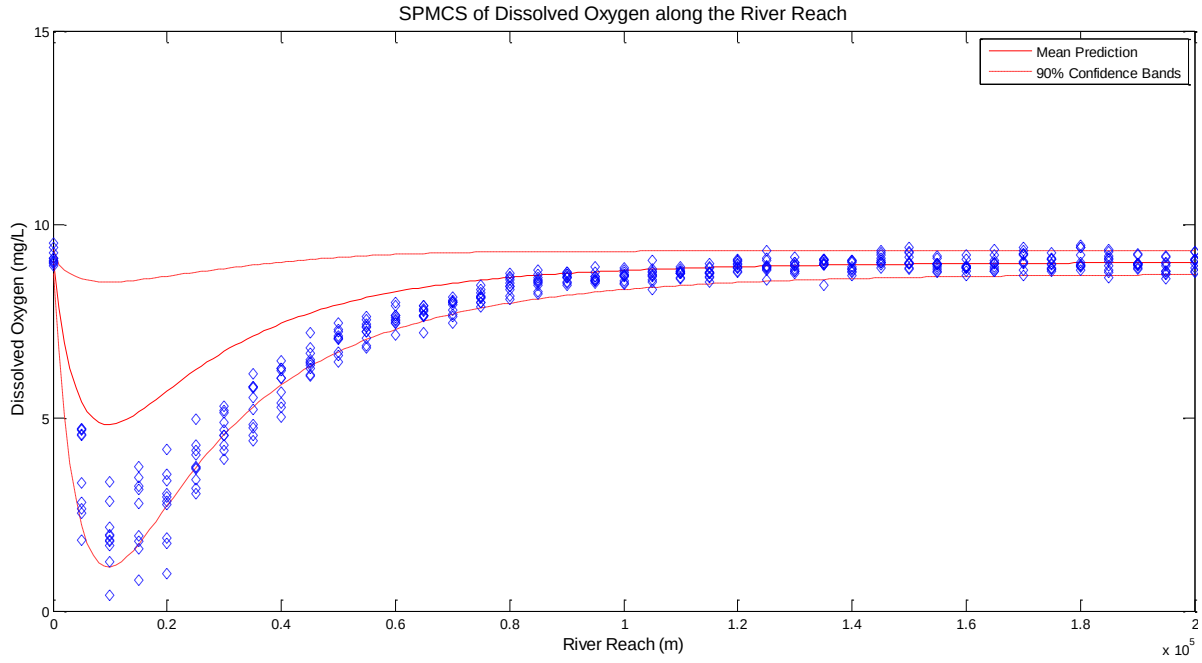

Figure 4.2 Results of the preliminary Single Phase Monte Carlo Simulation on the DO along the reach.

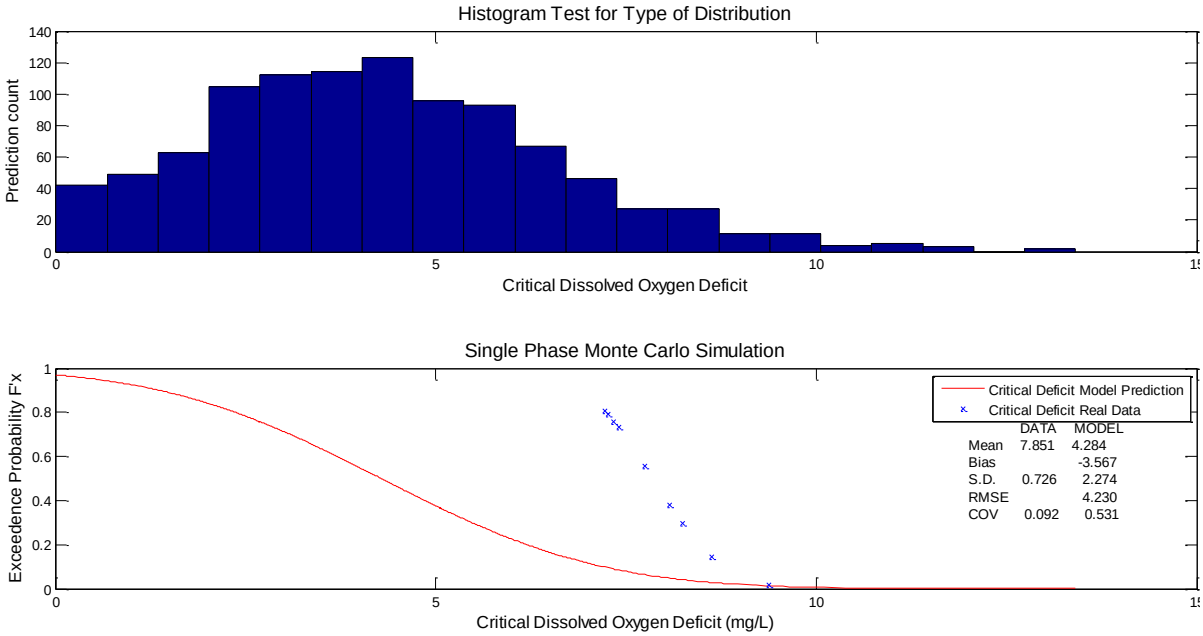

Figure 4.3 Results of the preliminary Single Phase Monte Carlo Simulation on the D_c.

At this stage a modeller has no idea which parameters are causing the uncertainty in the model's predictions, but it is known how it is caused. Wallach et al. (1998:344) stated that the bias is affected by non-linearities in the model while the model variance is affected by uncertainty (variation) in model input. This means that some of the input parameters' mean values are incorrect and they are also subjected to great uncertainty (variation). So, after the preliminary SPMCS, all that is known is that there is uncertainty (variance and error) in the model predictions and it will have to be reduced as much as possible if any decision making is going to depend on it.

4.4.2. Two Phase Monte Carlo Simulation Results

From the SPMCS it was determined that there is significant prediction uncertainty associated with the model output. What still had to be determined was which parameters were causing the problems. Before determining those parameters, it might prove enlightening to first determine what type of uncertainty is dominating the model. This piece of information is provided in **Figure 4.4** by the results of a TPMCS.

The TPMCS basically measures the aleatory uncertainty and epistemic uncertainty in the model and compares them. The most important step in a TPMCS is to correctly identify model input parameters as being either aleatory uncertain parameters or epistemic uncertain parameters. If it is determined that, according to the TPMCS, aleatory uncertainty dominates but the SPMCS delivered results of bad quality, there has obviously been a mistake in the identification of the parameters.

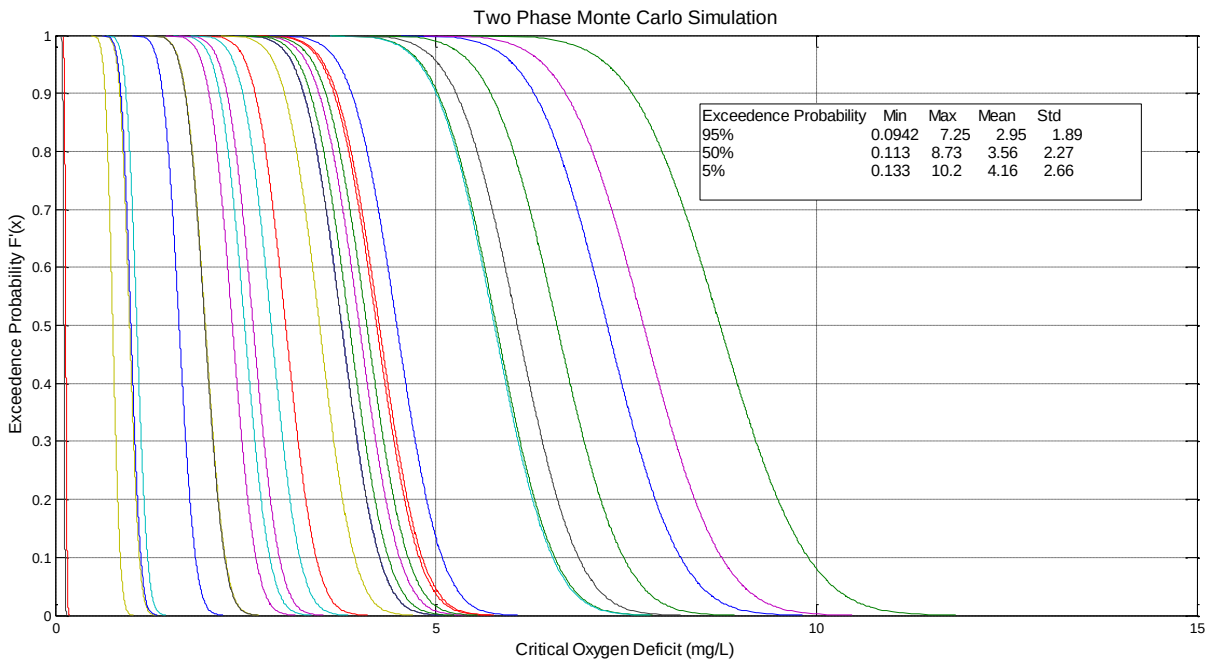

Figure 4.4 Results of the preliminary Two Phase Monte Carlo Simulation of D_c.

The results in **Figure 4.4** show that the epistemic parameters dominate the uncertainty in model predictions. It is shown that the individual exceedence plots that represent aleatory uncertainty are relatively vertical, meaning that they have little contribution to prediction uncertainty in terms of variance. Even if they did contribute significantly towards prediction uncertainty, there would have been nothing that one could do to reduce it except to design system interventions. This is because it was assumed that the knowledge component of their uncertainty was non-existent or already completely reduced.

The collective distribution of all the curves represents epistemic uncertainty and the values for D_c at the respective 95%, 50% and 5% exceedence probabilities vary greatly. According to the TPMCS, the value of D_c at a 5% probability of exceedence can be anything between 0.133mg/L and 10.2 mg/L. If a model's aleatory uncertainty is dominating the epistemic uncertainty, the variation in the individual exceedence plots should be greater than the collective variation of all the exceedence plots together. The general conclusion from the TPMCS results are that any attempts made to reduce the epistemic uncertainty in the model input will be beneficial to the model predictions.

