THE DEVELOPMENT OF A METHOD FOR THE INCLUSION OF SALINITY EFFECTS INTO ENVIRONMENTAL LIFE CYCLE ASSESSMENTS

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PREFACE

I, Anthony Leske, declare that unless indicated, this thesis is my own work and that it has not been submitted, in whole or in part, for a degree at another university or institution.

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A. Leske
November 2003

As the candidate's supervisor, I have approved this thesis for submission.

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Prof. C.A. Buckley
November 2003

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ABSTRACT

The work presented in this thesis stemmed out of the apparent lack of a method for incorporating salinity effects into environmental life cycle assessments. Salination of the water resources is a well-known problem in South Africa, and is of strategic concern. Any environmental decision support tool that does not allow the evaluation of salinity effects therefore has limited applicability in the South African context. The starting-point for the work presented in this thesis was to evaluate existing impact categories, and the characterisation models used to calculate equivalency factors for these impact categories, in an attempt to incorporate salinity effects into existing categories and/or characterisation models. The types of effects that elevated (above normal background levels) dissolved salt concentrations have on the natural and man-made environment were evaluated, and it was concluded that, although there was some overlap with existing impact categories, some of the salinity effects could not be described by existing impact categories. It was also concluded that there are clear and quantifiable causal relationships between releases to the environment and salinity effects. A separate salinity impact category was therefore recommended that includes all salinity effects, including; aquatic ecotoxicity effects, damage to man-made environment, loss of agricultural production (livestock and crops), aesthetic effects and effects to terrestrial fauna and flora. Damage to the man-made environment is evaluated in terms of effects on equipment and structures, interference with processes, product quality and complexity of waste treatment, and is used as an indicator for the environmental consequences derived from the caused additional activity in the man-made environment. Once a conceptual model for a separate salinity impact category had been formulated, existing characterisation models were evaluated to determine their applicability for modelling salinity effects. Salination is a global problem, but generally restricted to local or regional areas, and in order to characterise salinity effects, an environmental fate model would be required in order to estimate salt concentrations in the various compartments, particularly surface and subsurface water. A well-known environmental fate and effect model was evaluated to determine if it could be used either as is, or in modified form to calculate salinity potentials for LCA. It was however concluded that the model is not suitable for the calculation of salinity potentials, and it was therefore decided to develop an environmental fate model that would overcome the limitations of existing model, in terms of modelling the movement of salts in the environment. In terms of spatial differentiation, the same approach that was adopted in the existing model was adopted in developing an environmental fate model for South African conditions. This was done by defining a "unit South African catchment" (including the air volume above the catchment), which consists of an urban surface; rural agricultural soil (and associated soil moisture); rural natural soil (and associated moisture), groundwater (natural and agricultural) and one river with a flow equal to the

sum of the flows of all rivers in South Africa, and a concentration equal to the average concentration of each river in the country. A non steady-state environmental fate model (or, hydrosalinity model) was developed that can predict environmental concentrations at a daily time-step in all the compartments relevant to the calculation of salinity potentials. The environmental fate model includes all the major processes governing the distribution of common ions (sodium, calcium, magnesium, sulphate, chloride and bicarbonate) in the various compartments, and described as total dissolved salts.

The effect factors used in the characterisation model were based on the target water quality ranges given by the South African Water Quality Guidelines in order to calculate salinity potentials. The total salinity potential is made up of a number of salinity effects potentials, including; damage to man-made environment, aquatic ecotoxicity effects, damage to man-made environment, loss of agricultural production (livestock and crops), aesthetic effects and effects to terrestrial fauna and flora. The total salinity potentials for emissions into the various initial release compartments are shown in the table below.

Initial release compartment	Total salinity potential (kg TDS equ./kg)
Atmosphere	0.013
River	0.16
Rural natural surface	0.03
Rural agricultural surface	1.00

The salinity potentials are only relevant to South African conditions, and their use in LCA in other countries may not be applicable. This, in effect, means that the life cycle activities that generate salts should be within the borders of South Africa. It has been recognised that the LCA methodology requires greater spatial differentiation. Salination is a global problem, but generally restricted to local or regional areas on the globe, and it is foreseen that local or regional salinity potentials would need to be calculated for different areas of the earth where salinity is a problem. The LCA practitioner would then need to know something about the spatial distribution of LCA activities in order to apply the relevant salinity potentials. The LCA practitioner should also take care when applying the salinity potentials to prevent double accounting for certain impacts. Currently, this is simple because no equivalency factors exist for common ions, or for total dissolved salts as a lumped parameter.

The distribution of salinity potentials, which make up the total salinity potential, appears to be supported by the environmental policies and legislation of South Africa, in which irrigation using saline water is listed as a controlled activity, and subject to certain conditions.

The major recommendations regarding further work are focussed on the collection of data that will allow further refinement of the model, and to decrease the uncertainty and variability associated with the results. The values of the published equivalency factors are dependent on the mathematical definition of the local or regional environment, and these values have been calculated for Western European conditions. Equivalency factors may vary by several orders of magnitude, depending on how the local or regional conditions have been defined. It is therefore recommended that the model developed in this work ultimately be included into a global nested model that can be used to calculate equivalency factors for other compounds, including heavy metals and organic compounds. This would result in equivalency factors for all compounds that are relevant to South Africa.

CONTENTS

CHAPTER 3: CONCEPTUAL CHARACTERISATION MODEL DEVELOPMENT

CHAPTER 4: DETAILED FATE MODEL DEVELOPMENT

CHAPTER 5: ENVIRONMENTAL FATE MODEL VALIDATION AND PARAMETER SENSITIVITY

FIGURES

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GLOSSARY

Agreement index
The value of the agreement index is a measure of the degree to which a model's predictions are error free (defined by Equation 5-1).

Causal relationship
The relationship between an *intervention* (or release to the environment) and the effect that the *intervention* has on the environment.

Characterisation
A step in the environmental life cycle assessment methodology where contributions to each environmental *impact category* are quantified by using *equivalency factors*.

Characterisation model
A model that relates an *intervention* to an effect on the environment expressed as an *equivalency factor*.

Classification
A step in the environmental life cycle assessment methodology where all environmental *stressors* are classified according to the kind of environmental problem (or *impact category*) to which they contribute.

Common ions
In the context of this work, common ions include sodium, calcium, magnesium, chloride, sulphate and bicarbonate ions.

Compartment
The sub-units into which the environment is divided. The major compartments are air, water and soil. These compartments may be divided into sub-compartments such as fresh water, seawater, and so on.

Component
The substance that has a potential impact on the environment.

Effects factor
The reciprocal of the predicted *no-effect concentration* (defined by Equation 2-4).

Effects potential
In the context of this work, *effects potential* has the

	same meaning as *equivalency factor*.
Equivalency factor	An *equivalency factor* indicate how much a substance, or *component*, contributes to an environmental problem (*or impact category*). Mathematically, the *equivalency factor* is the product of the *fate factor* and the *effect factor*.
Fate factor	The *fate factor* is the *predicted environmental concentration* divided by the emission into an environmental *compartment*.
Functional unit	A criterion used to enable comparison of life cycle results of two alternatives. The most basic characteristic is the function that a product needs to fulfil. For example, comparison of a disposable paper cup with a china cup would not be valid since the life span of the two differ by a factor of at least 100. Instead, the function of the two alternatives, such as drinking one cup of coffee, could be compared.
Hydrosalinity model	A multimedia environmental fate model used to estimate concentrations of dissolved salts in the various aquatic and terrestrial *compartments*
Impact category	All environmental stressors are classified according to the kind of environmental problem to which they contribute, called impact categories. Examples include global warming, ecotoxicity, acidification and nutrification.
Initial release compartment	The *compartment* into which the *component* is emitted
Intervention	In the context of environmental life cycle assessment, release of a *component* into the environment is generally referred to as an *intervention*
No-effect concentration	The concentration of a *component* in a *compartment* at which no observable effects related to the impact categories are manifest.
Normalization	A step in the environmental life cycle methodology. The normalization step relates the scores obtained

	to the local, national or global situation, by dividing the impact scores by local, national or global figures for each *impact category*.
Predicted environmental concentration	The concentration of a *component* in a *compartment* after a release of the *component* in the same or any other *compartment*.
Risk characterisation ratio	Mathematically, the *risk characterisation ratio* is the *predicted environmental concentration* divided by the predicted *no effect concentration*.
Salination	The increase in concentration of soluble salts in the aquatic and terrestrial environment due to anthropogenic activities.
Salinity potentials	Salinity potentials are the same as *equivalency factors*, but for salinity effects. Salinity potentials include aquatic ecotoxicity, agricultural crop, natural vegetation, livestock, natural wildlife, material damage and aesthetic potentials.
Stressors	In the context of this work, *stressors* are defined as releases of *components* into the environment
Target water quality	The *no-effect concentration* is defined by the Department of Water Affairs and Forestry as the *target water quality*.
Threshold concentration	The concentration above which effects become observable.
Total dissolved salts	In the context of this theses, *total dissolved salt concentration is defined as the sum of the* common ion concentrations.
Total salinity potential	The sum of individual salinity potentials.
Valuation	A step in the environmental life cycle methodology where environmental profiles are reduced to a single score by applying weighting factors.

CHAPTER 1

INTRODUCTION

In this chapter, a brief introduction to environmental life cycle assessment is given, and the technique is briefly compared to other decision support techniques (Section 1.1). In Section 1.2, the salination of South African water resources is discussed in order to highlight the need for incorporating salinity effects into environmental life cycle assessments, in the South African context. The study objectives and the approach adopted in the study are discussed in Section 1.3, where references are made to the various chapters in the thesis.

1.1 INTRODUCTION TO ENVIRONMENTAL LIFE CYCLE ASSESSMENT (LCA)

Environmental life cycle assessment is a tool for the evaluation of the environmental burden of products at all the various stages in their life cycle, from the extraction of resources, the production of materials, product parts and the product itself, the use of the product to the management after discarding. Environmental burden covers all types of impacts on the environment, including extraction of different types of resources, emissions of hazardous substances and different types of land use. The term 'product' is used in its broadest sense, and includes physical goods as well as services. In comparative LCA studies, it is not the products themselves that form the basis for comparison, but the function provided by these products (Guinee et al., 2000).

The environmental life-cycle assessment technique for evaluating the environmental impact of products from cradle to grave is not new. Environmental assessments of products were carried out as far back as the 1960s. From the end of the 1980s, however, interest in LCA has grown strongly, and the methodological development has reached the point where standardisation has occurred through organisations such as the International Organisation for Standardisation (ISO) and SETAC (Wenzel et al., 1997). Table 1.1 gives examples of areas in which LCA can support decision-making.

LCA is one in a number of environmental decision support tools available, including environmental risk assessment, substance flow analysis, material flow accounting, input/output analysis, technology assessment and environmental auditing. Several authors have compared these tools (Sleeswijk et al., 1995; Udo de Haes et al., 2000; Olsen et al., 2001), the major distinguishing features of LCA being:

- LCA follows a holistic approach, bringing the environmental impacts of product functions into one consistent framework. Tools such as risk assessment and substance flow analysis typically focus on specific impacts related to single substances.
- Impact assessment in LCA is currently mostly done at a global scale and disregards time, while for most other tools impact assessment is typically at a regional or local scale and is defined for a given period of time.

Table 1.1: Examples of areas in which LCA can be used as a support in decision-making (Olsen et al., 2001)

Decision-maker	Strategic decisions	Construction and design	Purchase	Sales
Authorities	Support for legislation (e.g. in banning of products) and other instruments of control, studies on infrastructure (e.g. waste management, energy production), identification of research areas	In public service companies (water, energy, and other services); for studies and decision-making (similar to companies use)	When choosing between products and/or suppliers, issuing recommendations for "green procurement"	Eco-labelling, recommendations
Companies	When selecting central production processes, strategy, and business concepts	When selecting materials, process and production improvements, educational purposes	When choosing between products and/or suppliers	Marketing environmental declarations
Individuals	As voters; choosing a lifestyle	-	As consumers; using the eco-label	-
Non-government organisations	Political watch and lobbying	-	Recommendations	-

More detail on the LCA methodology is given in **Chapter 2**, however, a brief description of the methodology is given below.

LCA is commonly described as a four-step process. In the first step (goal definition and scoping), the problem and the intentions of the assessment are defined. The units of comparison are chosen, as well as the type of impacts that should be considered. The potential applications of the LCA determine the technical goals that are to be met. These in turn define the scope of the study. In the second step (inventory analysis) the processes required in the manufacture, use and eventual disposal of the product are specified. The inputs and outputs (such as resource or energy usage, and releases to the environment) for each process are defined. During the third step (impact assessment) the results of the inventory analysis are interpreted in terms of the impacts they have on the environment.

The impact assessment step typically consists of three sub-steps; in the classification step, all environmental stressors are classified according to the kind of environmental problem to which they contribute, called impact categories. In terms of the requirements of ISO 14042, the following impact categories and sub-categories are obligatory:

- Depletion of abiotic resources

- Effects of land use

    o Increase in land competition

- Climate change

- Stratospheric ozone depletion

- Human toxicity

- Eco-toxicity

    o Fresh-water aquatic

    o Marine

    o Terrestrial

- Photo-oxidant formation

- Acidification

- Nutrification

The following additional optional categories have been defined, and are not obligatory at this stage.