4.4.3. Parameter Monte Carlo Simulation Results

The PMCS is conducted to identify the parameters that contribute most to model prediction uncertainty. Only the parameters classified as epistemic uncertain parameters are investigated because it is assumed that the aleatory parameters are known to us and that the knowledge component of their uncertainty is completely reduced or non-existent. Thus, any further investigation into the uncertainty of the aleatory parameters will be pointless. When modelling real systems this is not the case; parameters may have aspects of both types of uncertainty such as natural variance but also measurement errors.

One might expect similar results to a conventional sensitivity analysis from the PMCS and it is similar in the sense that it considers each parameter's influence on the model output individually. There is a difference though; the sensitivity analysis only calculated some change in the model output due to change in the parameter input. In **Figure 4.5** the PMCS evaluates the DO's sensitivity to uncertainty in the model parameters rather than just change in the value of the parameters. Thus, the model's prediction uncertainty is mapped back to each parameter's contribution of uncertainty. This analysis gives a report on the prior influence of each parameter's uncertainty on model prediction uncertainty.

In each of the graphs in **Figure 4.5**, the mean DO prediction is depicted along with the standard deviation of the DO predictions. The standard deviations characterize model prediction uncertainty and are represented by the error bars.

The uncertainty of the kinetic parameters before the calibration (prior uncertainty) can be compared by calculating their Coefficients of Variation (COV). **Table 4.4** summarizes each parameter's uncertainty and compares it to the other parameters.

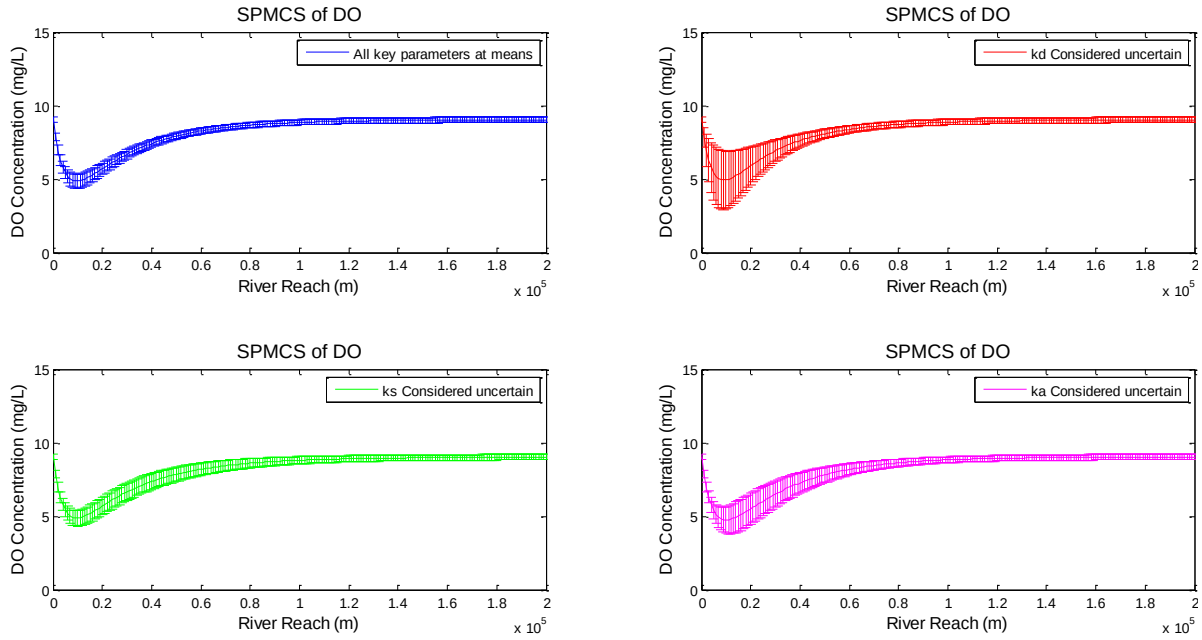

Figure 4.5 Results of the preliminary Parameter Monte Carlo Simulation of the DO along the reach.

Table 4.4 Comparison of the kinetic parameters' Prior Uncertainty.

	k_d	k_s	k_a
Mean	0.7	0.5	7
Standard Deviation	0.4	0.3	1.5
COV	0.57	0.6	0.21

In **Table 4.4** k_s appears to be the most uncertain parameter, however, in **Figure 4.5** its uncertainty seems to make the least contribution to the prediction uncertainty. This coincides with the sensitivity analysis' result for k_s. The uncertainty of k_a is much smaller than the other two parameters' uncertainty but its big contribution to prediction uncertainty is very clear in **Figure 4.5**. The uncertainty in k_d is considerable and its contribution to prediction uncertainty is also large, especially in the vicinity of D_c.

The results in **Figure 4.5** are a fine example of how an uncertainty analysis can increase knowledge of how a model or system behaves. What is interesting is the fact that the uncertainty analysis identified

the regions in the river where decay and reaeration dominates, exactly as the theory explained in Chapter 3.2. Decay dominates in the first section of the DO prediction, up to the point where the critical oxygen deficit is reached. Then reaeration dominates from the critical point to the end of the reach. If a different model was evaluated, and this kind of knowledge wasn't familiar to the modeller, the modeller would quickly have identified it. The uncertainty analysis is very similar to the sensitivity analysis in this sense, but keep in mind that the sensitivity analysis would not have considered the prior situation of uncertainty in the parameters. Thus it would not be able to determine by how much the uncertainty in the kinetic parameters did dominate the model's behaviour at this stage.

It can sometimes happen that model output is less sensitive to change in a specific parameter than to others, but the uncertainty associated with the specific parameter has a larger influence on the model output than the more sensitive parameters with less uncertainty. This becomes apparent if one compares the results of the study's sensitivity analysis with the results in **Figure 4.6**. The sensitivity analysis determined that when the values of parameters k_d, k_s and k_a are increased with 20%, k_d is more sensitive than k_a. When the values were decreased with 20%, k_a proved to be more sensitive than k_d.

By conducting the PMCS on the D_c equation, the results in **Figure 4.6** quickly conclude that the current state of uncertainty in k_d has the greatest effect on the D_c equation's prediction uncertainty. The uncertainty in k_d caused the standard deviation in the model output to increase from 0.431 to 1.98 while the uncertainty in k_a caused the standard deviation in the output to increase from 0.431 to 0.94.

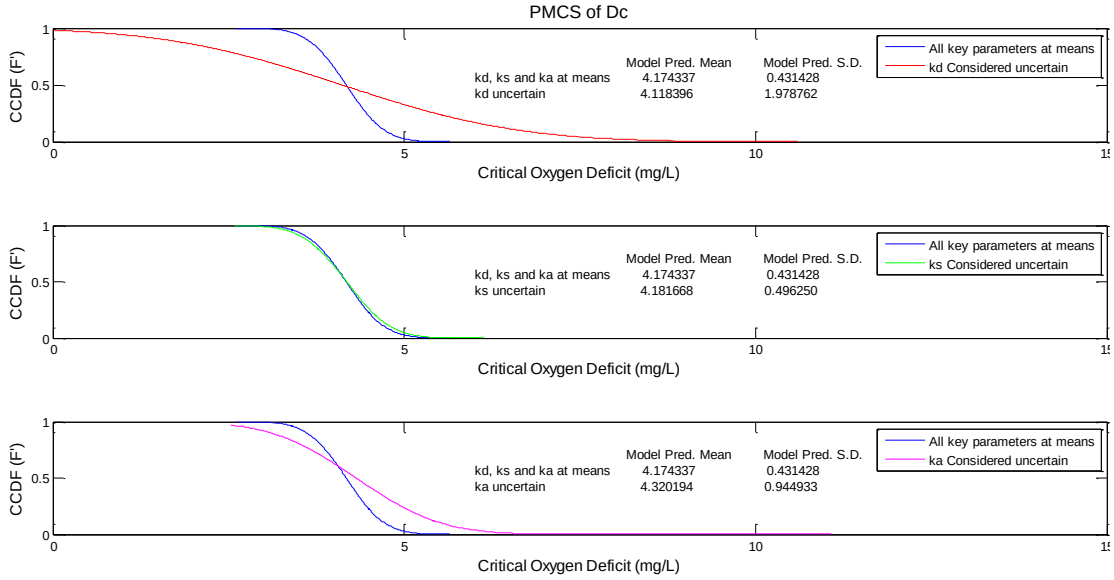

Figure 4.6 Results of the preliminary Parameter Monte Carlo Simulation of D_c.

This information is much more enlightening than the information from the conventional sensitivity analysis and one is immediately aware of both parameters' influence on the output and decision making is much easier. Keep in mind that the constituent of interest in both the sensitivity analysis and **Figure 4.6** was D_c and not DO. It was decided that it would be more convenient to compare the uncertainty analysis and sensitivity analysis in the context of D_c because it is a point estimate.

The sensitivity of the model output to change in k_s proved to be negligibly small and this is also confirmed in the results of **Figure 4.5** and **Figure 4.6**. Even though the COV in k_s is 60%, which represents a lot of parameter uncertainty, the effect of this uncertainty on prediction uncertainty is very small. In this situation the sensitivity analysis was correct in its analysis of k_s but this might not always be the case and an uncertainty analysis definitely has an advantage over the sensitivity analysis. It must be mentioned that sensitivity analysis also has one distinct advantage over an uncertainty analysis using MCS; it is much cheaper in terms of computer calculations. A sensitivity analysis will consist of much fewer model runs than a proper uncertainty analysis using MCS.

One might argue in this case that any further reduction of k_s' uncertainty in this model would be a waste of time and money. Spending time and money on the determination of k_d and k_a, however, would not.

4.5. Calibration Results

The calibration was used as the only method of reducing parameter uncertainty. It is only one of a couple of methods to reduce parameter uncertainty. It was assumed that the only epistemic parameters in the model were the kinetic rate coefficients and they are generally determined by calibration. The prior and posterior distribution characteristics of the kinetic parameters can be viewed in **Table 4.5** and **Table 4.6**. Both tables also contain the covariance matrix that describes the coefficients' interrelationships.

Table 4.5 Prior distribution characteristics (covariance matrix included) of the kinetic parameters including the summer input characteristics.

	L_0	Q	T	k_d	k_s	k_a
Means	60	3	20	0.7	0.5	7
S.D.	6	0.3	1	0.4	0.3	1.5
COV	0.1	0.1	0.05	0.5714	0.6	0.2143
	k_d	k_s	k_a			
k_d	0.16	0	0			
k_s	0	0.09	0			
k_a	0	0	2.25			

Table 4.6 Posterior distribution characteristics (covariance matrix included) of the kinetic parameters including the winter input characteristics.

	L_0	Q	T	k_d	k_s	k_a
Means	40	15	10	0.9636	0.2694	5.2335
S.D.	8	1.5	1	0.0916	0.1145	0.5116
COV	0.2	0.1	0.1	0.0951	0.4252	0.0978
	k_d	k_s	k_a			
k_d	0.0084	-0.0054	0.0343			
k_s	-0.0054	0.0131	-0.0493			
k_a	0.0343	-0.0493	0.2618			

From **Table 4.5** and **Table 4.6** a notable change in all three coefficients' values is clear from before to after calibration. What is very interesting now is that the posterior distributions can be compared with the parameter distributions used in the generation of the synthetic data. That means the calibrated values for the kinetic coefficients can be compared with their 'true' values. In reality this is never possible. **Table 4.7** summarizes and compares the prior and posterior distributions for the kinetic parameters with each other as well as with the 'true' parameter characteristics. All parameter distributions were assumed to be normally distributed. Keep in mind that the prior distributions of the

parameters were causing the unacceptable model prediction uncertainty in the preliminary uncertainty analysis.

Table 4.7 Comparison between true parameter distributions and the prior -and posterior distributions.

Parameter	True Mean	True SD	Prior Mean	Prior SD	Posterior Mean	Posterior SD
k_d	0.9	0.12	0.7	0.4	0.96	0.09
k_s	0.3	0.03	0.5	0.3	0.27	0.11
k_a	5	0.25	7	1.5	5.23	0.51

The Monte Carlo method of calibration was very accurate in determining the mean values of the coefficients. The true mean value for k_d was 0.9 and its posterior mean value 0.96. Both k_s and k_a were calibrated with the same level of accuracy; true mean values of 0.3 and 5 for k_s and k_a versus calibrated values of 0.27 and 5.23 for k_s and k_a respectively. From the covariance matrix it can be established that the interdependency between the parameters is very little. All three parameters were calibrated within less than 10% error of their true values. Notice the accuracy with which the mean value of k_s was calibrated although the model shows very little sensitivity to it. It is hard to think that this kind of accuracy would have been possible in a successive-substitution type calibration.

The Monte Carlo method of calibration was slightly less successful in calibrating the coefficients' standard deviations although it still performed satisfactory. It should be noted that the posterior standard deviation for k_d is less than the true standard deviation for k_d. This means that after the reduction of this parameter's uncertainty, one is under the impression that its uncertainty is much less than what it truly is. The posterior distributions' standard deviations reflect the kinetic parameters' aleatory uncertainty, which is also its true standard deviation. Models are supposed to predict with accurate stochastic variability and with little epistemic uncertainty. Using the posterior standard deviation of k_d will in fact mean that the model will predict with the wrong stochastic variability, which leads back to a model predicting with epistemic uncertainty! This doesn't matter now because it will be shown shortly that aleatory uncertainty dominates the epistemic uncertainty after the calibration and the effect that the remaining epistemic uncertainty has on the model is acceptable and manageable. Any further reduction of uncertainty is pointless as the model already predicts with good quality.

From the results discussed above it can be concluded that the Monte Carlo method, of repeatedly simulating the model with a range of possible values for the kinetic parameters, was successful in its numerical approximation of the true values of the kinetic parameters. It is important though that the true values of the parameters must be within the parameter ranges specified in the calibration.

Otherwise there would be no way for the method to randomly sample the correct values of the kinetic parameters.

4.6. Model Confirmation Results

Before using a calibrated model for decision making it must be confirmed. This is done by running the model with the calibrated kinetic coefficients and comparing the results with a second set of data that is different than the first set used for the calibration of the model. Chapra (2008:324) explains that the forcing functions and boundary conditions in the confirmation are supposed to be different values than in the calibration of the model and supposed to correspond with the second set of data. The second set of data that was used in the model confirmation was the winter data. The corresponding forcing functions and boundary conditions are summarized in **Table 4.8**.

Table 4.8 Forcing functions and boundary conditions corresponding to the winter data.

Parameter	Units	Mean	Standard Deviation
L_0	mg/L	40	8
Q	m^3/s	15	1.5
T	$°C$	10	1

Figure 4.7 shows the mean prediction of the DO model and it can be concluded that graphically it compares very well to the system's winter observations.

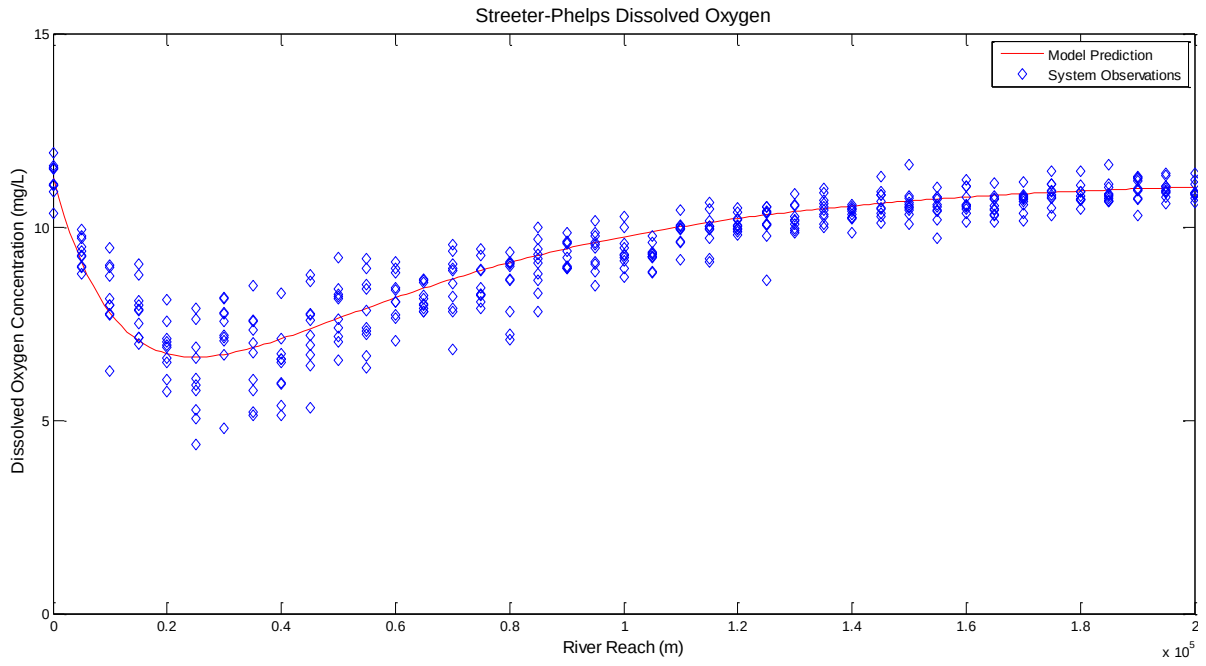

Figure 4.7 Comparison of the confirmatory application of DO with the second set of system observations (winter data).

4.7. Confirmation Uncertainty Analysis Results

The objective of this uncertainty analysis is to confirm that the epistemic parameters in the model have indeed been reduced and that the model is now fit for use in a management application. The confirmation uncertainty analysis was conducted in exactly the same way as the preliminary uncertainty analysis. The only difference was that the posterior distributions for the kinetic parameters were used in the confirmation uncertainty analysis. The results are compared with the winter data, so the forcing functions and boundary conditions corresponding to the winter data were also used in the analysis. **Table 4.9** and **Table 4.10** summarize the parameter characteristics used to generate Model Parameter Input for this uncertainty analysis and are updated versions of **Table 3.10** and **Table 3.11**.

Table 4.9 Summary of the characteristics used to generate Model Parameter Input for the confirmation uncertainty analysis.

Parameter	Units	Mean	Standard Deviation	Coefficient of Variation	Distribution	Type of uncertainty
L_0	mg/L	40	8	0.2	Normal	Aleatory
Q	m^3/s	15	1.5	0.1	Normal	Aleatory
T	$°C$	10	1	0.1	Normal	Aleatory
k_d	d^{-1}	0.96	0.09	0.0938	Normal	(Reduced) Epistemic
k_s	d^{-1}	0.27	0.11	0.4074	Normal	(Reduced) Epistemic
k_a	d^{-1}	5.23	0.51	0.0975	Normal	(Reduced) Epistemic

Table 4.10 Covariance Matrix of posterior distributions.

	k_d	k_s	k_a
k_d	0.004	-0.0031	0.0212
k_s	-0.0031	0.0088	-0.0358
k_a	0.0212	-0.0358	0.1923

4.7.1. Single Phase Monte Carlo Simulation Results

Figure 4.8 shows the result of the confirmation SPMCS of the DO model. Based on the mean values the model seems to be predicting with acceptable bias and the 90% confidence interval confirms that the model is also predicting with improved precision. This confidence interval is short enough and 90% probability is confident enough for decision making purposes.