- Effects of land use
    - o Loss of life support
    - o Loss of biodiversity
- Toxicity
    - o Fresh-water sediment
    - o Marine sediment
- Radiation
- Depletion of biotic resources
- Desiccation
- Noise
- Waste heat
- Casualties

Releases to the environment can contribute to several impact categories. In the characterisation step, contributions to each impact category are quantified. Several environmental models, called characterisation models, are available for this purpose. These models are used to calculate equivalency factors, which indicate the relative contribution to a specific impact category. Characterisation results in a list of impact profiles, which specify the quantified contribution of the functional unit to each impact category. The impact profiles are not easy to compare since they are usually presented in different units. A normalisation step (which is optional) is therefore sometimes used to identify the size of the impact of the function compared to the size of the total impact. This of course means that the size of the total impact must be known.

The last step (interpretation and improvement assessment) includes an assessment of uncertainties and key assumptions, as well as recommendations for actions. In some cases LCA practitioners take the process one step further by assigning weights to the various impact categories in order to derive a single, weighted average score for the product or function. Several methods have been proposed to derive the weighting factors, but all are based on value judgements (Guinee et al., 2000).

The original intent of this work was to use the LCA technique to evaluate different effluent treatment technologies at a large pulp and paper manufacturing operation that disposes highly

saline effluent by means of irrigation onto agricultural land. The irrigation of saline effluent has, over many years, resulted in elevated salt levels in nearby surface-water resources, and as a result pressure is being placed on the operation by environmental authorities to discontinue irrigation practices. In reviewing the literature on LCA, however, it was soon discovered that there is currently no apparent method available for incorporating the effects of salinity into life-cycle assessments. The objective of the work therefore changed to the development of a method for incorporating salinity effects into life-cycle assessment.

1.2 SALINATION OF SOUTH AFRICAN WATER RESOURCES

Salinity is a global problem. Nearly 40% of the agricultural land in the world is experiencing serious productivity reduction due to soil degradation. In some areas it is as much as 75%. As much as 70% of water use is for irrigation and nearly one third of the 260 million hectares of irrigation land world wide is now affected by salination (UNEP, 2002). In general, however, salination limited to local areas, particularly in industrialised countries that are arid or semi-arid, such as Australia and South Africa. Salinity problems within a country are furthermore generally limited to specific catchments where industrialisation has taken place to a significant degree, or where extensive irrigation takes place

South Africa is classified as a semi-arid country, with an annual rainfall of approximately 497 mm, which is well below the world average of 860 mm. A comparatively narrow region along the eastern and southern coastlines is moderately well watered, but the greater part of the interior and the western portion of the country are arid or semi-arid. Sixty five percent of the country receives less than 500 mm rain annually, which is usually regarded as the minimum for successful dry-land farming. Twenty one percent of the country receives less than 200 mm annually (DWA, 1986).

The quality of many water resources in South Africa is declining. This is primarily as a result of salination, and to a lesser extent because of eutrophication and pollution by trace metals and micro-pollutants (DWA, 1986). In the State of the Environment report published by the Department of Environmental Affairs and Tourism in 1999 (DEAT, 1999), salination of surface water resources is listed as a major concern, particularly in the western Cape, eastern Cape, Kwa-Zulu Natal, and the Vaal River. The total dissolved solids concentrations in many rivers exceed 2 000 mg/L. Maize is the largest commercial crop grown in South Africa. The threshold salinity level (above which yield loss begins) for maize is 1 100 mg/L.

Although little information is available on the extent of groundwater pollution in South Africa, salination of groundwater is also recognised as a threat, particularly in the eastern and southern Cape, and the Northern Province.

In the 1999 State of the Environment report, the major contributions to salinity due to human intervention includes; discharge of municipal and industrial effluent, irrigation return water, urban storm-water runoff, surface mobilisation of pollutants from mining activities and industrial operations and seepage from waste disposal sites, mining and industrial operations. Rapid population growth has led to urbanisation, intensification of agricultural production, and industrialisation. In addition, government policies that have encouraged monoculture and intensive use of agrochemicals have resulted in over-use of land, and degradation of vegetation and soils. Effects of increased salinity include salination of irrigation soils, reduction in crop yields, increased scale formation and corrosion in domestic and industrial water conveyance systems, increased requirement for pre-treatment of selected industrial water uses, and changes in biota. It is estimated that 10% of the 1.2 million ha of land that is irrigated is severely affected by salination (DEAT, 1999).

In August 1998, a White Paper on Integrated Pollution and Waste Management for South Africa was tabled in parliament. Salination of fresh water is listed as a key issue in this policy.

It is evident from this brief introduction to the extent of the salinity problem in South Africa, and its strategic threat to the limited water resources of the country that the exclusion of salinity from any environmental decision support tool would severely undermine its applicability in the South African context.

1.3 STUDY OBJECTIVES AND APPROACH

In broad terms, the objective of the study is to develop a method for incorporating salinity into the environmental life-cycle assessment methodology. This could be achieved in a number of possible ways as indicated in the logic diagram used in the development of the method, shown in Figure 1.1. The numbers in **bold** in Figure 1.1 reference the sections of this document in which the detailed discussions are given. In **Section 2.1** the LCA methodology and the types of decisions that LCA results may support is demonstrated by means of a simple worked example. The example is repeated in **Section 7.2**, in order to demonstrate the effects of incorporating the additional salinity impact category developed during the study.
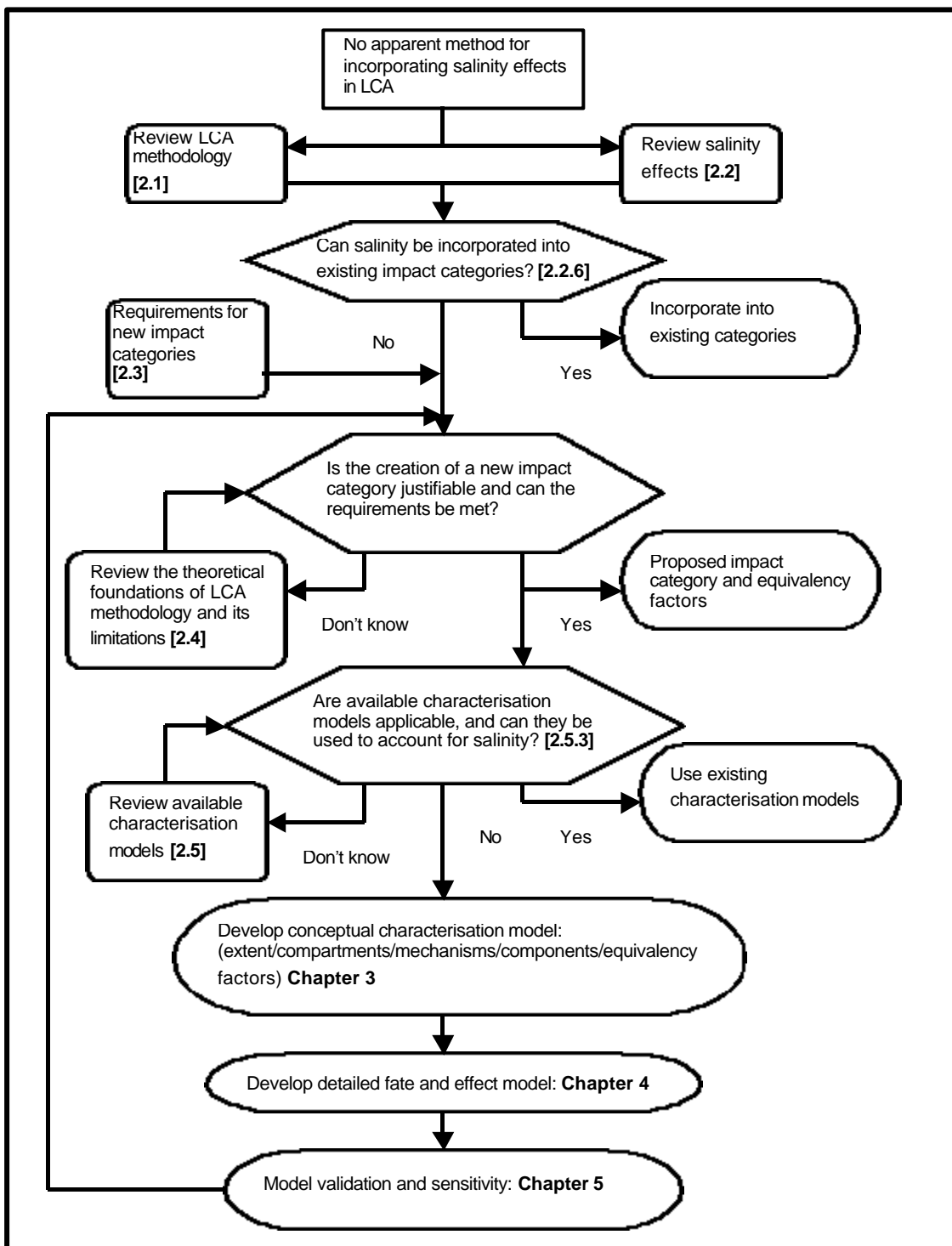
Figure 1.1: Logic diagram for the development of a method for incorporating salinity into LCA

In **Section 2.2**, the term *salinity* is defined, and the effects of salinity on the natural and man-made environment are discussed in detail. The objectives of this literature review are threefold; firstly to establish what the potential salinity impacts on the natural and man-made environment are; secondly to establish whether there are clear causal relationships between releases to the environment, midpoints and endpoints; and lastly to determine if there are any potential impacts that could not be included into existing impact categories. At this point it is established that there are clear and quantifiable causal relationships between releases to the environment and effects for salinity, and that although existing impact categories included some of the salinity effects, others were not included in any of the existing impact categories.

In **Section 2.3** the literature is reviewed to determine the requirements for establishing new impact categories, and in **Section 2.4** the theoretical foundations of the LCA methodology and its limitations are reviewed. It is concluded that, within the framework of the LCA methodology, separate impact category for salinity can be established that meet these requirements (**Section 2.2.6**). These findings were published in May 2003 (Leske and Buckley, 2003).

Once it is established that a separate salinity impact category is justifiable, a characterisation model is needed to calculate equivalency factors for the proposed salinity impact category. The starting point is to evaluate existing characterisation models (**Section 2.5**) in terms of the approach followed, their applicability to South African conditions, their ability to model inorganic ions, and their ability to incorporate all potential salinity effects. It is concluded that although the approach adopted in developing the existing characterisation models was scientifically sound in terms of the theoretical foundations of LCA (**Section 2.4**), the models can not be used to calculate equivalency factors for salinity in the South African context (**Section 2.5.3**), and that a characterisation model is required for South African conditions, using the same approach adopted in existing characterisation models.

In light of the review and conclusions made in **Chapter 2**, there are some general considerations that must be examined before a characterisation model for salinity can be developed. For example, which of the salinity impacts should be included in the model, what geographical extent should the model cover, and what degree of spatial differentiation should be applied? What compartments, components and mechanisms should be included? These questions are addressed in **Section 3.1**. In **Section 3.2**, a conceptual framework for an environmental fate model for salinity is proposed, based on the issues addressed in **Section 3.1**. In **Section 3.3** the fate and exposure components are linked in a conceptual method for characterising salinity effects.

In **Chapter 4**, the conceptual environmental fate model proposed in **Chapter 3** is developed in more detail. The chapter is sub-divided into two sections; **Section 4.1** deals with the atmospheric deposition model, and **Section 4.2** deals with the hydrosalinity model. Existing atmospheric deposition models are not used in this study. A simple atmospheric deposition model is developed and therefore a detailed review of the literature relating to the generation, removal and transport mechanisms of aerosols over South Africa is presented in **Section 4.1.1**. The modelling approach and model development is presented in **Section 4.1.2**. The hydrosalinity model is, however, based on existing models and a detailed literature review is not given. The approach adopted in developing the hydrosalinity model is given in **Section 4.2.1**, and the development of the model itself is given in **Section 4.2.2**.

In **Chapter 5** the environmental fate model developed is validated, based on published data and calculated surface water flow and quality data for the "unit South African catchment". The chapter is divided into four sections. In **Section 5.1**, the approach adopted and the rationale for adopting the approach in validating the environmental fate model is presented. The environmental fate model essentially consists of two sub-models; an atmospheric deposition model, and a hydrosalinity model. These sub-models are covered in **Sections 5.2** and **5.3** respectively. The hydrosalinity model in turn consists of a catchment hydrology (or rainfall-runoff) component, and a salt transport component (which includes a sediment transport component). Each component of the fate model is addressed in the same way in this chapter. Firstly, the parameters used in the model component and, as far as possible published values are presented. Secondly, the calibration results, based on several indices correlating observed to predicted values are presented. A simple sensitivity analysis is conducted to determine the most sensitive parameters, and these parameters are adjusted in order to further refine the calibration of the model. The results of the calibrated model are then presented and discussed. In **Section 5.4** the influence of the identified sensitive parameters on the salinity fate factors is evaluated.

In **Chapter 6** the methodology for determining no-effect concentrations (reciprocal of effect factors) used to determine salinity potentials is presented. In **Section 6.1** the methodology generally adopted for determining effect factors is presented and the differences in methodology and approach adopted in this study are highlighted. The fate factors for the various salinity impacts defined in **Chapter 3** are discussed and presented in **Section 6.2**. The no-effect concentrations used to calculate salinity potentials are summarised in **Section 6.3**.