Figure 4.9 shows the results from the confirmation SPMCS of the model D_c. The histogram shows that a normal distribution of the model output accurately characterizes the distribution of the

predictions. From the CCDF graph it is clear that the model still predicts with some bias (-1.4 mg/L). It also predicts with greater standard deviation but in general the results are much better than in the preliminary uncertainty analysis of D_c. The overall quality of the model predictions is acceptable in comparison with the results from the preliminary uncertainty analysis; since the reduction of parameter uncertainty, the RMSE decreased from 4.23 mg/L to 1. 7 mg/L.

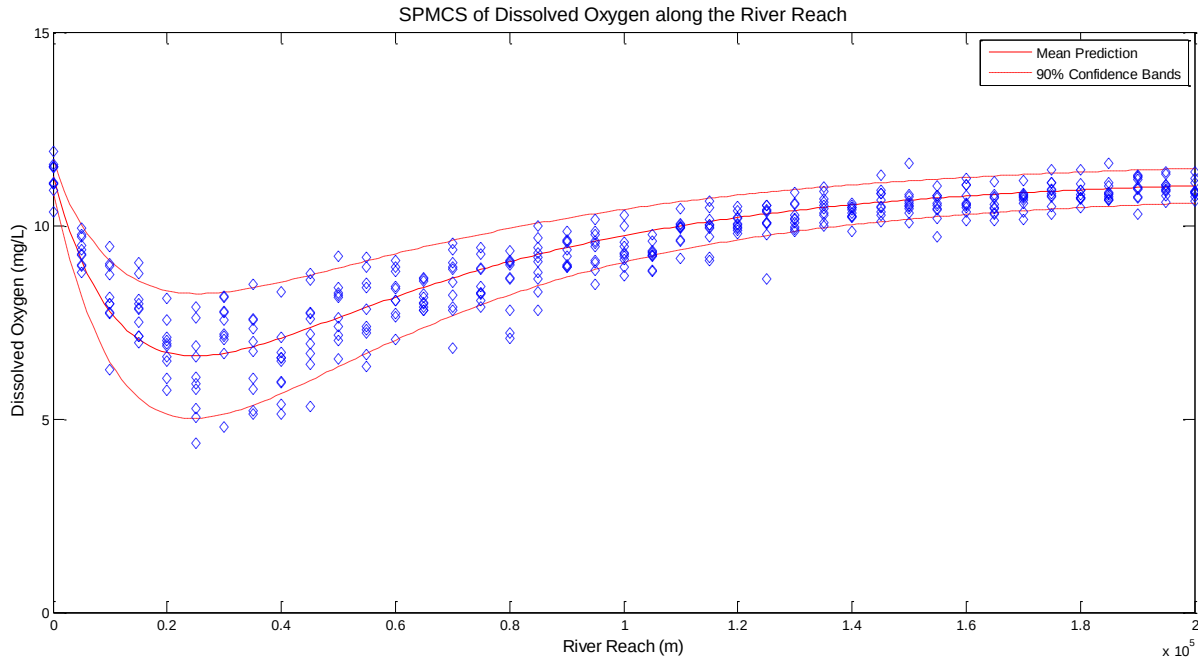

Figure 4.8 Results of the confirmation Single Phase Monte Carlo Simulation of DO along the river reach.

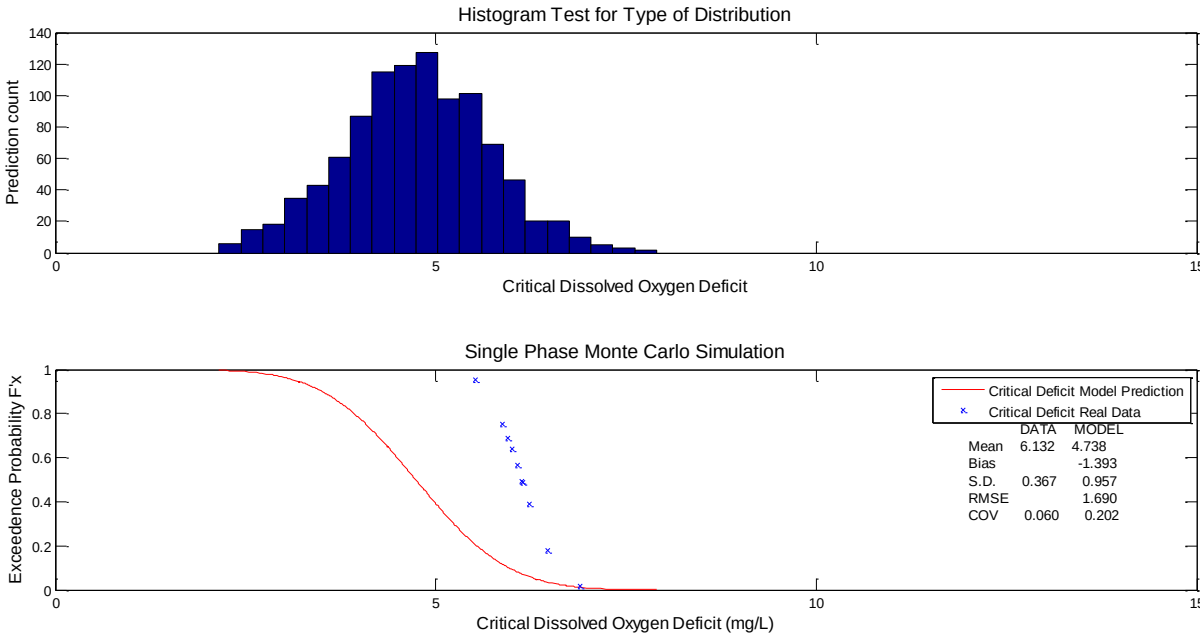

Figure 4.9 Results of the confirmation Single Phase Monte Carlo Simulation of D_c.

The reasons for the difference between the model predictions and the system observations can be any of the following three: Firstly, the way the system observations of D_c were collected was by subtracting the observed DO concentrations from the expected DO_{sat} and determining the 10 maximum D_c concentrations in the river. This might lead to discrepancies because the mean temperature was used to calculate the expected DO_{sat} and not the temperature corresponding to each individual DO sample. The temperature at the time of the specific DO data collection was disregarded which is probably not scientifically correct. Situations like these occur in real life modelling and modellers will have to judge for themselves how they will manage uncertainties caused by inadequate data collection like this.

Secondly, the equation used for the calibration of the kinetic parameters was the DO equation while **Figure 4.9** shows the results of the D_c equation. This means that one model was used in the calibration of the parameters and another used when the calibrated parameters were applied. This is also not 100% correct and the values of the kinetic parameter might not be exactly appropriate for use in the D_c equation. The DO equation and the D_c equation were derived together in the Streeter-Phelps theory and they are supposed to model related water quality constituents. In practice the D_c -and t_c equations of Streeter-Phelps are used to calibrate the kinetic parameters because they can often be determined from a river's data (Chapra, 2008:398). So this second explanation should actually not be the reason for the difference in the model predictions and the system observations. The Streeter-Phelps kinetic parameter values are supposed to be interchangeable between the DO -and D_c equations.

Thirdly, the number of system observations might be too few to get an accurate representation of the D_c concentrations in the river. McBean & Rovers (1998:13) mention that statistical procedures must be sensitive to the fact that observed data only represent a sample from a population. As sample size increases, its description of the population should improve, but it is expensive and time consuming to collect large numbers of samples.

4.7.2. Two Phase Monte Carlo Simulation Results

From **Figure 4.10** it is clear that the epistemic uncertainty in the model has been reduced and the dominance of model uncertainty has shifted from being epistemic to being aleatory. At a 5% probability of exceedence the minimum and maximum values for D_c differ by 1.13 mg/L. This still represents some epistemic uncertainty but it is a huge improvement on the results of the preliminary TPMCS. It is interesting to see that the relatively little epistemic uncertainty in the kinetic parameters still causes some variation in the collection of CCDF curves in **Figure 4.10**. It should be possible to manage this epistemic uncertainty with appropriate margins of safety in any potential intervention designs. Any additional reduction of epistemic uncertainty will be a waste of time and money and the only way of reducing total uncertainty now is by changing the physical system. The importance of correctly classifying the model parameters as either aleatory or epistemic must be emphasized. If the classification of the model parameters is wrong, the results of the TPMCS will give a wrong impression of the model's uncertainty and decision making could be affected.

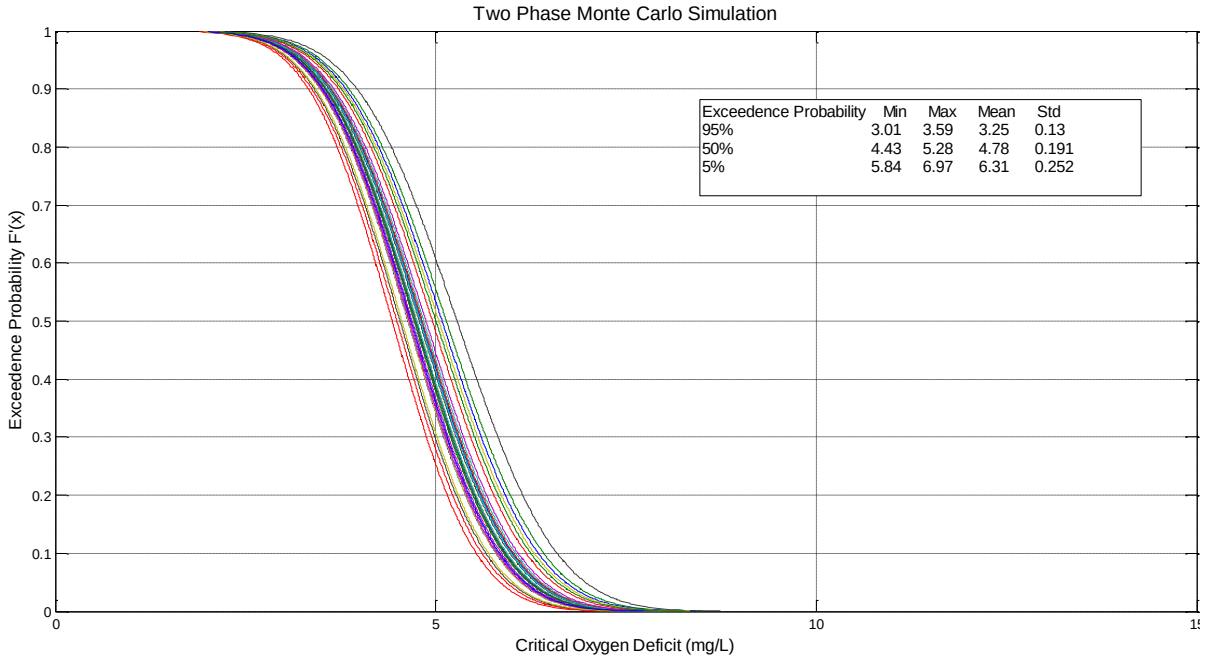

Figure 4.10 Results of the confirmatory Two Phase Monte Carlo Simulation of the D_c equation.

4.7.3. Parameter Monte Carlo Simulation Results

Figure 4.11 and **Figure 4.12** relate each kinetic parameter's contribution to the prediction uncertainty in each Streeter-Phelps equation. They confirm that the kinetic parameters' uncertainty has been reduced.

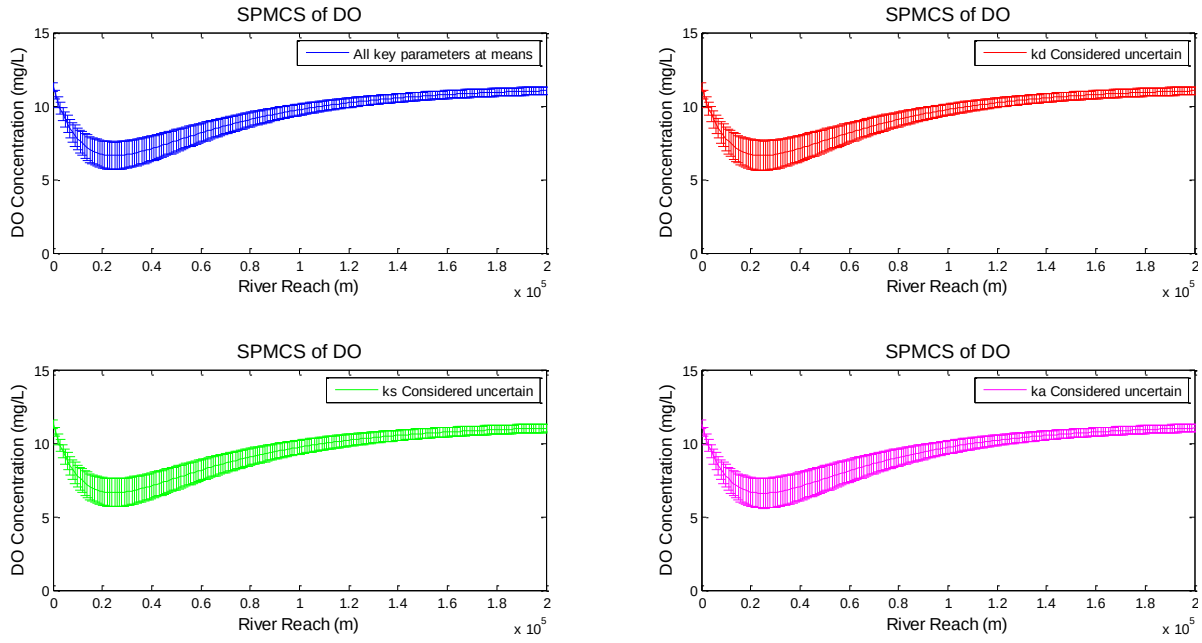

Figure 4.11 Results of the confirmation Parameter Monte Carlo Simulation of the DO along the river reach.

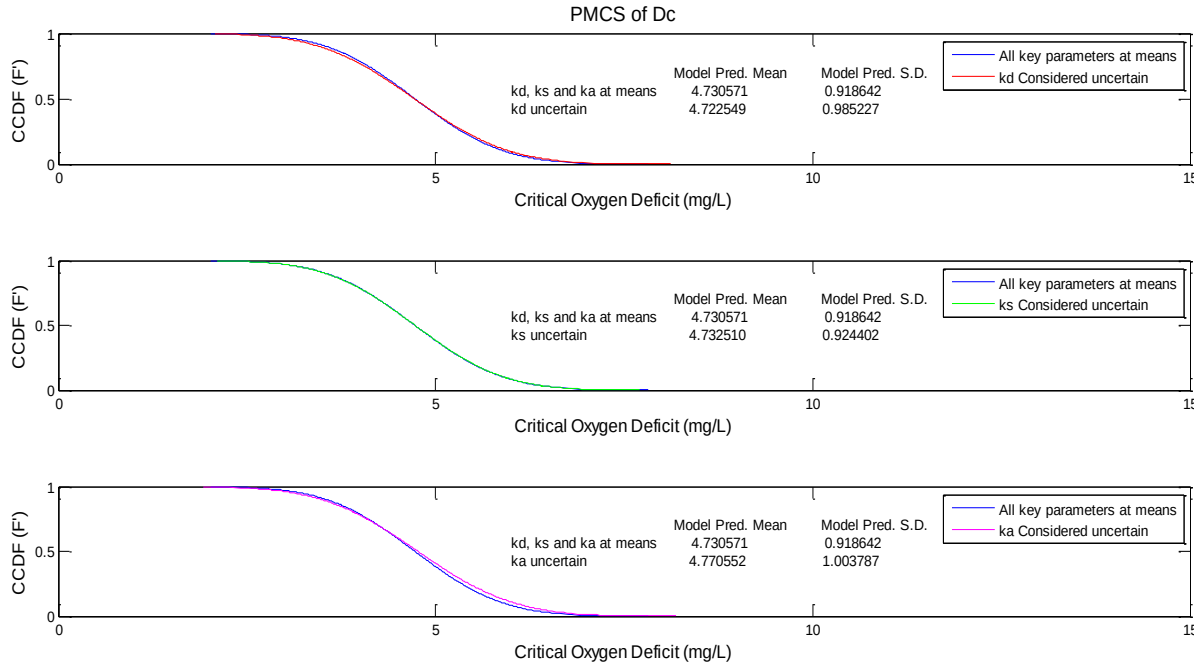

Figure 4.12 Results of the confirmation Parameter Monte Carlo Simulation of D_c.

If one compares the standard deviation bars in **Figure 4.11**, it is apparent that the spread of the error bars hardly increases from case 1 to the other three cases. In comparison to **Figure 4.5** there has been an immense improvement with regards to each parameter's individual contribution to the DO equation's prediction uncertainty. Note that **Figure 4.11** and **Figure 4.5** are the results of the winter and summer flows respectively. Their forcing functions and boundary conditions are different.

Figure 4.12 shows that the standard deviations of the D_c predictions hardly changes for the different cases of parameter uncertainty. The uncertainty of k_a seems to be contributing the most of the prediction uncertainty in the D_c equation by increasing the standard deviation from a base prediction of 0.92 mg/L to 1 mg/L. As expected, the uncertainty of k_s contributed the least to the model prediction uncertainty.

One must be careful not to get too confident with the results by misinterpreting them. In section 4.5 it was mentioned how the calibration of k_d resulted in an accurate value for its mean value but its stochastic variability was smaller than that of the 'true' k_d. Thus the results in **Figure 4.11** and **Figure 4.12** might give the wrong impression of the parameters uncertainty and this can have an effect on the overall quality of the model's predictions. It is important for a model to predict with reduced epistemic uncertainty but with the correct stochastic variability.

MCS proved to be very effective in the PMCS configuration of uncertainty analysis, although the initial feeling of it might seem very familiar to a sensitivity analysis. After all, it was executed in the same order as a conventional sensitivity analysis, but the MCS conducted repeated simulations of sensitivity runs and considered parameter distributions and variation rather than just a fixed change in parameter values. It is true that this process could also have been completed by using FOAMs but keep in mind that if the parameters' distributions are not conventional, FOAMs will not characterize the effect of parameter uncertainty on prediction uncertainty so well. The reason for this is that FOAMs use the first-, second -and possibly, the third moments (3rd moment represent a distribution's skewness) of the parameters to propagate parameter uncertainty. Thus, FOAMs will not be able to assess the effects of any complex shapes of non-normal distributions on the model's prediction uncertainty.

4.8. Management Application

Once a model's prediction uncertainty has been quantified, how does one go about making decisions with the newly acquired knowledge concerning the uncertainty associated with the model? This subsection focuses on a suggestion of how this knowledge can be applied in the design of a TMDL intervention option.

4.8.1. Introduction to Total Maximum Daily Loads and Margin of Safety

WQMs are used to assess the effectiveness with which TMDLs can be implemented to improve the water quality of impaired waters. The uncertainty associated with the models' predictions is of great concern though (Shirmohammadi et al., 2006:1034). Despite this concern, there is a lack of well-defined and practiced processes for the incorporation of uncertainty into TMDL calculations (Shirmohammadi et al., 2006:1045).

A TMDL is defined as the load that a water body can assimilate without violating water quality standards (Shirmohammadi et al., 2006:1046). Sexton et al. (2011:2202) explain that the TMDL for the water body is the resultant load after the load has been reduced enough to meet the water quality standard. One of the main problems of calculating the TMDL is model uncertainty, and decision makers would like some sense of reliability in model predictions when designing intervention options.