In **Chapter 7** the calculated salinity potentials are presented and discussed. In environmental life cycle assessment, the magnitude of the emission impulse is determined during the life cycle inventory step. The temporal distribution of the impulse emission is, however, not known. In

Section 7.1 the effects that impulse characteristics have on the values of the salinity potentials are evaluated in order to confirm that salinity potentials are linearly related to impulse magnitude, and that salinity potentials are not a function of the temporal distribution of the impulse emission. In **Section 7.2**, the calculated salinity potentials are presented and discussed. The effect that the inclusion of a salinity impact category has on the types of decisions that life cycle assessment support are evaluated by means of the worked example presented in **Chapter 2**. The methodology and results of the method developed to include salinity in environmental life cycle assessment are evaluated in terms of the requirements for defining new impact categories, presented in **Section 2.3**. Finally, in **Section 7.3**, a discussion of the uncertainty associated with the results is presented and forms the basis for determining recommendations for further work.

Conclusions and recommendations for further work are given in **Chapter 8**.

CHAPTER 2

LITERATURE REVIEW

In this chapter a number of literature reviews are presented. In Section 2.1 the LCA methodology is demonstrated by means of a simple worked example. The example not only demonstrates the methodology, but also highlights the type of information provided by LCA, upon which decisions regarding environmental management are based. The example also provides a basis for comparison with results of the same LCA including the salinity impact category developed during this study, which is presented in Chapter 7. In Section 2.2 the term salinity is defined in the context of this study, and the literature on salinity effects on the natural and man-made environments is reviewed. The purpose of this literature review is also to establish if there are clear and quantifiable causal relationships between releases to the environment and the effects of salinity, as well as to determine, and present a conclusion, on whether the salinity impacts could be incorporated into existing impact categories. In Section 2.3 the literature is reviewed in order to determine the requirements for defining new impact categories. The literature on the theoretical foundations of LCA, upon which the characterisation models are based, is reviewed in Section 24. In Section 2.5 an existing characterisation model is evaluated in terms of its suitability for use in characterising salinity effects in the South African context, and a conclusion in this regard is presented.

2.1 INTRODUCTION TO LCA METHODOLOGY

The simplest method of demonstrating the LCA methodology is by means of a simple worked example, using hypothetical emission values. The example will highlight the sequential steps that are followed when conducting an LCA, the calculation methods, and the interpretation of the LCA results, and will also be used to highlight shortcomings of the LCA methodology, particularly with regard to salinity. Several guidelines have been published for conducting LCAs. The guideline published by UNEP (UNEP, 1996) has been used as a basis for demonstrating the methodology.

The worked example is repeated in **Chapter 7** in order to demonstrate the effects that incorporating the additional salinity impact category that was developed during the study would have on the types of decisions that are made based on information provided by LCA.

The framework for conducting LCAs is shown in Figure 2.1. The steps shown in the framework are followed for the worked example given below.

Background to the LCA worked example.

Pressure is being placed on a large water intensive, manufacturing operation, by environmental authorities, to reduce the amount of water used. The operation is self sufficient with respect to electrical energy, which is generated on site by the combustion of coal and other organic material. The operation has a small discharge of wastewater directly into a nearby river, but the bulk of the effluent generated by the operation is irrigated on agricultural pastures. Environmental authorities do not regard the disposal of wastes by means of irrigation as good management practice, and the operation is considering the installation of an effluent treatment plant. Treated effluent will be recycled into the operation, resulting in a reduction in water use and a significant reduction in the amount and contaminant loads requiring irrigation. The project will, however, result in an increase in emissions to atmosphere due to an increased energy demand.
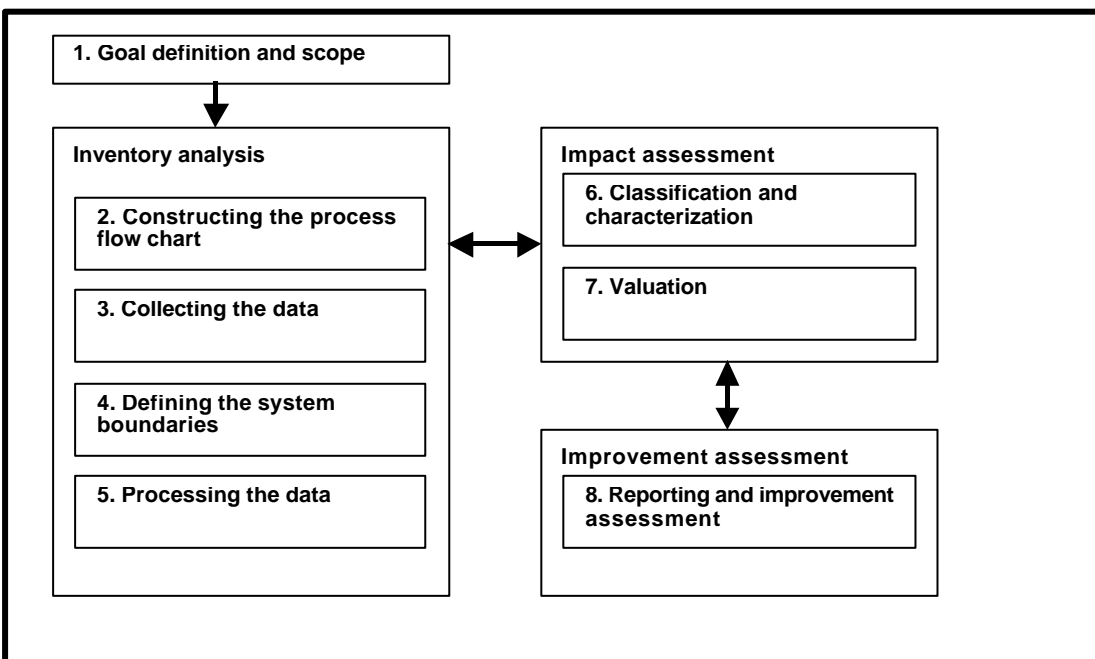
Figure 2.1: The framework for life cycle assessment (UNEP, 1996)

Step 1: Goal definition and scope

Management at the operation would like to use the results of an LCA to assist them in deciding whether to implement the effluent treatment project or not. In particular, they would like to know what the environmental impacts of the current operation are, and how these will change if the project is implemented. A particular question that must be addressed is, do the advantages of reduced effluent loads outweigh the disadvantages of increased atmospheric emissions? Based on these objectives, it was decided that one ton of product will be used as the functional unit.

Steps 2 – 5: Inventory analysis

Based on the objectives of the LCA, and the fact that the quantity of raw materials (excluding coal) and products would remain unchanged, a "gate-to-gate" LCA would be conducted, and that individual unit processes within the operation would not be evaluated separately. The process flow chart for the example is therefore simple, and is shown in Figure 2.2.

From atmospheric emission and effluent monitoring data gathered by the operating personnel, the specific pollutant loads (in kg/ton product) were calculated, and are shown in Table 2.1, which is known as the life cycle inventory.

Step 6: Classification and characterisation

In the classification step, all environmental 'stressors' (emissions in this example) are classified according to the kind of environmental problem (or impact category) to which they contribute. Each release to the environment can contribute to several types of problems. Table 2.2 is a matrix showing which of the emissions in the example contributes to the environmental impact categories shown. To simplify the calculations, not all possible impact categories or contributions to impact categories were selected.

In the characterization step, contributions to each environmental impact category are quantified by using equivalency factors, which indicate how much a substance contributes to a problem compared to a reference substance. The life cycle inventory results (Table 2.1) are multiplied with the corresponding equivalency factors (shown in Table 2.3) and added per impact category to give a list of figures called an impact profile, shown in Table 2.4 and illustrated graphically in Figure 2.3.
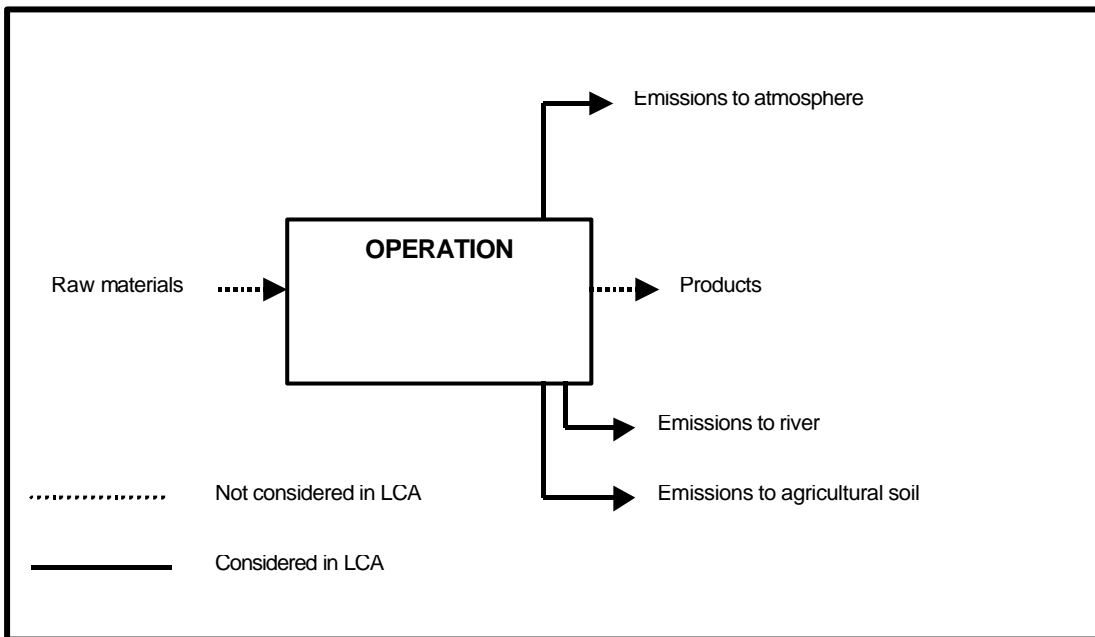
Figure 2.2: Process flow chart for LCA worked example

The various impact categories in the impact profile shown in Figure 2.3 cannot be compared with each other since they are expressed in different units. It can, however, be deduced that implementation of the proposed water treatment plant will significantly increase the global warming potential (by 40%), acidification potential (by 30%), nutrification potential (by 15%) and to a lesser extent the photochemical oxidation potential (by 9%). On the other hand however, the fresh water aquatic ecotoxicity potential will decrease by 21%, the fresh water sedient ecotoxicity potential will decrease by 25%. Based on this information, management may decide that the magnitude of the increase in some of the environmental effects outweigh the magnitude of the decrease in other effects, and may therefore decide not to build the effluent treatment plant.

To be able to directly compare the various impact scores, a normalization step is required. The normalization step relates the scores obtained to the local, national or global situation, by dividing the impact scores by local, national or global figures for each impact category. Thus the magnitude of the impact in relation to the total problem can be gauged. Normalisation is a recommended step, but is not obligatory in terms of the ISO standards.

In the worked example the normalization step is not included since the example is used to demonstrate the effect that inclusion of a salinity impact category (refer to **Chapter 7**) may have on the types of decisions that may be made based on life cycle assessment results. In order to

normalise the impacts, impact scores on some geographical scale would be needed and there are currently no impact scores for salinity.

Table 2.1: Life cycle inventory for worked example

	Specific pollutant loads (kg/ton product)	
	Base case	With treatment
Emissions to air		
Carbon dioxide	3.0	4.2
Carbon monoxide	1.20	1.56
Oxides of nitrogen (NOx)	0.90	1.17
Sulphur dioxide	1.30	1.69
Particulate matter (PM10)	1.0	1.3
Hydrogen sulphide	0.5	0.65
Ammonia	0.10	0.13
Carbon disulphide	0.20	0.22
Emissions to fresh water		
Ammonia	0.001	0.001
Phosphate	0.002	0.002
Chemical oxygen demand	0.1	0.1
Lead	0.001	0.001
Total dissolved salts	1.0	1.0
Emissions to agricultural soil		
Chemical oxygen demand	2.0	0.4
Carbon disulphide	0.0010	0.0002
Hydrogen sulphide	0.010	0.002
Lead	0.00002	0.00001
Cadmium	0.000030	0.000026
Copper	0.00030	0.0002
Dichloromethane	0.00004	0.00008
Total dissolved salts	6.0	1.0

Step 7: Valuation

In the valuation step, the environmental profiles are reduced to a single score by applying weighting factors. Weighting factors are largely subjective, and give an indication of the relative value of one impact category compared to another. For example, national environmental policies may dictate that in the short term pollution of water resources is more important than atmospheric pollution. Global warming will therefore have a lower weighting that fresh water ecotoxicity, for example. In the worked example, assuming all categories were equally weighted, the total score

for the base case is 11.1, and with effluent treatment 11.0. There is thus not a strong case to implement the effluent treatment project.

Step 8: Reporting and improvement assessment

This step is self-explanatory. The results can be presented in a number of ways. For example, the contribution to each impact category by each pollutant can be examined in order to prioritise environmental management strategies for dealing with these contaminants.