In TMDL calculations, the uncertainty associated with models is usually accounted for by the Margin of Safety (MOS). Mathematically, a TMDL is written as (Mishra, 2011:1; Shirmohammadi, 2006:1034):

$$TMDL = \sum WLA + \sum LA + MOS$$

$\sum WLA$ = waste load allocation (point sources)

$\sum LA$ = load allocation (non-point sources)

MOS = margin of safety

In the context of TMDL calculations, MOS accounts for the uncertainty in the water body's response by adjusting the load allocation. This adjustment is made by decreasing the loads (contrary to what the equation above might lead one to believe). The value of MOS in this case should always be negative. There are two ways of assigning a MOS to a TMDL (Sexton et al., 2011:2197):

1. The MOS can be considered explicitly, which involves assigning an arbitrary fixed percentage, factor of safety, to the point –and non-point sources.

2. The MOS can be considered implicitly, which involves increasing the threshold water quality criterion above which is necessary. For example; the water quality standard for dissolved oxygen of a water body might be a value of say 5 mg/L, but the goal of the engineer might be to design a load that would result in a dissolved oxygen concentration of 6.5 mg/L.

It is suggested that MOS should be determined by calculations supported by scientific information, rather than being arbitrary assigned factors of safety. The use of formal uncertainty analysis methods can provide a scientifically correct platform for determining MOS. A Monte Carlo method will provide a probability based stochastic approach of which the output distribution can be used to make water quality impairment decisions for conventional pollutants (Sexton et al., 2011:2198; 2201).

It is better to fully utilize an output distribution for the inclusion of uncertainty into TMDL calculations because uncertainty is included directly into the determination of WLA and LA, and in cases where model performance is satisfactory, a MOS is not even necessary (Shirmohammadi et al., 2006:1046). The rest of this subsection discusses an approach for determining MOS and calculating a TMDL using uncertainty analysis methods.

4.8.2. Case Study

In the case of the hypothetical environment modelled in this study, the TMDL is a BOD load that has to be calculated. The hypothetical stream must be capable of assimilating this load in order to maintain or exceed a water quality standard of 4.5 mg/L DO. The uncertainty associated with the model must be taken into account when calculating the TMDL.

The management application of the model is the final step of the modelling protocol and by this stage the model has undergone a preliminary uncertainty analysis, calibration and a confirmatory uncertainty analysis. The confirmatory uncertainty analysis confirmed that the epistemic uncertainty associated with the model has been reduced to a point where it can be managed. For the purpose of calculating the TMDL, the worst case scenario, which happens to be the summer months, is considered. Due to the ecosystem's vulnerability, the water body is said to be impaired if 5% of the model predictions are in violation of the water quality standard.

Recall that the Streeter-Phelps model was calibrated and that the results from the calibration were confirmed to be satisfactory. **Figure 4.13** is a confirmatory SPMCS of the DO equation. The summer characteristics and calibrated kinetic coefficients (**Table 4.11**) were used as input and the results were compared with the summer data for the hypothetical river.

Table 4.11 Posterior distribution characteristics (covariance matrix included) of the kinetic parameters including the summer input characteristics.

	L_0	Q	T	k_d	k_s	k_a
Means	60	3	20	0.9636	0.2694	5.2335
S.D.	6	0.3	1	0.0916	0.1145	0.5116
COV	0.1	0.1	0.05	0.0951	0.4252	0.0978
	k_d	k_s	k_a			
k_d	0.0084	-0.0054	0.0343			
k_s	-0.0054	0.0131	-0.0493			
k_a	0.0343	-0.0493	0.2618			

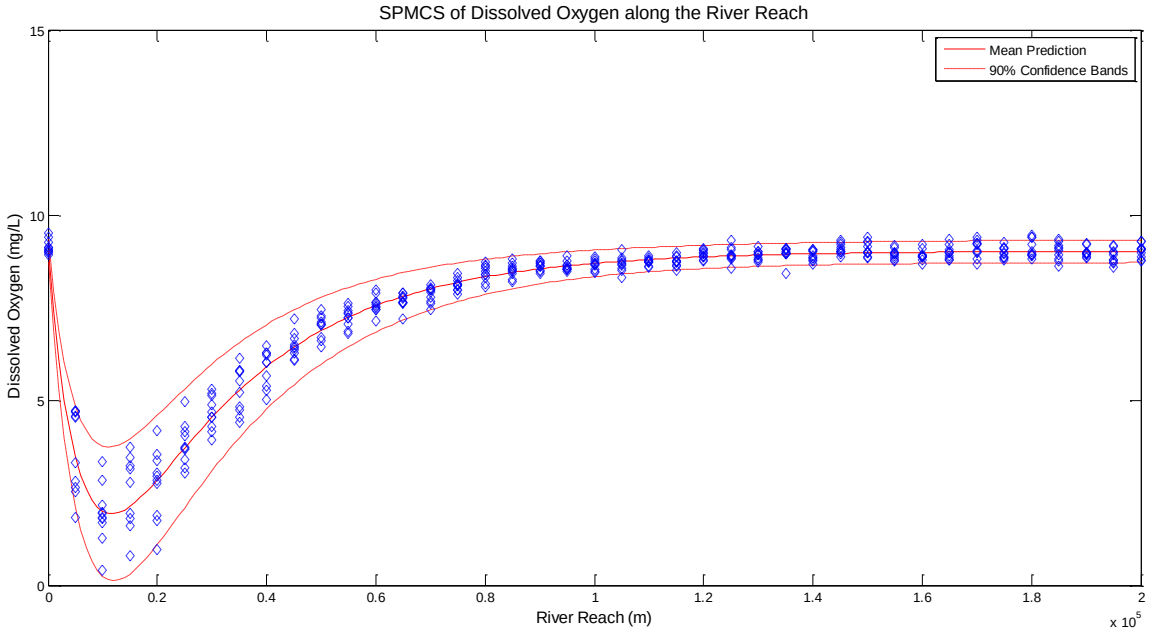

Figure 4.13 Confirmatory SPMCS of the DO equation using summer characteristics and calibrated kinetic coefficients.

From **Figure 4.13** it is clear that the model calibration is satisfactory. The focus of the decision maker should now be centered on determining a BOD load that will lift the 90% confidence bands above the water quality standard of 4.5mg/L. In the current situation it is being violated for almost 400m of the river's travelling distance. Keep in mind that in real environmental situations there are much more point – and non-point sources of pollution and that water quality standards are constantly being violated.

To determine a BOD load that the river will be able to assimilate, it is better to use the critical deficit equation, as it focuses on the critical point in river where the DO concentration is at its lowest. Critical deficit is, however, not the best water quality constituent to model because it cannot be

directly related to the water quality standard which is expressed in dissolved oxygen concentration levels. Therefore the critical deficit equation is transformed to rather provide a solution for the critical DO concentration:

$$DO_c = DO_{sat} - D_c$$

Figure 4.14 shows the results of a SPMCS of the critical DO equation and compares the results with the system observations for the minimum DO concentrations in the summer months.

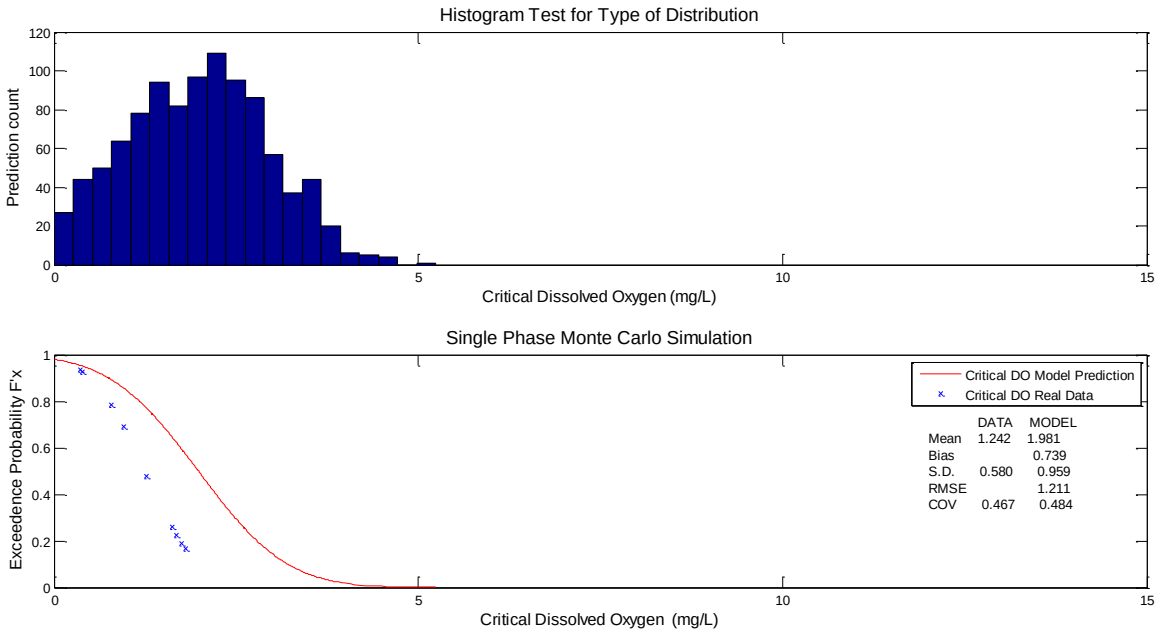

Figure 4.14 SPMCS of the critical DO equation and the comparison of its results with the DO data for the summer months.

Although the model does not predict with complete accuracy it can still be used in the determination of the BOD load. The model prediction is not perfect, but the remaining uncertainty can be accounted for by an appropriate MOS.

According to Shirmohammadi et al. (2006:1046) the WLA is usually the sum of the point sources with no uncertainty assumed (LA is disregarded for the purpose of this illustration). This means that the water quality standard of 4.5 mg/L DO can be plugged into the DO_c equation along with the mean values of all the input parameters (**Table 4.11**) and solved for BOD. The solution in this case is a BOD load of 38.44 mg/L. This means that a load of 38.44 mg BOD/L should result in a mean DO concentration of 4.5mg/L.

To assess the effectiveness of implementing a TMDL of 38.44mg BOD/L one can perform another SPMCS using the same system characteristics (**Table 4.11**) but with the newly determined TMDL (assume a COV of 10% for L_0). The results are shown in **Figure 4.15**:

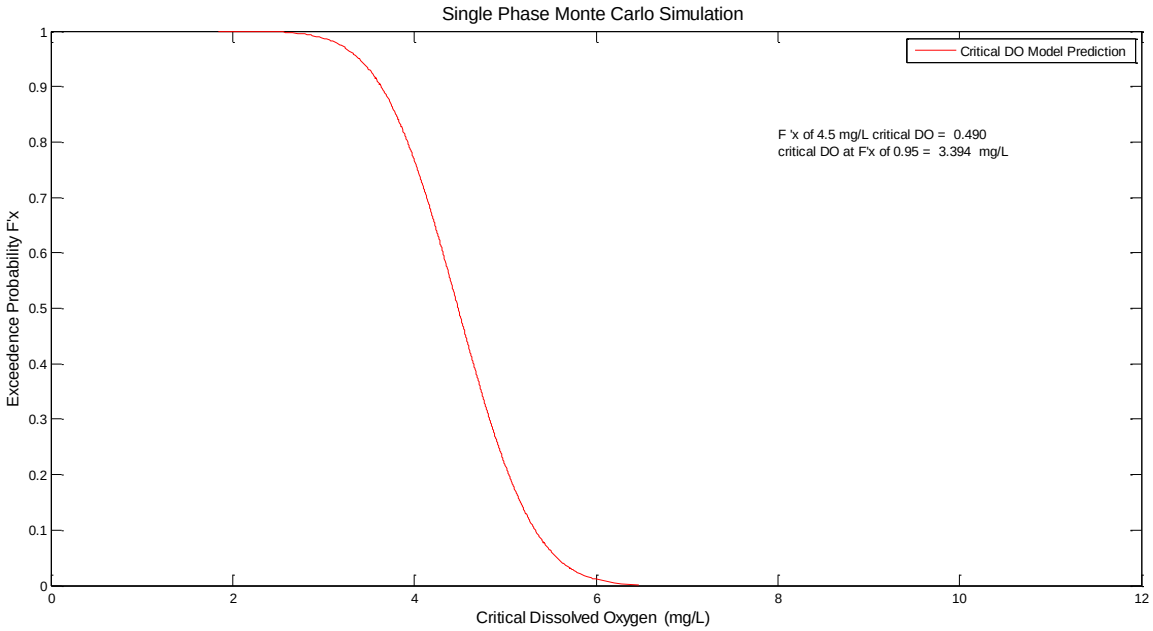

Figure 4.15 SPMCS of the critical DO equation using 38.44mg BOD/L as the TMDL.

The expected mean DO prediction is 4.5mg/L, but due to the randomness of MCS, the probability of exceeding a DO concentration in **Figure 4.15** is 0.49 and not 0.5. This is not of concern now and a properly determined MCS size (n) should result in the model predictions converging to a probability of 0.5 for a DO concentration of 4.5 mg/L.

What should rather be of great concern now is the fact that due to the natural variability of the system, there is still a chance of 0.51 of violating the water quality standard. The risk associated with designing a load of 38.44 mg/L is too great and the stochastic variability of the environment needs to be taken into account when determining the TMDL. This is achieved by using a MCS of the critical DO equation and solving for BOD, resulting in an output distribution for a TMDL.

A very important point that needs to be remembered now, is the fact that the model's over prediction (**Figure 4.14**) of DO needs to be taken into account. The model's bias should be subtracted from the water quality standard of 4.5mg/L to compensate for the fact that the model over predicts on average. This creates a new water quality goal for the TMDL designer. The TMDL should rather be designed for achieving a water quality standard (read goal) of 3.761mg/L (4.5-0.739).

The bias is used rather than the RMSE because the RMSE is a measure of the model's total uncertainty. The standard deviation of the RMSE term is already taken into account in the MCS method for determining the output distribution for the BOD load. Keep in mind that the standard deviation term in the RMSE accounts for both the aleatory uncertainty of the natural system as well as part of the model's epistemic uncertainty. The inclusion of the model's bias in the water quality goal should compensate for the other part of the epistemic uncertainty. If one subtracted the RMSE,

instead of the bias, from the water quality standard and then determined an output distribution for the BOD load, part of the epistemic uncertainty would have been taken into account twice, resulting in an unnecessary low BOD load that could increase costs dramatically.

Figure 4.16 shows the result for the MCS method of determining an output distribution for the BOD load. From the figure it can be seen that the subtraction of the bias from the water quality standard resulted in a TMDL of 32.369 mg BOD/L. However, this load does not take into account the aleatory uncertainty of the system being modeled or the remaining inherent epistemic uncertainty of the model.

It is now better to determine a load from the distribution that would minimize the risk of violating the water quality standard. For this purpose a BOD load of 25.972 mg BOD/L at a probability of exceedence of 0.95 should be better suited. This means that a decision maker can be 95% sure that a BOD load of 25.972 mg BOD/L or less will result in the water quality standard being maintained.

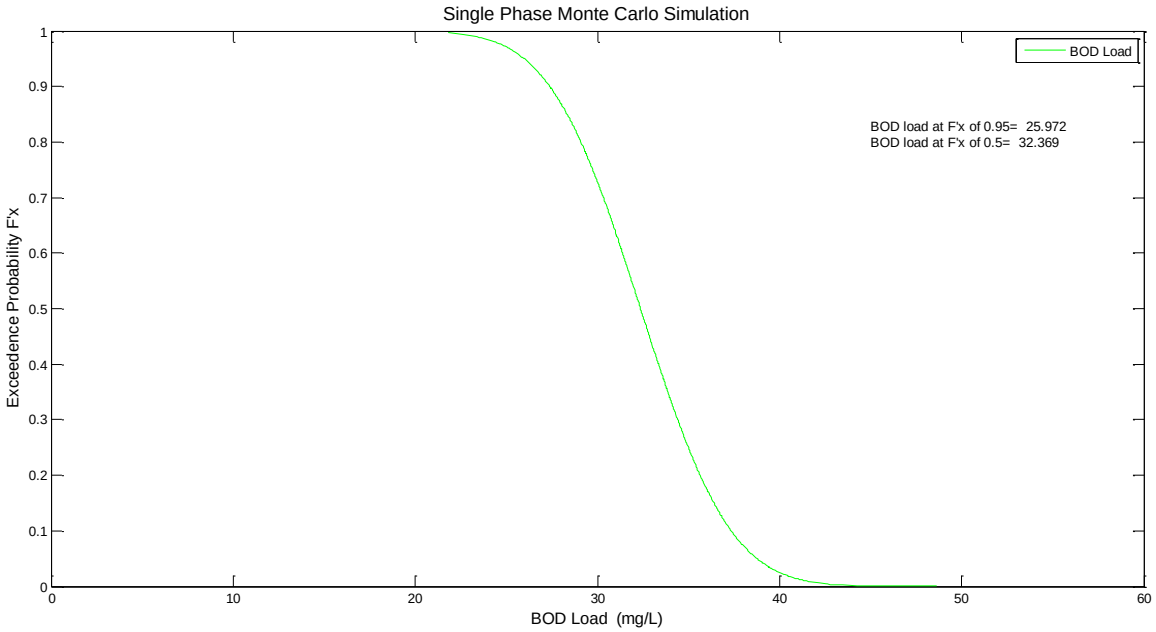

Figure 4.16 MCS determined output distribution for the BOD load.

The statement in the previous paragraph can now be tested by performing another SPMCS of the critical DO equation, using the TMDL of 25.972 mg BOD/L (assume COV of 10% for L_0) as input for L_0. The rest of the input parameters stay the same as in **Table 4.11**. **Figure 4.17**shows the results of the SPMCS of the critical DO equation using a TMDL of 25.972 mg BOD/L. At a probability of exceedence of 0.95, the model predicts a DO concentration of 5.155 mg DO/L. This exceeds the water quality standard of 4.5 mg DO/L, meaning that the water quality standard is likely to be maintained with this TMDL discharged into the river.

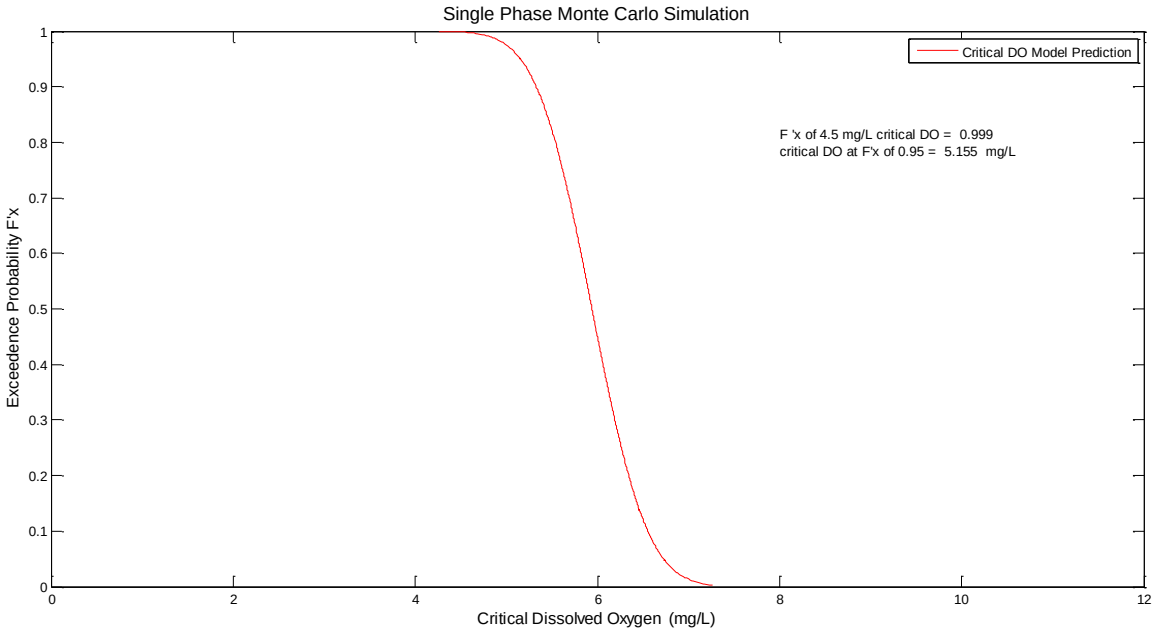

Figure 4.17 SPMCS of the critical DO equation using 25.972mg BOD/L as the TMDL.