Table 2.2: Classification matrix for worked example, excluding salinity

	GWP	HTP	FAETP	FSETP	TETP	POCP	AP	NP
Emissions to air								
Carbon dioxide	X							
Carbon monoxide		X				X		
Oxides of nitrogen (NOx)		X				X	X	X
Sulphur dioxide		X				X	X	
Particulate matter (PM10)		X						
Hydrogen sulphide		X						
Ammonia		X					X	X
Carbon disulphide		X	X	X	X			
Emissions to fresh water								
Ammonia								X
Phosphate		X						X
Chemical oxygen demand								X
Lead		X	X	X	X			
Total dissolved salts								
Emissions to agricultural soil								
Chemical oxygen demand								
Carbon disulphide		X	X	X	X			
Hydrogen sulphide								
Lead		X	X	X	X			
Cadmium		X	X	X	X			
Copper		X	X	X	X			
Dichloromethane		X	X	X	X			
Total dissolved salts								

GWP = global warming potential, HTP = human toxicity potential

FAETP = fresh water ecotoxicity potential, FSETP = fresh water sediment ecotoxicity potential

TETP = terrestrial ecotoxicity potential, POCP = photochemical oxidant formation

AP = acidification potential, NP = nutrification potential

Table 2.3: Equivalency factors for worked example, excluding salinity

	GWP	HTP	FAETP	FSETP	TETP	POCP	AP	NP
Emissions to air								
Carbon dioxide	1							
Carbon monoxide		**0.012**				0.027		
Oxides of nitrogen (NOx)		**0.78**				0.028	0.5	0.13
Sulphur dioxide		0.096				0.048	1.2	
Particulate matter (PM10)		0.82						
Hydrogen sulphide		0.22						
Ammonia		0.1					1.6	0.35
Carbon disulphide		1.6	0.33	0.0027	0.0051			
Emissions to fresh water								
Ammonia								0.33
Phosphate		0.00052						1.0
Chemical oxygen demand								**0.022**
Lead		12	9.6	250	4.8×10^{-22}			
Total dissolved salts								
Emissions to agricultural soil								
Chemical oxygen demand								
Carbon disulphide		3.6	0.34	0.28	1.6			
Hydrogen sulphide								
Lead		3300	6.5	170	330			
Cadmium		20000	7800	2000	1700			
Copper		94	5900	1500	140			
Dichloromethane		2.4	0.00016	0.00011	0.00025			
Total dissolved salts								

GWP = global warming potential (kg CO_2 eq./kg)

HTP = human toxicity potential (kg 1,4-DCB eq./kg)

FAETP = fresh water ecotoxicity potential (kg 1,4-DCB eq./kg)

FSETP = fresh water sediment ecotoxicity potential (kg 1,4-DCB eq./kg)

TETP = terrestrial ecotoxicity potential (kg 1,4-DCB eq./kg)

POCP = photochemical oxidant formation (kg ethylene eq/kg)

AP = acidification potential (kg SO_2 eq./kg)

NP = nutrification potential (kg PO_4 eq./kg)

Values in **bold** are taken from UNEP (1996), all other values are taken from Guinee et al. (2000)

Table 2.4: Impact profile for the worked example LCA, excluding salinity

Impact category	Impact score	
	Base case	**With effluent treatment**
Global warming (kg CO_2 equ.)	3.000	4.200
Human toxicity (kg 1,4-DCB equ.)	2.811	3.240
Fresh water exocoxicity (kg 1,4-DCB equ.)	2.021	1.400
Fresh water sediment ecotoxicity (kg 1,4-DCB equ.)	0.764	0.604
Terrestrial ecotoxicity (kg 1,4-DCB equ.)	0.102	0.077
Photochemical oxidant formation (kg ethylene eq.)	0.120	0.131
Acidification (kg SO_2 eq)	2.170	2.821
Nutrification (kg PO_4 eq)	0.157	0.202

The simple worked example above demonstrates the methodology that is followed when conducting a LCA, and the type of information that is provided by the technique. In practice, in this particular example, other decision support tools such as environmental impact assessment could have been used in conjunction with LCA. The example does however highlight the fact that there is currently no method of incorporating salinity into the LCA. One of the major emissions from the operation in the worked example is dissolved salts, which could not be taken into account because no impact category exists for salinity and no equivalency factors are available for common ions.
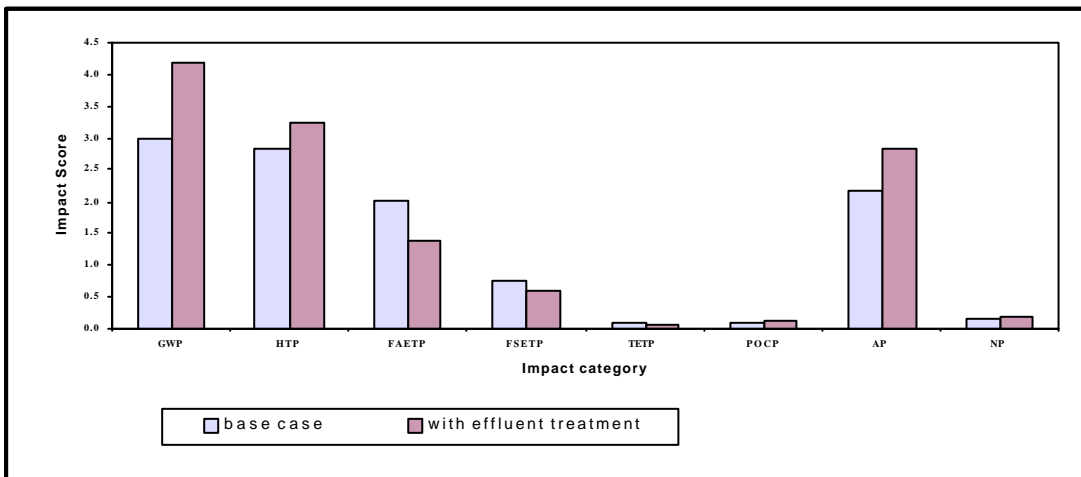
Figure 2.3: Impact profile for the LCA worked example, excluding salinity

2.2 SALINITY EFFECTS

In this section the term *salinity* is defined in the context of this study, and the literature on salinity effects on the natural and man-made environments is reviewed. The purpose of this literature review is also to establish if there are clear and quantifiable causal relationships between releases to the environment and the effects of salinity, as well as to determine, and present a conclusion, on whether the salinity impacts could be incorporated into existing impact categories.

2.2.1 Definition of salinity

In order to determine whether the creation of a salinity impact category has merit and meets the requirements for new categories, it is prudent to define the term "salinity" in the context of environmental LCA, and to review the effects of salinity.

In the Water Quality Guidelines for Aquatic Ecosystems (DWAF, 1996) salinity, described as total dissolved salts (TDS), is classified as a non-toxic inorganic constituent. Non-toxic inorganic constituents are in turn defined as ones which may cause toxic effects at extreme concentrations, but which are generally system variables in that their natural concentrations depend on localised geochemical, physical and hydrological processes.

A distinction is therefore made between toxic inorganic constituents (such as heavy metals) that are toxic at low concentrations (in the order of up to several mg/L, van Vuuren et al., 1994), and so called non-toxic inorganic constituents, or common ions (such as sodium, calcium, magnesium, chloride, sulphate, and bicarbonate) that only exhibit toxic and other effects at high (in the order of hundreds to thousands of mg/L) concentrations that are above normal background levels (DWAF, 1996). In defining a salinity impact category in the context of LCAs, "salinity impacts" are therefore defined as those impacts caused by elevated (above natural background levels) common ion concentrations.

Sodium, calcium, magnesium, chloride, sulphate and bicarbonate ions make up the major fraction of the total ionic concentration in South African waters. Using Maucha diagrams, Day and King (1995) classify surface water in South Africa into four categories, based on proportional concentrations of dominant ions:

Category 1: Dominant ions are Ca^{2+}, Mg^{2+}, HCO_3^- (Na^+ is less than 25% of cations). These waters are "rock dominated", and are restricted to the regions of

the high altitude basalt cap of Lesotho/Kwa-Zulu-Natal and the dolomite and Pretoria Series of the Northern Transvaal.

Category 2:   Dominant ions are Ca^{2+}, Mg^{2+}, HCO_3^- (Na^+ is greater than 25% of cations). These waters are "rock dominated", mostly encircling Category 1 at lower altitudes. It also occurs on Karoo and Waterberg sedimentary rocks and igneous rocks of the Basement Complex and the Bushveld Igneous Complex.

Category 3:   Dominant ions are Ca^{2+}, Mg^{2+}, HCO_3^-, Na^+, Cl^- (more or less co-dominant). These waters are widespread and not apparently associated with any particular geological formations.

Category 4:   Dominant ions are Na^+ and Cl^-. Dilute waters in Category 4 are rainfall dominated, and concentrated water is evaporation-rainfall dominated. Occurs in the south-western Cape on Table Mountain Sandstones, in the western arid regions on Karoo sediments, and in coastal Kwa-Zulu-Natal on a variety of substrata.

The categories defined show clear regional patterns that are attributed to geological influences. The pH of water does not affect the TDS concentration in water significantly. Changing the pH of water does, however, change the concentration of both H^+ and OH^-, which in turn affects the ionic and osmotic balance of aquatic organisms. Relatively small changes in pH are not normally lethal, although sub-lethal effects may occur. Most often, lethal effects are related to the mobilisation of toxic substances (Dallas and Day, 1994). The pH values for natural waters in South Africa usually range between 6.5 and 8.0 (Dallas et al., 1998).

Elevated salt levels in South African surface waters (Dallas and Day, 1994) and groundwater (Du Preez et al., 2000) have been widely reported and are of national concern (DEAT, 1991).

2.2.2 Effects on soil and plants

Both the inherent permeability and hard-setting characteristics of a soil can be modified by irrigation with highly saline water. The sodium adsorption ratio (SAR) is an index of the potential of irrigation water to induce sodic soil conditions. The SAR is calculated as follows:

$$SAR = \frac{Na^+}{[(Ca^{2+} + Mg^{2+})/2]^{0.5}}$$

[2-1]

Ion concentrations in the above expression are expressed as mmol/L. An increase in SAR will result in a decrease in the permeability of the soil, thereby increasing runoff and decreasing the amount of water available for plant growth, and hence lowering the crop yield. Data on the effects of SAR on crop yields and quality are available (Du Preez et al., 2000).

Irrigation using saline water induces soil salinity, which results in a reduction of crop yields once a threshold soil salinity, which is specific to each crop, is exceeded. A plant's tolerance to salt depends not only on the salinity, but also on many other factors such as soil, climate, plant variety and growth stage, agronomic and irrigation practices. Plant parts are also not affected equally; shoot growth is usually influenced more than root growth. The leaf-to-stem ratio is also often affected.

Salinity in the root zone can adversely affect growth due to either a decrease of the osmotic potential (decreased water availability) caused by the high concentration of soluble ions and/or specific ion effects, which include toxicity of specific ions and/or unfavourable ratios of such ions. In addition, salinity disrupts nutrition by decreasing the activity of nutrient ions due to ionic strength, regardless of the substrate (Barnard *et al*., 1998).

Published data on the effects of elevated concentrations of dissolved salts, and individual ions on plants (including various crops, ornamental shrubs, trees and ground-covers) are available (Maas, 1990). These data are usually expressed as threshold concentrations at which no yield loss occurs, and concentrations at which different yield losses occur.

High salt levels in surface water may also cause a decrease in the abundance and diversity of riparian vegetation. This in turn may modify temperatures, sediment inputs, organic material

sources. Very little information is available on South African species, however: some data are available on Australian species (WRC, 2000b).

Phytoplankton communities may change slightly with an increase in salinity, with less tolerant species giving way to more tolerant species (WRC, 2000b).

2.2.3 Effects on animals and humans

Saline water may detrimentally affect animal health by rendering the water unpalatable. Palatability is also influenced by the types of salts present. Magnesium sulphate is more harmful than sodium chloride or sodium sulphate. The main water quality constituents implicated in palatability effects are chloride, sulphate, magnesium, bicarbonates and calcium. Direct effects of unpalatability include the refusal to consume water, consumption below the physical requirement, or in extreme cases, over consumption. The main toxicological effects of high-salinity waters on animals include symptoms of diarrhoea and dehydration. Acute toxic effects related to specific ions are often indirectly due to the increased water intake and can elicit a toxic response at levels normally safe. Different species have different tolerances for saline water, and can adapt to a certain degree (DWAF, 1996).

Published data on salinity tolerances for livestock are available (Casey et al., 1998); however, very few data are available for wild animals. One report (WRC, 2000b) suggests that wildlife is not affected at salinity levels of up to 1 200 mg/L TDS.

Low concentrations of particularly calcium and magnesium salts have nutritional value, although water with an extremely low dissolved salts concentration is objectionable due to its flat, insipid taste. Human health effects related to dissolved salts are minimal at concentrations of below 2 000 to 3 000 mg/L. In contrast, high concentrations of salts impart an unpleasant taste to water and may also adversely affect the kidneys. Some of the human physiological effects that may be directly related to high salt concentrations include (DWAF, 1996):

- Laxative effects, mainly from sodium sulphate and magnesium sulphate.
- Adverse effects of sodium on certain cardiac patients and hypersensitive individuals.
- Effects of sodium on women with toxaemia associated with pregnancy
- Some effects on kidney function

Target water quality objectives are published for human health and taste effects for TDS, and for selected ions (DWAF, 1996).

2.2.4 Effects on aquatic ecosystems

Each species of aquatic organism is adapted to living in water of a certain quality, although some can tolerate wide differences in concentration of a wide variety of constituents, whereas others cannot (Dallas and Day, 1994). Changes in the dissolved salt concentration can have an effect on individual species, community structures and on microbial and ecological processes such as rates of metabolism and nutrient cycling (Dallas *et al*., 1998)

In a review done by Jooste et al. (2000), the lack of data on the sensitivity of freshwater plants and animals to salinity increases was highlighted. In general, however, it was concluded that for microbial communities, small changes in salinity have little effect. Many macrophytes are, however, sensitive and exhibit many sub-lethal responses. Invertebrates are most sensitive to increasing salinities. The most sensitive insects include stones, some may-flies, caddis-flies, dragon-flies and water-bugs. The most sensitive molluscs are pulmonate gastropods. Fish are generally tolerant to salinities in excess of 10 000 mg/L TDS, however, larval fish are more sensitive than adults, and eggs are more tolerant than larvae. There is some evidence of low breeding success in water birds where salinity levels are above 3 000 mg/L. Fresh-water turtles are most at risk.

Results on salinity tolerances of selected macro-invertebrates of the Sabi River in the Kruger National Park of South Africa done by Palmer and Scherman (2000) linked mortality to increasing salinity and the nature of the salt used to elevate the salinity.

The South African Water Quality Guidelines for Aquatic Ecosystems (DWAF, 1996) state that the rate of change of salt concentration, and the duration of change appear to be more important than absolute changes in concentration. Guidelines are given in terms of concentration increase.

2.2.5 Effects on man-made environment

In conjunction with pH value, TDS values play a major role in the corrosion or scaling potential of water. Depending on the nature of the dominant cations and anions, the water will either have a tendency to scale (carbonates, sulphates, silica, calcium and magnesium) or corrode (chlorides and sulphates). High levels of dissolved salts can also indirectly interfere with the proper functioning of several industrial processes and may affect product quality. In addition, wastes containing high salt levels discharged from industrial processes will require more sophisticated

and expensive treatment to remove the salts. Target water quality guidelines are published for different categories of industries (DWAF, 1996).

Several indices (such as the Langelier Saturation Index and calcium carbonate precipitation potential) can be used to indicate a water's tendency to scale or corrode; however, a detailed analysis of the water is required (WRC, 2000b).

From the above review, a simplified causal relationship diagram for salinity has been constructed and is shown in Figure 2.4.

2.2.6 Conclusions

In the review of the literature, only one reference could be found that deals with the inclusion of salinity into life cycle assessment. Feitz and Lundie (2002) developed a salinity potential based purely on the potential of irrigation water to adversely affect the structure of soil. The method, which is based on the calculation of the sodium adsorption ratio in the soil, requires detailed information on the quality of the irrigation water and individual equivalency factors must be calculated for each relevant life cycle step. By the authors' own admission, the proposed method has severe limitations.

From the literature review of LCA methodology and the impacts of salinity given above, the following can be concluded:

- There is currently no separate impact category for salinity; however, some salinity impacts do fall within some of the existing impact categories, in particular fresh water and terrestrial ecotoxicity effects. Material damage and aesthetic effects cannot be included into existing impact categories.
- There are clear and quantifiable causal relationships between releases to the environment and salinity effects.
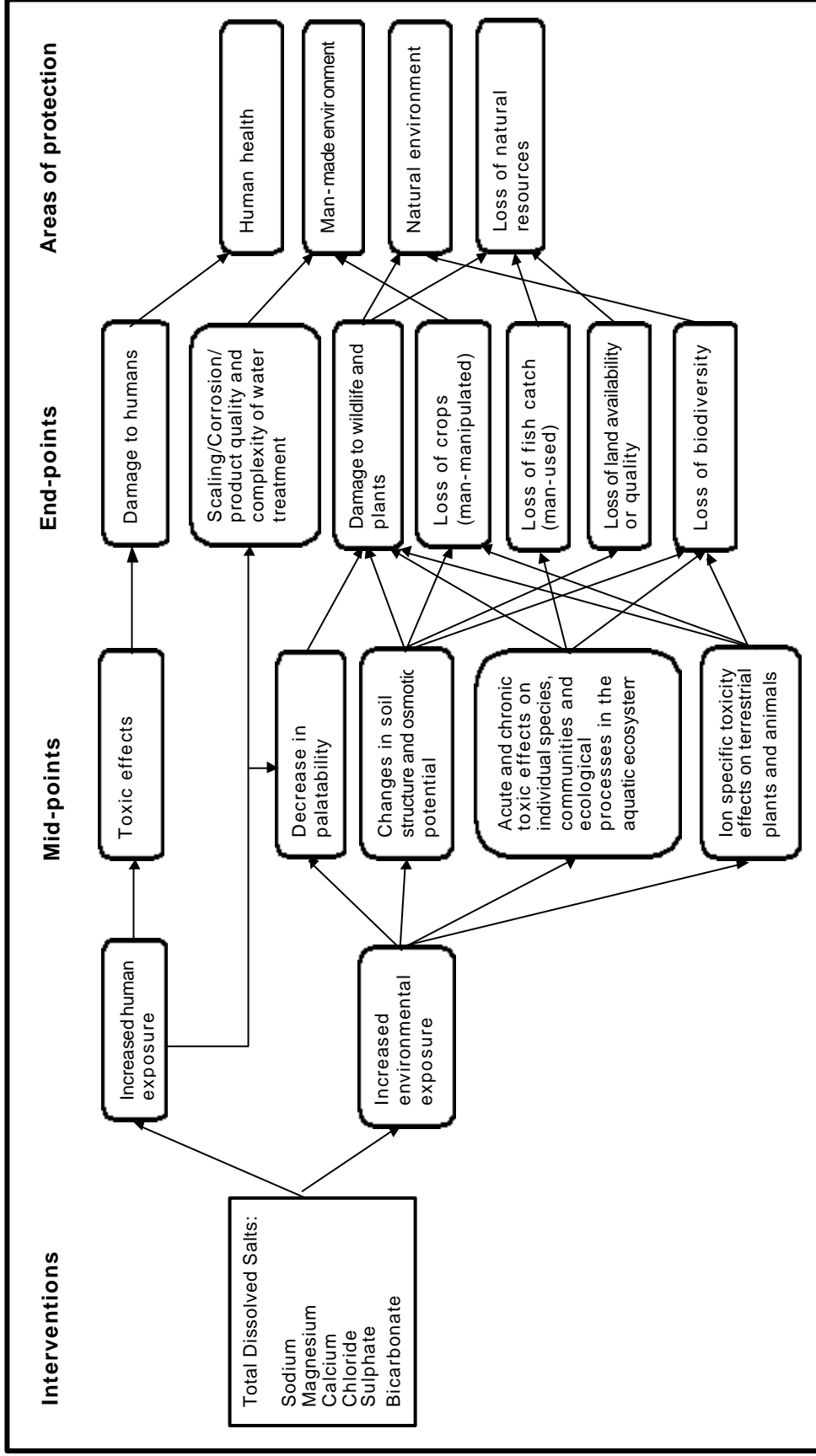
Figure 2.4: Causal relationships between mid-points, end-points and areas of protection for salinity

2.3 REQUIREMENTS FOR DEFINING NEW IMPACT CATEGORIES

A number of requirements for definition of new impact categories have been defined by the Society of Environmental Toxicology and Chemistry (SETAC), and are shown in Table 2.5.

An important limitation set by ISO in defining new impact categories is that value choices are not allowed in comparative assertions. The SETAC-Europe working group may, however, deviate from this ISO requirement. The number of impact categories has to be limited by practicality. One possible way to split categories that are too heterogeneous and do not allow for scientifically valid aggregation is to use sub-categories (Udo de Haes *et al*., 1999).

The requirements for defining new impact categories are listed in Table 2.5 and are re-visited in **Chapter 7.**

Table 2.5: Requirements for defining new impact categories (Udo de Haas *et al*., 1999)

General starting point:
1. A framework shall be developed which is open to further scientific progress and further detailing of new information.

Starting points for total categories:
2. The categories shall together enable encompassing assessment of relevant impacts, which are known today.
3. The categories should have the least overlap possible (independence).
4. The total of the impact category should amount to a not too high number (practicality).

Starting points for separate impact categories:
5. The category indicator can be chosen anywhere in the environmental mechanism of an impact category, from releases to the environment to category end-points.
6. The category indicator should be modelled in a scientific and technically valid way in relation to the releases to the environment (i.e. using a distinct identifiable environmental mechanism and / or reproducible empirical observation)
7. The category indicator shall be environmentally relevant (i.e. it shall have sufficiently clear links to the category end-points)
8. It must be possible that characterisation factors are multiplied by mass or other units indicating the magnitude of the release to the environment.

2.4 THEORETICAL FOUNDATIONS OF LCA

There are two fundamentally different methodologies for developing methods for LCA. On the one hand, there is the methodology in which a comparison of theoretical predictions and actual phenomena provides the benchmark for the adequacy of the LCA theory. A usual approach in

this methodology is to analyse the complicated structure in a number of simpler steps. These steps correspond to portions of accepted models, disciplines and causal relationships, such as multi-media fate models. This approach is suitable to change-oriented LCA, where the environmental consequences of different options for fulfilling a certain function are compiled and evaluated. On the other hand, there is descriptive LCA, which is not based on scientific method and cannot be tested empirically. Although there is one ultimate benchmark for testing the predictions of change-oriented LCA, it is clear that this benchmark is useless in practice due to the complicated autonomous developments in society, economy and the environment. The comparison of the predictions of LCA with reality is therefore practically unattainable (Guinee et al., 2000). The predictions made with change-oriented LCA are based on model calculations, and a model is a simplified representation of real mechanisms and phenomena. The choices in modelling are however not fully subjective. Depending on the questions asked or answers required, some models are more appropriate than others. The approach adopted should be as explicit as possible in the assumptions and simplifications that are introduced in modelling the environmental consequences of change.

2.4.1 A general model for LCA

When studying the change in environmental interventions (release into the environment) or effects it is necessary to specify the time pattern and reference situation, as shown in Figure 2.5.

The LCA analysis is between two parallel systems (e_1 being the predicted future state without the environmental intervention – or reference situation, and e_2 being the predicted future state with the environmental intervention); not a before-after comparison, but a with-and-without comparison.

A general equation for describing the change in environmental effects ($\Delta_{s,t}$) would include not only time (t), but also space (represented by dimensions x, y and z), as shown in Equation [2-2]:

$$\Delta_{s,t} = \int\limits_{t_0}^{\infty} \int\limits_{world} \int \int [e_2(x,y,z,t) - e_1(x,y,z,t)]dx\,dy\,dz\,dt \qquad [2-2]$$

Choosing one point in time (e.g. time t_1 in Figure 2.5) will discard many effects from the life cycle. If all effects over time are required, it is necessary to integrate over time. In the spatial domain, it is theoretically possible to restrict the analysis to one location, modelling of spatial differentiation

within a number of regions, or as shown in Equation [2-2] integrating over the entire spatial domain.
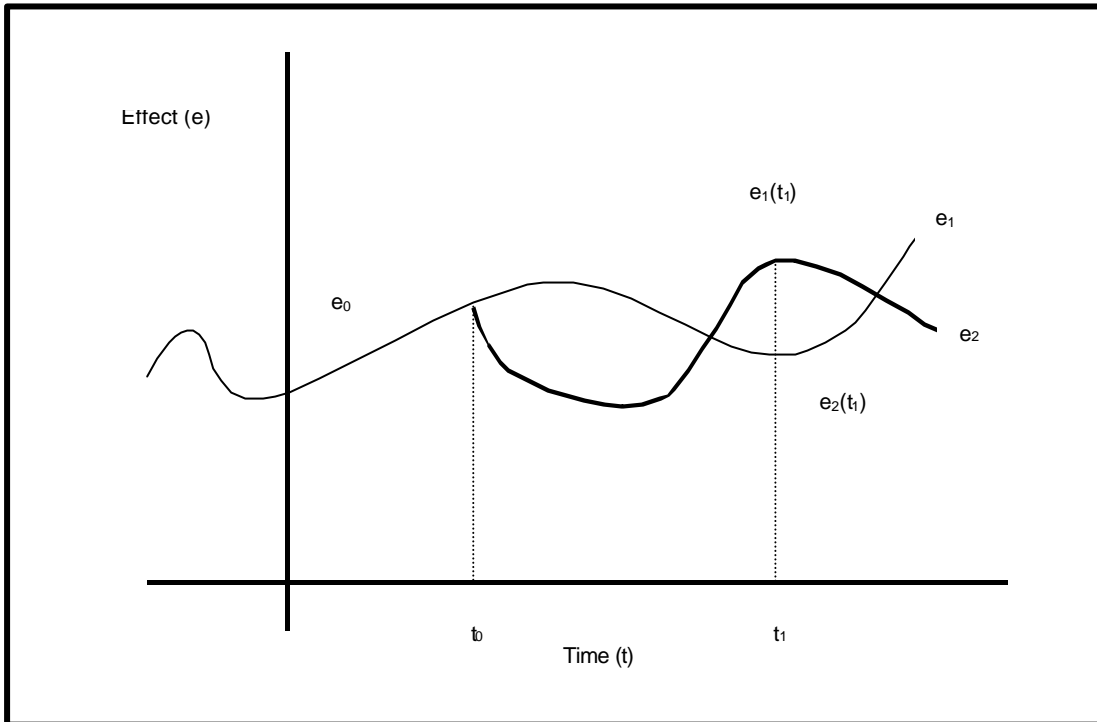
Figure 2.5: Time pattern of effect (e) before a choice (e_0 to the left of t_0), after the choice not implemented (e_1, to the right of t_0) and after the choice is implemented (e_2, to the right of t_0) (adapted from Guinee _et al_., 2000).