Recall that in the calculation of a BOD load, the model's bias was subtracted from the water quality standard to compensate for the model's tendency to over predict critical DO. Subtracting the bias from the critical DO of 5.155 mg/L now gives a concentration of 4.416 mg/L. Although strictly speaking this violates the water quality standard, it is right in the vicinity of a DO concentration of 4.5mg/L. Looking at the uncertainty analysis in the **Figure 4.14**, this should not be a problem as the observations and model predictions start to converge at a probability of 0.95, so in all likelihood, the water quality standard will be maintained. Whether this will be the case in practice we do not know and the only way of finding out would be to implement the intervention action.

So what was the calculated value of the MOS included in the TMDL? The MOS equals the difference between the load required to maintain the water quality standard, and the load required to maintain the water quality goal (Sexton et al., 2011:2202). MOS due to the model bias is thus (38.44 - 32.369) = 6.071mg/L. MOS due to the aleatory uncertainty and remaining epistemic uncertainty is (32.369 - 25.072) = 7.297 mg/L. The total MOS included in the TMDL was (6.071 + 7.297) = 13.368 mg BOD/L (or a subtraction of 34.78% of the WLA).

5. Conclusion

This study focused on investigating MCS and its use in the quantification of prediction uncertainty associated with WQMs. It explained how different configurations of MCSs can achieve different objectives of uncertainty analysis. Three different configurations of MCSs were explained and illustrated. These included Single Phase Monte Carlo Simulation (SPMCS), Two Phase Monte Carlo Simulation (TPMCS) and Parameter Monte Carlo Simulation (PMCS).

The three Monte Carlo configurations were applied to a Streeter-Phelps model of a hypothetical river. Each MCS was applied to the model in a preliminary uncertainty analysis and then in a confirmatory uncertainty analysis once parameter uncertainty was reduced. From the uncertainty analyses applied to the Streeter-Phelps model it became clear how each configuration of integrated MCSs could be used to increase a modeler's knowledge in order to improve the model or to make informed decisions concerning the environment.

First the SPMCS was conducted to determine the overall quality of the model's predictions. A SPMCS assesses a model's total prediction uncertainty by considering both epistemic and aleatory uncertainty together in a single MCS.

Once it was established that the model predictions were unsatisfactory, the dominant type of uncertainty was determined. The objective of a TPMCS is to determine which type of uncertainty dominates the model. A TPMCS separates the aleatory and epistemic uncertainty in a WQM. This is achieved by two MCSs, one nested within the other. The result of a TPMCS is a graph with an ensemble of CCDFs. The distribution of the ensemble of CCDFs illustrates the extent of the epistemic uncertainty associated with the model and the distribution of each individual CCDF quantifies the aleatory uncertainty associated with the model. The kinetic rate coefficients were considered to be the parameters with significant epistemic uncertainty and the TPMCS also proved the dominance of their epistemic uncertainty over the rest of the model's aleatory uncertainty.

Finally the key uncertain parameters were determined with the application of the PMCS. It achieves this objective by considering each parameter in the model, one parameter at a time, and completing a full MCS by varying the parameter and keeping the rest of the parameters constant. By assessing the standard deviations in the model results, one can determine the effect of the parameter's uncertainty on the model's total prediction uncertainty. The rates of decay (k_d) and reaeration (k_a) proved to be the coefficients contributing the most to the model's prediction uncertainty. The contribution from the settling rate (k_s) of organic matter was negligible.

The parameter uncertainty in the rate coefficients was then reduced by calibrating the model with an automated technique using a Monte Carlo method. This entailed varying the model's coefficients until

an optimal agreement between the model predictions and the observed data could be established by the minimization of the sum of squares residuals.

Once parameter uncertainty was reduced, a confirmatory uncertainty analysis was conducted to prove that the uncertainty was reduced. Each configuration of MCS was applied for the second time in exactly the same way as the preliminary uncertainty analysis. The SPMCS established that the overall quality of the model's predictions improved. The TPMCS determined that the dominant type of uncertainty associated with the model shifted from being epistemic uncertainty to being aleatory uncertainty. Finally the PMCS confirmed that the key uncertain parameters' contribution to prediction uncertainty was reduced.

The fundamental principles of MCS are very easy to understand and a basic knowledge of statistical methods is all that is needed to conduct an uncertainty analysis using MCS. Monte Carlo methods are robust and thorough in its analysis of a model and it provides full distributions of model predictions in association with probability of occurrence, which is very convenient in any engineering problem where optimization and risk management is important.

Although slightly understated, a highlight of this study is in Chapter 4.8 where it is illustrated how the quantification of a model's prediction uncertainty aided in the determination of a Margin of Safety (MOS) in a management application of the model. The objective of the management application was to determine a TMDL for the hypothetical river. The TMDL had to include a MOS due to the uncertainty associated with the model and the natural system. The MOS was determined by using an implicit approach where by the threshold of the water quality criterion was increased by the amount with which the model over-predicted the critical DO levels in the river. In combination with the implicit approach, the method also involved using a MCS produced output distribution for the TMDL, which included the aleatory and remaining epistemic uncertainty in the TMDL calculations. The total MOS included in the TMDL turned out to be almost 35% of the point source waste load allocation (WLA). Thus the TMDL = WLA + (-0.35) WLA.

The calculation of the MOS was based on a scientific approach rather than an arbitrary assumption of MOS, thus the unnecessary over- or under design of intervention options could be avoided. The use of an uncertainty analysis in the determination of a MOS illustrated the benefits that an uncertainty analysis could provide for any ecological system under environmental management. Any practical decision maker would rather be aware of the uncertainty and assumptions associated with his/her model than be ignorant of it.

6. Recommendations

6.1. General Recommendations

The first and foremost recommendation that always needs to made when discussing mathematical modelling is the proper collection of data. Without proper data collection, model uncertainty spirals out of control. It is impossible to manage an environmental system effectively if it is not known what and how much needs to be managed. The importance of sufficient and high-quality data cannot be overemphasized.

The use of basic uncertainty analysis methods and the associated statistics must never be underestimated. WQMs can become very complex and the use of complex statistical methods can confuse a model user even more. The use of a basic uncertainty analysis method can contribute greatly to the good communication of uncertainty to decision makers and other stakeholders.

When it comes to the management of sensitive environments and making decisions based on WQMs, honesty is the best policy. A model's assumptions and uncertainties must always be made known to decision makers and stakeholders. Modelling honesty in the uncertainty analysis itself is also very important; otherwise the whole point of an uncertainty analysis is undermined.

6.2. Future Research Recommendations

MCS is often criticized as being an approximate technique, which is true, but the accuracy of a MCS can be improved by increasing the number of model runs in the simulation. This however leads to more computer resources being used and time consuming calculations, which can become a problem when large and complex WQMs are employed. Alternative sampling methods such as Latin Hypercube Sampling (LHS) exists and offers some improvements on MCS. Further research on the use of LHS in WQMs could prove insightful on the potential benefits of LHS, especially concerning the convergence of complex WQM results.

The uncertainty analysis performed in this study took place under controlled conditions. The model was calibrated to fit data that was artificially generated. Although this had the advantage of determining the effectiveness with which the Monte Carlo based uncertainty analysis achieved its objectives, it will now be interesting to see how the procedure performs under real conditions. It is therefore suggested that a real environmental system be modeled and an uncertainty analysis of the model be conducted. Sufficient and appropriate data would be needed and a simple and suitable environmental system would have to be identified for this study.

It is often emphasized that environmental management can only benefit from the analysis of a model's uncertainty. These benefits can be economic advantages in terms of modelling and data collection;

can have positive practical implications for the system (e.g. the reduction of risk); and can be time saving in terms of modelling and data collection. Despite all these benefits being mentioned, they haven't been thoroughly assessed in this study. There is obviously also a tipping point when the costs of uncertainty analyses and the reduction of model uncertainty outweigh their benefit. For example, it can sometimes make financially more sense to design TMDLs with outrageous arbitrary margins of safety, rather than undertaking the costs of scientifically determining margins of safety and reducing uncertainty. When does the execution of an uncertainty analysis lose its benefit? It is therefore suggested that a study be undertaken to determine the cost and benefit of a model's uncertainty analysis.

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Appendix A

MATLAB

MATLAB was used to program the experimental simulation and uncertainty analysis of the model in this thesis.

MATLAB is a mathematical software package that was initially designed for numerical linear algebra but it has become a tool for all types of mathematical calculations. MATLAB offers extremely valuable and cost-effective tools that improve the productivity of the programmer. In the context of solving equations, it is considered to be a major improvement in comparison to programming tools such as FORTRAN because there is no need to program the algorithms and only a basic understanding of the mathematics and programming is needed. Using MATLAB minimizes the risk of programming errors and allows the user to immediately visualize simulation results. It has been applied in almost every field of scientific and technical calculations and is also very effective at performing basic statistics. In addition to being very effective, it is also generally available at most academic institutions (Holzbecher, 2007: VII; 3).

A general point of critique though, is the fact that it is very expensive to obtain a user's licence, which limits its use to universities and companies with sufficient funds as well as a real need for it.

MATLAB proved to be very useful in this study due to the mathematical nature of environmental modelling and the need for basic statistical functions in an uncertainty analysis. In addition to that, the costliness of MCS and the effectiveness with which MATLAB could conduct a MCS made MATLAB the ideal software package to use in this study.