2.4.2 Model simplifications

Equation [2-2] emphasises the idealistic concept that a full temporal and spatial integration of emissions/effects of pollutants and extraction of resources is required in LCA methodology. Equation [2-2] is however of little practical use. LCA deals with complex interwoven networks of mining, industrial, agricultural, household and waste management activities. The patterns of these activities are dispersed over many locations and may span decades. The mathematical relationships that describe these real mechanisms are in principle, non-linear, dynamic and will often show hysteresis and irreversibility. No such model of "full reality" exists.

Practitioners of LCA are happy if simplifying assumptions are made so that modelling can be done with reasonable accuracy that include the total release into the environment, integrated over all locations and infinite time in an assumed steady state. The omission of economic mechanisms

and spatial detail leads to a great simplification, but it reduces the quality of the results of the analysis. The inherent simplifications in Equation [2-2] are:

- *Omission of spatial detail.* For example, emissions in the vicinity of different types of ecosystems are not distinguished from one another. This does not mean that distances between unit processes are set equal to zero, but only that transport is taken into account. It also does not mean that all unit processes are assumed to operate according to the technological state that is epresentative of one region. We may still distinguish between emission characteristics for electricity production at different places. We only do not specify where the emissions occur. The only default spatial details that are kept are those along a short list of environmental media: air, surface water, soil, sea and sediment. The implicit value judgement made in the spatial integration step is, however, that similar effects in different places count the same in the ultimate evaluation of effects. The reliability and validity of LCA results may be much improved by the introduction of further spatial differentiation. Although space specific data will almost never be available for all processes within the product life cycle, a space specific assessment may be preferable for those processes for which the required information is available. In order to make spatial differentiation generally applicable to any process in a product life cycle, spatially specific equivalency factors are needed. This has not been achieved yet.
- *Omission of temporal detail.* This means that emissions are specified as total time-integrated emissions over the time span covered by the functional unit.
- *Omission of non-linearity.* This means, for example, that when the production of 1 kg of steel is associated with an emission of 5 kg of a substance, the production of 2 kg of steel will result in the emission of 10 kg of that substance.

Multi-media fate models in risk assessment relate continuous emission fluxes to environmental concentrations. Since multi-media fate models depend on geographical and climatological parameters, it is almost impossible to use them without applying some form of spatial differentiation. The use of single values for such parameters may lead to large deviations. Spatial differentiation with respect to fate comes down to the further division of each media into a number of different compartments. All these compartments together compose the so-called *unit world*. The spatially non-differentiated unit world consists of a small number of homogeneously mixed media, and the spatially differentiated unit world consists of a larger number of homogeneously mixed compartments.

The default simplification of full space and time integration results in no information on spatial and temporal detail being available in the model. One only specifies the total life cycle loadings, in the form of aggregated amounts of releases. Hence any attempt to interpret the contribution of these

substances to environmental impact categories, such as ecotoxicity and acidification, can only be made without incorporating spatial and temporal details.

In LCA, it is the **capacity** of causing harmful effects that forms the basis for the assessment, and not so much the extent to which this capacity has become **effective**. If we move away from full space and time integration to add more details with respect to spatial and temporal characteristics of release and receiving environment, then we are entering the area of **actual** impacts, as opposed to **potential** impacts. In general, for an assessment in completely potential terms, it suffices to use a smaller number of model parameters. For an assessment in completely actual terms, a larger number of parameters are required.

The normal practice of LCA currently remains placing the emphasis on completeness rather than elaborateness of mechanisms (Guinee et al., 2000).

2.4.3 Exposure and effect

An *exposure* (or intake) factor is a parameter that relates a standard (time-integrated) amount of a substance in a single environmental medium or compartment to the relative amount of this substance that eventually becomes bioavailable for organisms in this medium or compartment (for the evaluation of toxicity effects). *"Exposure"* in LCA terminology thus means a discrete event caused by a discrete (mass-loading) emission in LCA. Exposure is also a collective, rather than individual measure. If the population exposed is doubled, the exposure itself is considered to be doubled.

An *effect* factor is a parameter that relates a standard exposure level of a species or ecosystem to a certain effect level. The presence of sensitive species and background concentrations are all effect-related aspects. The concept of sensitivity is strongly connected to dose-response relationship. A numerical representation of sensitivity may be based either on the exposure value at which a species starts to show adverse effects to a substance (e.g. no-effect concentration) or on the relative size of the response to a standard increase of the dose in the response area. Both the no-effect levels and the slope of the dose-response curve vary between species and substances. Since dose-response relationships are seldom linear and homogeneous, the dose/response ratio is not independent of background concentrations. In regions of low background concentrations, effects may not occur, despite the presence of sensitive species. It is a matter of choice whether the purely potential effects in such *"below threshold"* areas are taken into account, especially for naturally occurring substances such as minerals, which may even be benevolent at low concentrations (Guinee et al., 2000).

2.4.4 Linking fate and exposure

Steady-state environmental fate models, based on the theoretical principles outlined in **Section 2.4.1,** and applying the simplifying assumptions outlined in **Section 2.4.2** are used to estimate a fate, or distribution factor. For a continuous emission E (in kg/y) into an environmental compartment, the fate model is used to estimate the concentration of the pollutant in the compartment (PEC in kg/m^3). The *Fate Factor* (in y/m^3), for effects that are a function of concentration, is given by:

$$Fate\ Factor = \frac{PEC}{E}$$ [2-3]

Where PEC is the predicted environmental concentration.

Following on from the discussion on exposure and effect in **Section 2.4.3**, an *Effect Factor* (in m^3/kg) is given by (for effects related to concentration, such as salinity effects):

$$Effect\ Factor = \frac{1}{PNEC}$$ [2-4]

Where $PNEC$ is the predicted no effect concentration (in kg/m^3).

The product of the *Fate Factor* and the *Effect Factor* is called the equivalency factor. The environmental impact ("impact scores" in Table 2.5) due to the activity being assessed is then the product of the *Fate Factor*, the *Effect Factor* and the mass emitted (taken from the life cycle inventory). Environmental fate and exposure models used to calculate equivalency factors are called characterisation models, and are reviewed in more detail in **Section 2.5** below.

2.4.5 Characterisation models

Several characterisation models are available for estimating equivalency factors for each compound contributing to a specific impact category. These are shown in Table 2.6. Equivalency factors are generally estimated using environmental fate and exposure models, and are indicators of the probability of exposure and probability that the exposure leads to an effect (i.e. risk). The impact parameters (or release) for each compound and each compartment are multiplied by the

respective equivalency factors and the results are added to give a total score for each impact category. These scores are, however, not easy to compare since they are usually presented in different units. A normalisation step can therefore be added to identify the size of the contribution to an impact category in terms of the size of the total problem. An additional step is sometimes included, where the normalised values are weighted in order of importance (usually determined subjectively) (Guinee, 2000).

The causal relationships in an environmental mechanism are shown in Figure 2.6. From Table 2.6 and Figure 2.6 it can be seen that, at this point in the development of the LCA methodology, most models have been developed for characterisation of the environmental impacts at mid-point level only. There are, however, still several mid-points that have not been described by means of models. Furthermore, the quantitative links between mid- and end-points (called damage functions) are only in the beginning stages of development.

In general, definition of an indicator closer to the point of release into the environment will result in more transparent modelling, but will render the indicator less environmentally relevant. In contrast, definition closer to the end-points will make the indicator more environmentally relevant, but will render it less transparent in its relationship to releases to the environment. Definition of an indicator at the level of the end-points themselves implies maximum environmental relevance.

Choosing indicators at different levels, however, will require very close attention to the consistency of the impact framework as a whole, avoiding as much as possible any overlap between categories, or missing types of impact. This can be difficult if some indicators are defined at end-point level and others at levels earlier in the mechanism. The environmental themes (impact category) approach at mid-point level is currently considered to be best practice (Guinee, 2000).

In considering how to incorporate salinity into the LCA methodology therefore, one must take into account the current LCA best practice, but also the way in which LCA best practice is developing. Ultimately, it is envisioned that salinity damage functions will be developed, that link end-points to mid-points.

Table 2.6: Characterisation models available for selected categories (Guinee et al., 2000)

Impact Category	LCI result	Characterisation model	Category indicator	Characterisation factor	Indicator result
Abiotic depletion	Extraction of minerals and fossil fuels	The concentration reserves and rate of de-accumulation approach	Reserve depletion	Abiotic depletion factor (ADF) for each extraction of minerals and fossil fuels (kg antimony equivalents/kg extraction)	kg of antimony equivalents
Increase in land competition	m^2 per year of land use	-	-	-	m^2 per year of land use
Climate change	Emissions of greenhouse gases to air	Model as developed by the International Panel on Climate Change (IPCC) defining the global warming potential of different greenhouse gases	Infrared radiative forcing (W/m^2)	Global warming potential 100 year time horizon (GWP100) for each greenhouse gas emission to air (kg CO_2/kg emission)	kg CO_2 equivalents
Depletion of stratospheric ozone	Emission of ozone-depleting gases to air	Model as developed by the World Meteorological Organisation (WMO) defining the ozone depletion potential of different gases	Stratospheric ozone breakdown	Ozone depletion potential in the steady state emission of each substance to air	kg CFC-11 emissions
Human toxicity	Emissions of toxic substances to air, water and soil	USES fate and exposure model developed by RIVM	Ratio of acceptable to predicted daily intake	Human toxicity potential (HTP) for each emission to air, water and soil	kg 1,4-dichlorobenzene equivalents
Eco-toxicity	Emissions of toxic substances to air, water and soil	USES fate and exposure model developed by RIVM	Ratio of predicted Environmental Concentration (PEC) to Predicted No Effect Concentration (PNEC) (for sub-categories; fresh water aquatic, fresh water sediment, marine, marine sediment and terrestrial)	Eco-toxicity potentials for each sub-category	kg 1,4-dichlorobenzene equivalents
Photo-oxidant formation	Emissions of substances (VOC, CO) to air	UNECE Trajectory Model	Tropospheric ozone formation	Photochemical ozone creation potential for each emission to air	kg ethylene equivalents
Acidification	Emissions of acidifying substances to air	The RAINS 10 model, developed at IIASA, describing the fate and deposition of acidifying substances	Deposition/Acidification critical load	Acidification potential (AP) for each emission to air	kg SO_2 equivalents
Nutrification	Emissions of nutrients to air, water and soil	Stoichiometric procedures, which identify the equivalence between N and P for both terrestrial and aquatic systems	Deposition/N/P equivalents in biomass	Nutrification potential (NP) for each emission to air, water and soil	kg PO_4 equivalents
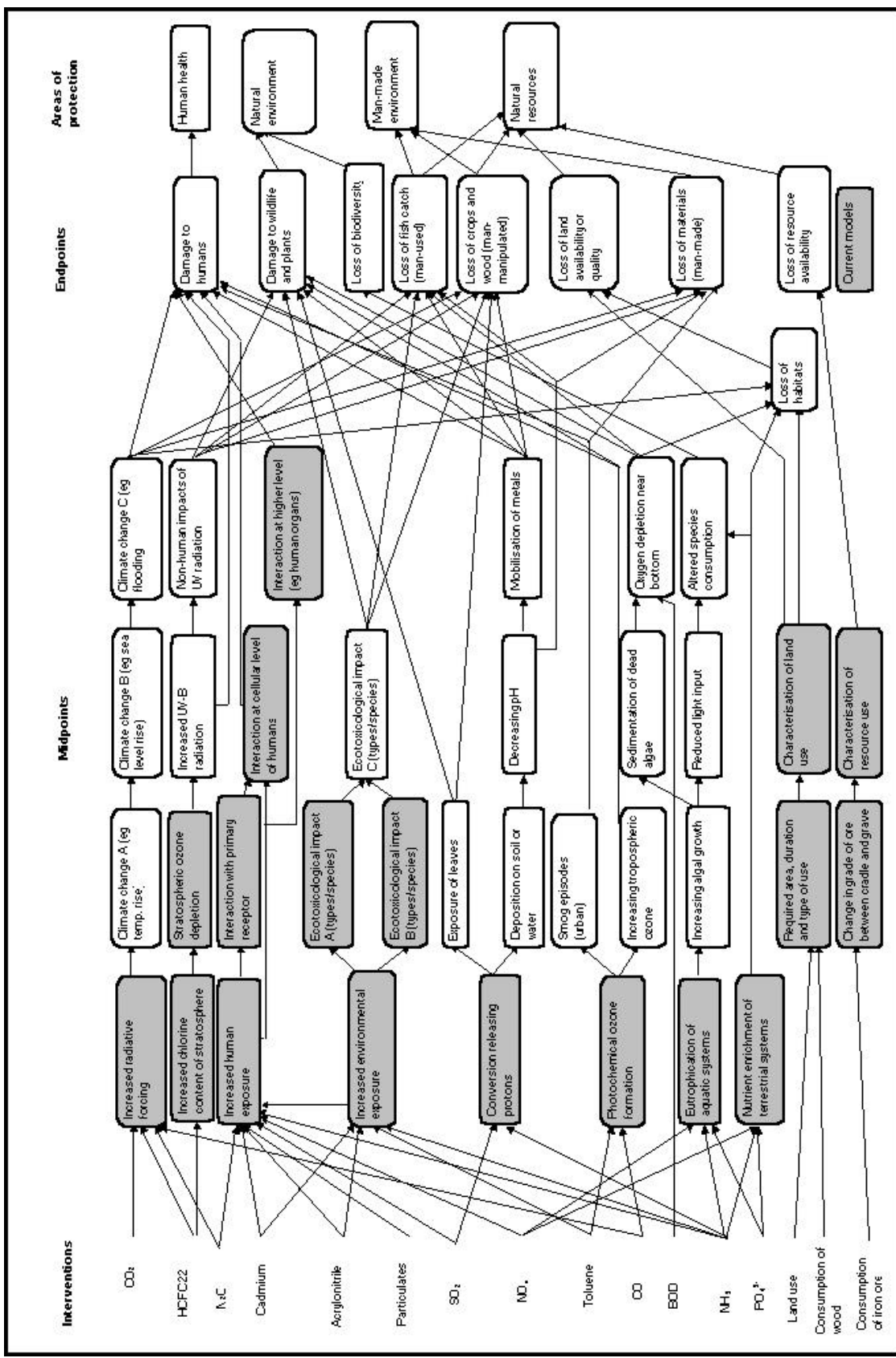
Figure 2.6: Causal relationships between interventions, midpoints and endpoints (Guinee et al., 2000)

2.5 ENVIRONMENTAL FATE AND EXPOSURE MODELS

In this section an existing characterisation model is evaluated in terms of its suitability for use in characterising salinity effects in the South African context, and a conclusion in this regard is presented.

2.5.1 USES-LCA model description and approach

A good starting point in developing a characterisation model for salinity would be to examine existing models, specifically to determine their applicability to being used either with or without modification, to characterise salinity effects. Several multi-media fate and effect models are available, such as EUSES 2.0 (EC, 1996), CalTox and USES-LCA (Huijbregts, 1999). The USES-LCA model is based on the USES 2.0 model and is the most recently developed model, and is considered by some to be best practice for characterisation of toxicity (Guinee., et al 2000). For this reason, the USES-LCA model has been evaluated in some detail.

In the USES-LCA model, the globe is modelled as a closed system, as shown in Figure 2.7. The globe has 5 spatial scales, a regional, a continental and a global scale consisting of three parts, reflecting arctic, moderate and tropic geographic zones of the Northern hemisphere. In turn the regional and continental scales each consist of six compartments: air, fresh water, sea water, natural soil, agricultural soil and industrial soil. All three climate-zones of the global scale each consist of three compartments: air water and soil.
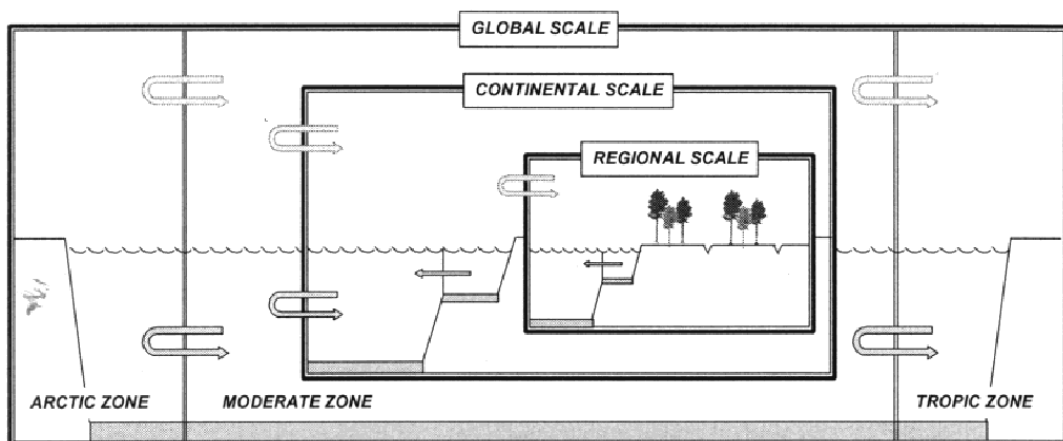
Figure 2.7: Schematic representation of the USES-LCA multi-media fate model boundaries (Huijbregts, 1999).

The model is used to calculate the predicted environmental concentrations (PEC) of the substance in each compartment of each scale by using the substance independent data shown in Table 2.7 and substance dependent data shown in Table 2.8. Table 2.9 shows the environmental mechanisms accounted for in the USES-LCA model to predict movement of pollutants between compartments and scales/zones and hence the predicted environmental concentrations in the various compartments at all scales.

Weighted Risk Characterisation Ratios (RCR) are calculated for each environmental compartment as follows:

$$WeightedRCR_{i,x,e} = \frac{(PEC_{i,x,e,c/s})W_{i,c/s}}{PNEC_{x,c}}$$ [2-5]

Where i denotes the impact category, x denotes the substance, c denotes the environmental compartment and s denotes the scale. $W_{i,c/s}$ are impact specific weighting factors for compartments (c) or scales (s). Weighting factors are based on population densities and compartment masses or volumes, and are used to aggregate the $RCRs$ on different geographical scales per impact category. The predicted no-effect concentrations ($PNEC$) are obtained from toxicological information. The equivalency factors used in the characterisation stage of life cycle assessments are calculated as follows:

$$EQ_{x,e} = \frac{WeightedRCR_{x,c,e}}{Weighted(RCR_{x,c,e})_{reference}}$$ [2-6]

Where $Weighted(RCR_{x,c,e})_{reference}$ is the weighted risk characterisation ratio for a reference substance (usually 1,4- dichlorobenzene).

Table 2.7: Substance independent model parameters used in USES-LCA (Huijbregts, 1999).

- Areas of all scales/zones
- Volume fraction of water in plant roots
- Bulk density of plant leaves
- Human intake of drinking water
- Human intake of leaf crops
- Human intake of meat
- Human inhalation rate
- Human soil ingestion
- Temperatures at all interfaces
- Fraction of solids, air, water and organic carbon in suspended matter, sediments and soil
- Fraction of sediment that is aerated
- Wind speeds at all scales
- Average daily precipitation at all scales
- Fraction of all scales that are fresh water, seawater, natural soil, agricultural soil and industrial soil
- Suspended solids concentration in water
- Settling velocity of suspended matter
- Fraction rain water that infiltrates soil
- Mass transfer coefficients

- Volume fraction of fat in plant roots
- Bulk density of plant roots
- Compartment pH values
- Human intake of fish
- Human intake of root crops
- Human intake of dairy products
- Human body weight
- Density of air, water and solid phase
- Surface area of aerosols
- Concentration of OH^- radicals in atmosphere
- Atmospheric mixing heights
- Aerosol deposition velocities and collection efficiencies at all scales
- Concentration of biota in water in all scales
- Water depth at all scales
- Sediment mixing depth at all scales
- Generation rate of suspended matter
- Soil erosion rates

Table 2.8: Substance dependent model parameters used in USES-LCA (Huijbregts, 1999).

- Oral human limit value
- Aquatic predicted no effect concentration
- Molecular mass
- Partitioning coefficients

- Inhalatory human limit value
- Terrestrial predicted no-effect concentration
- Melting point
- Bioconcentration factors, biotransfer factors and human bioavailability factors

Table 2.9: Environmental mechanisms modelled by USES-LCA (Huijbregts, 1999)

Compartment	Mechanism		
	Advective	**Diffusive**	**Reactive**
Air	Flow (based on wind speed and pollutant concentration)	Adsorption by water and soil from air	Degradation due to photochemical reactions
	Aerosol deposition	Volatilisation into air from water and soil	
Water	Flow (based on water flow and pollutant concentration)	Volatilisation into air	Degradation due to hydrolysis, photolysis and biodegradation
	Runoff	Desorption from sediment to water	
Soil	Deposition onto soil from air	Volatilisation to air from soil	Degradation due to hydrolysis and biodegradation
	Erosion	Adsorption by soil from air	
	Leaching		
Sediment	Sedimentation and re-suspension from and to water	Adsorption from water	Degradation by hydrolysis and biodegradation
	Burial	Desorption to water	

2.5.2 Limitations of USES-LCA in terms of salinity effects

In the context of LCA, salinity effects have been defined as those effects caused by elevated (above natural background levels) concentrations of common inorganic ions (particularly sodium, calcium, magnesium, chloride, sulphate and bicarbonate). Toxic effects caused by ions at low concentrations (for example, heavy metals) are therefore not considered to be salinity effects. The major categories of salinity effects identified in **Section 2.2** are:

- Material damage (scaling, corrosion, product quality changes)
- Aesthetic effects (taste)
- Aquatic ecosystem effects (chronic and acute effects on individual species, communities and/or ecological processes)
- Terrestrial ecosystem effects (chronic and acute effects on terrestrial animals, change in soil structure and loss of crop yield)

The limitations of current toxicity characterisation models have been well documented (van Beelen, 1998, Huijbregts, 1999), however in terms of salinity effects, the following limitations are of particular importance:

Spatial differentiation

Since multi-media fate models depend on geographical and climatological parameters, it is almost impossible to use them without applying some form of spatial differentiation. In the USES-LCA model, equivalency factors are relevant to Western Europe, and values at other locations may differ by orders of magnitude. The reliability and validity of LCA results may be much improved by the introduction of further spatial differentiation, to calculate spatially specific equivalency factors (Guinee., et al 2000). This is particularly valid for salinity effects. Salinity is a global problem. Nearly 40% of the agricultural land in the world is experiencing serious productivity reduction due to soil degradation. In some areas it is as much as 75%. As much as 70% of water use is for irrigation and nearly one third of the 260 million hectares of irrigation land world wide is now affected by salination (UNEP, 2002). In general, however, salination limited to local areas, particularly in industrialised countries that are arid or semi-arid, such as Australia and South Africa. Salinity problems within a country are furthermore generally limited to specific catchments where industrialisation has taken place to a significant degree, or where extensive irrigation takes place. Salination (as defined) is furthermore limited to terrestrial and fresh water aquatic environments. In terms of salinity effects, the sea can be seen as an infinite sink of common ions.

Idealistically, salinity potentials could be calculated for each catchment in an area or country where salinity effects are significant. This would require detailed data (fate model parameters) for each catchment, and would require that the spatial distribution of life cycle inventory emissions is known, which is most often not the case. A compromise is therefore required between more relevant and reliable LCA results from characterisation models using a high degree of spatial differentiation (with associated high data demand), and less relevant and reliable LCA results from characterisation models using a lower degree of spatial differentiation.

Salinity impacts

The USES-LCA model calculates 6 toxicity potentials; fresh water ecotoxicity, marine ecotoxicity, fresh water sediment ecotoxicity, marine sediment ecotoxicity, terrestrial ecotoxicity and human toxicity, for release of emissions into 5 possible initial release compartments; air, fresh water, sea water, agricultural soil and industrial soil. In terms of the toxicity effects of salinity it may therefore be possible to account for salinity effects, however, salinity (as defined) impacts do not only

include ion specific toxic effects, but also include other effects such as crop yield loss, aesthetic and material damage effects.

Sub-surface water modelling

Existing toxicity characterisation models make use of very simple rainfall-runoff relationships to estimate the steady state concentrations of sub-surface water. The lack of an adequate sub-surface modelling component in the USES-LCA model has been identified as a limitation (Huijbregts, 1999). Adequate modelling of the sub-surface water component is critical when evaluating salinity impacts because the salt concentration of sub-surface water has a direct influence on crop production, and also has a direct influence on surface water salt concentration, which in turn affects many of the other salinity sub-impacts. Published data on threshold salt concentrations, and yield loss as a function of salt concentration are available, and in order to calculate realistic effects potentials, sub-surface salt concentrations should be calculated with a corresponding degree of accuracy and scientific relevance.

Ionising substances

Models such as USES and USES-LCA were designed to evaluate the risks of neutral organic compounds, where the toxicity, risk of bioaccumulation and partitioning of the compound between solid and aqueous phase can be estimated from the octanol/water partitioning coefficient of these compounds. These estimations are only valid for neutral organic compounds showing baseline toxicity but not for other types of compounds like organic cations, anions, surfactants and inorganic compounds (van Beelen, 1998). Although these models have been used to estimate toxicity potentials for some metals (particularly heavy metals), they have not been used to calculate potentials for common ions such as sodium, calcium, magnesium, chloride, sulphate and carbonate/bicarbonate.

2.5.3 Conclusions

The USES-LCA characterisation model was evaluated in terms of its applicability to be used as a basis for incorporating salinity into the LCA methodology. The USES-LCA model was chosen because it is a well developed and accepted environmental fate model that has been adapted to calculate toxicity potentials for LCA, and intuitively would be suited for calculating salinity effects, some of which are toxicological in nature. It is however concluded that the USES-LCA model is not suitable for the calculation of salinity potentials. The reasons for this are discussed in detail above, but in summary, are:

- In the USES-LCA model the globe is modelled as a closed system using a series of nestled multi-media fate models on different geographical scales, with Western Europe being defined as the smallest regional (or "starting") scale. Substance independent model parameters used may result in equivalency factors that are therefore not necessarily valid to South African conditions. Furthermore, salination is a local or regional problem, and that a higher degree of accuracy is required in modelling on a smaller spatial scale.

- Although the USES-LCA model accounts for some of the salinity impacts, it does not account for all.

- Sub-surface water and solute transport modelling in the USES-LCA model is inadequate for the degree of accuracy and relevance needed to account for salinity effects.

- Perhaps the biggest obstacle in using the USES-LCA model in some modified form to account for salinity effects is that it has been developed to handle organic compounds, and is not suited for estimating the fate of ionic compounds.

CHAPTER 3

CONCEPTUAL CHARACTERISATION MODEL DEVELOPMENT

In light of the review and conclusions made in Chapter 2, there are some general considerations that need to be examined before a characterisation model for salinity can be developed. For example, which of the salinity impacts should be included in the model, what geographical extent should the model cover, and what degree of spatial differentiation should be applied? What compartments, components and mechanisms should be included? These questions are addressed in Section 3.1. In Section 3.2, a conceptual framework for an environmental fate model for salinity is proposed, based on the issues addressed in Section 3.1. In Section 3.3 the fate and exposure components are linked in a conceptual method for characterising salinity effects.

3.1 GENERAL CONSIDERATIONS

An *exposure* (or intake) factor is a parameter that relates a standard (time-integrated) amount of a substance in a single environmental medium or compartment to the relative amount of this substance that eventually becomes bioavailable for organisms in this medium or compartment (for the evaluation of toxicity effects). An *effect* factor is a parameter that relates a standard exposure level of a species or ecosystem to a certain effect level. Multimedia environmental fate and expose models are used to predict the concentrations of substances in the various media, and to use effect factors to characterise the impact (as discussed in **Sections 2.4.3** and **2.4.4**)

It is pertinent to consider the following in the development of a conceptual characterisation model:

- which salinity impacts to include.
- the level spatial differentiation and geographical extent.
- which compartments to include, and
- which components need to be modelled

These general considerations are discussed in **Sections 3.1.1** to **3.1.4**

3.1.1 Salinity impacts

Conceptually, it is proposed that the salinity characterisation model be as all-inclusive as data availability and modelling constraints allow. Salinity effects are discussed in **Section 2.2**, and in light of the availability of no-effect concentration data it is proposed that the following effects be accounted for in the methodology:

- Aquatic ecotoxicity effects
- Effects on agricultural crop production
- Material damage effects
- Aesthetic effects
- Effects on livestock
- Effects on natural vegetation
- Effects on natural terrestrial ecosystems

3.1.2 Spatial differentiation and extent

The issue of spatial differentiation is discussed in **Sections 2.4.2** and **2.5.2**. In general, multi-media fate models have been developed for the globe as a closed system. Multi-media fate models however depend on geographical and climatological parameters, and it is almost impossible to use them without applying some form of spatial differentiation. It appears to be the general consensus that the reliability and validity of LCA results may be much improved by the introduction of further spatial differentiation (Guinee., et al 2000; Potting and Hauschild, 1997a and 1997b, Sleeswijk and Heijungs, 1996, Huijbregts, 1998). As discussed in **Section 2.5.2**, this is particularly valid for salinity effects. Salinity is a global problem (refer to **Section 1.2**), but in general is limited to local or regional areas, and is prevalent in industrialised countries that are arid or semi-arid, such as Australia and South Africa. Salinity problems within a country are furthermore generally limited to specific catchments where industrialisation has taken place to a significant degree, or where extensive irrigation takes place. Salination is furthermore limited to terrestrial and fresh water aquatic environments. In terms of salinity effects, the sea can be seen as an infinite sink of common ions.

Most toxicity characterisation models are steady-state models. Predicted environmental concentrations are calculated based on continuous emission fluxes imposed on the various initial

release compartments. Various methods have been proposed (Guinee., et al 1996) to overcome the difference between the emission flux necessary to implement in a steady state multimedia fate model and the artificial emission pulse resulting from a life cycle inventory. The most common method is to use a reference substance. Heijungs (1995) published a paper on the harmonization of methods for impact assessment. In this paper the following important conclusions were made:

- Provided there is a linear relationship between continuous fluxes and steady-state concentrations, the total time integrated exposure due to an emission pulse can be found by simply multiplying the amount of pulse emission by the coefficients that link fluxes to concentrations. A consequence of this is that pulse-oriented techniques, like LCA, need not (under certain conditions) employ complicated time-dependent unsteady-state models for impact prediction, but can use the much simpler steady-state models that have been developed for flux-oriented techniques, like risk assessment.
- The existence of equivalency factors had previously been proven assuming that the impacts of the products are marginal compared with the total impacts. Heijungs (1995) proves that, in fact, almost every linear exposure and/or impact prediction model gives rise to equivalency factors, which can be used in every LCA, regardless of the marginality of the product's impacts.
- The impact scores calculated in LCA bear no relation to factually occurring impacts, as discussed in **Section 2.4.2**
- A reference substance is not required when calculating equivalency factors.

In the development of the characterisation model, it was decided to develop a non steady state model for the following reasons:

- At the outset, it was uncertain as to whether there would be a linear relationship between continuous fluxes and steady-state concentrations.
- Existing non steady-state models were available, familiar, and accepted for general use in South Africa. Many of the model parameters for these models were available for each catchment, at quaternary level. These models have been used and validated for a number of catchment studies in South Africa.
- The steady state coefficients that link fluxes to concentrations were not known for the defined "unit catchment".

Idealistically, salinity potentials could be calculated for each catchment in an area or country where salinity effects are significant. This would require detailed data (fate model parameters) for

each catchment, and would require that the spatial distribution of life cycle inventory emissions is known, which is most often not the case. A compromise is therefore required between more relevant and reliable LCA results from characterisation models using a high degree of spatial differentiation (with associated high data demand), and less relevant and reliable LCA results from characterisation models using a lower degree of spatial differentiation. It is therefore proposed that, as a starting point, an environmental fate and effect model be developed on a South African scale. This model would have to account for movement of salts across natural and political borders.

3.1.3 Compartments

Most multi-media fate models include, at a minimum an air, soil and water compartment for estimating the ultimate fate of compounds in the environment (Mackay, 1991). In the USES (Guinee et al., 1996b) and USES-LCA (Huijbregts, 1999) models the water compartment is further sub-divided into fresh water and seawater. The soil compartment is divided into industrial, natural and agricultural in the USES model, and into industrial and agricultural soil in the USES-LCA model. Some models include a sediment model, sometimes consisting of natural sediment and marine sediment components.

In considering compartmentalisation of the environment, the potential effects of salinity (refer to **Section 2.2**) need to be considered. Arguably the highest potential impact of salinity is on agriculture, particularly on irrigated crops. Salt levels in agricultural soils are higher than natural soils due not only to the concentration effects of evaporation, but also due to the application of salts in the form of inorganic fertilizers. It is therefore essential that a distinction be made between natural soil and agricultural soil. In South Africa, most water users (including domestic, industrial and agricultural) use surface water. The agricultural sector is the biggest user of groundwater. It is estimated that 78% of all groundwater abstracted is used for irrigation, 7% for rural purposes and 6% for stock watering. Only 4% of groundwater abstracted is used in the urban environment. Approximately 16% of irrigated lands use groundwater (Conrad et al., 1999). The flow and quality of surface water is in turn influenced by the flow and quality of groundwater. It is therefore unavoidable, and in fact desirable (due to the use of groundwater, particularly in the agricultural sector of South Africa), to include a groundwater compartment, also sub-divided into a natural and agricultural components. The generation of salt (aeolian, terrestrial or aquatic) and the deposition of aeolian salt, and the storage and removal of salt from surfaces are influenced to a large degree by land-use practices. It is therefore proposed that a further sub-division into urban and rural (natural and agricultural) components be made. It is also proposed that sediment be included in the model only as far as it affects the transport of sorbed salt, including transport via

eroded sediments from surfaces, and via bed and suspended load in rivers. The sea can be considered as an infinite sink of salts, and is therefore not included in the model.

3.1.4 Components and mechanisms

Numerous hydrosalinity models have been developed and applied to various studies of South African catchments. These models range from simple models requiring very few input parameters to complex three-dimensional groundwater and solute transport models that require a large number of input parameters (Hughes, 1997). It is proposed that a hydro-salinity model be developed based on the rainfall-runoff model originally developed by Pitman (Pitman, 1973) and later expanded to include salinity by Herold (Herold, 1981). The Pitman model has become the most widely used rainfall-runoff model in South Africa. The current official version is referred to as WRSM90, and was used to model rainfall-runoff in all catchments within South Africa to the quaternary level. Monthly rainfall and evaporation data as well as simulated river flows and model parameters are therefore available for all catchments in the country (Midgely et al., 1994).

The environmental mechanisms included in the USES-LCA model are given in Table 2.10. For salinity, as defined in **Section 2.2**, common ions comprise sodium, calcium, magnesium, chloride sulphate and bicarbonate. Collectively, these components are defined (in the context of this study) as total dissolved salts (or, TDS). It is proposed that in this study TDS be modelled as a lumped parameter, for the following reasons:

- There are more data available on the effects of salinity expressed as a function of TDS, than there are expressed as a function of the concentrations of individual ions.
- There are more surface and groundwater quality data available as TDS (or electrical conductivity, which is a linear function of TDS) than there are of individual ions.
- The availability of models as described above.

Modelling of TDS as a lumped parameter does, however, present certain challenges, particularly with respect to parameters such as solubility limits and adsorption constants. These are discussed in **Chapter 5** It is envisaged that eventually the model be used to develop salinity potentials for individual ions. This is discussed in more detail in **Chapter 8**.

The major physical and chemical mechanisms that may influence the fate of dissolved salts are briefly described below, and are shown schematically in Figure 3.1. More detailed discussions are given in **Sections 4.1** and **4.2**.

Atmosphere: Marine and/or terrestrial aerosols (a fraction of which will be in a form that will dissolve in water) are transported into, across and out of the air space over South Africa by advection. During this process, additional aerosol mass may be generated, either naturally or due to the activities of man. These aerosols are dispersed into the air space, but are generally limited in their vertical extent of dispersion by stable inversion layers. Deposition of aerosols occur through several mechanisms; wet deposition is the removal of aerosols by rainfall, either in-cloud or below cloud scavenging; dry deposition is the deposition of gases and particles from the atmosphere by processes other than dissolution in rain, cloud or fog.

Surfaces: Salt is generated on urban and agricultural surfaces from anthropogenic activities. This salt is either discharged into the air (as mentioned above), discharged into surface water or onto soils. On impervious areas some or all of the salt deposited from the atmosphere is washed off via surface runoff and generally enters surface water. In pervious areas, some or all of the salt deposited via deposition or discharge by man enters the surface water via surface runoff and the balance enters the soil via infiltration. During rainfall events, erosion takes place, and a small fraction of the salt will adsorb onto the eroded soil that enters the surface water. In the case of irrigated surfaces, additional salt load is applied to the surface from the salts present in the surface water.

Soil and soil water: A number of processes occur in the soil. Depending on the amount of water entering the root zone, the amount of evapotranspiration occurring, and on the soil characteristics, some of the water will be stored in the root zone, some will move towards the surface water as interflow, and some will percolate into the groundwater. Inorganic ions will be generated through the process of leaching. Adsorption and ion exchange will occur between the soil matrix and the soil water, and if the sufficient water is lost by means of evapotranspiration, the solubility limit of certain salts may be exceeded and these will precipitate out in the soil matrix, and will re-dissolve if sufficient water becomes available.

Groundwater: Groundwater is either stored (accumulates), enters the surface water as base-flow, or enters deep-seated groundwater. The mechanisms that govern solute transport in groundwater are the same as for soil water.

Surface water: Surface water flow is made up of a surface runoff component, an interflow component and a groundwater flow component. Evaporation from the surface water occurs, and a small fraction of water is lost as bed-loss. In addition to the liquid phase, sediment is transported either as suspended sediment or as bed load. This sediment will contain adsorbed salt.

3.2 CONCEPTUAL FATE MODEL

It is proposed that a multimedia environmental fate model be developed, and that the model be developed to the level at which data is available. The characterisation of a "unit South African catchment" and the development of a conceptual fate model are described in this section.

3.2.1 The "unit South African catchment"

It is proposed that the same approach be adopted as was adopted in the USES-LCA model where a "unit environment" was defined. The difference, however, is that a "unit South African catchment" is defined, as shown schematically in Figure 3.2. This is a hypothetical catchment (including the air space above it) that has the same surface area as the surface area of the country, but has one single river with a flow equal to the sum of the flows of all rivers in the country and a salt load equal to the sum of the salt loads of all rivers in the country. The land use distribution remains unchanged from actual practices, but is confined to one single urban area, one single rural natural area and one single rural agricultural area. Rainfall on and evaporation from this catchment occur at average rates for the country. It is proposed that the data available in the WR90 series of reports published by the Water Research Commission (Midgley et al., 1994) be used to determine the monthly average flow of the "unit river", the monthly average evaporation for the country, and the monthly average rainfall.

A large database of surface water quality in South African rivers exists (refer to **Appendix B**), that can be used to calculate the monthly average dissolved salt concentration in the "unit South

3.2.2 Atmospheric deposition model

It is proposed that a simple atmospheric deposition model be developed that could be used to calculate salt deposition rates at a daily time step, without resorting to complex air dispersion modelling, with its associated data demand. The seasonal variations in salt deposition rates, and the influence of rainfall on salt deposition should be taken into account. The concentration *per se* of common inorganic salts in the atmosphere does not play a significant role in the salinity impacts as defined.
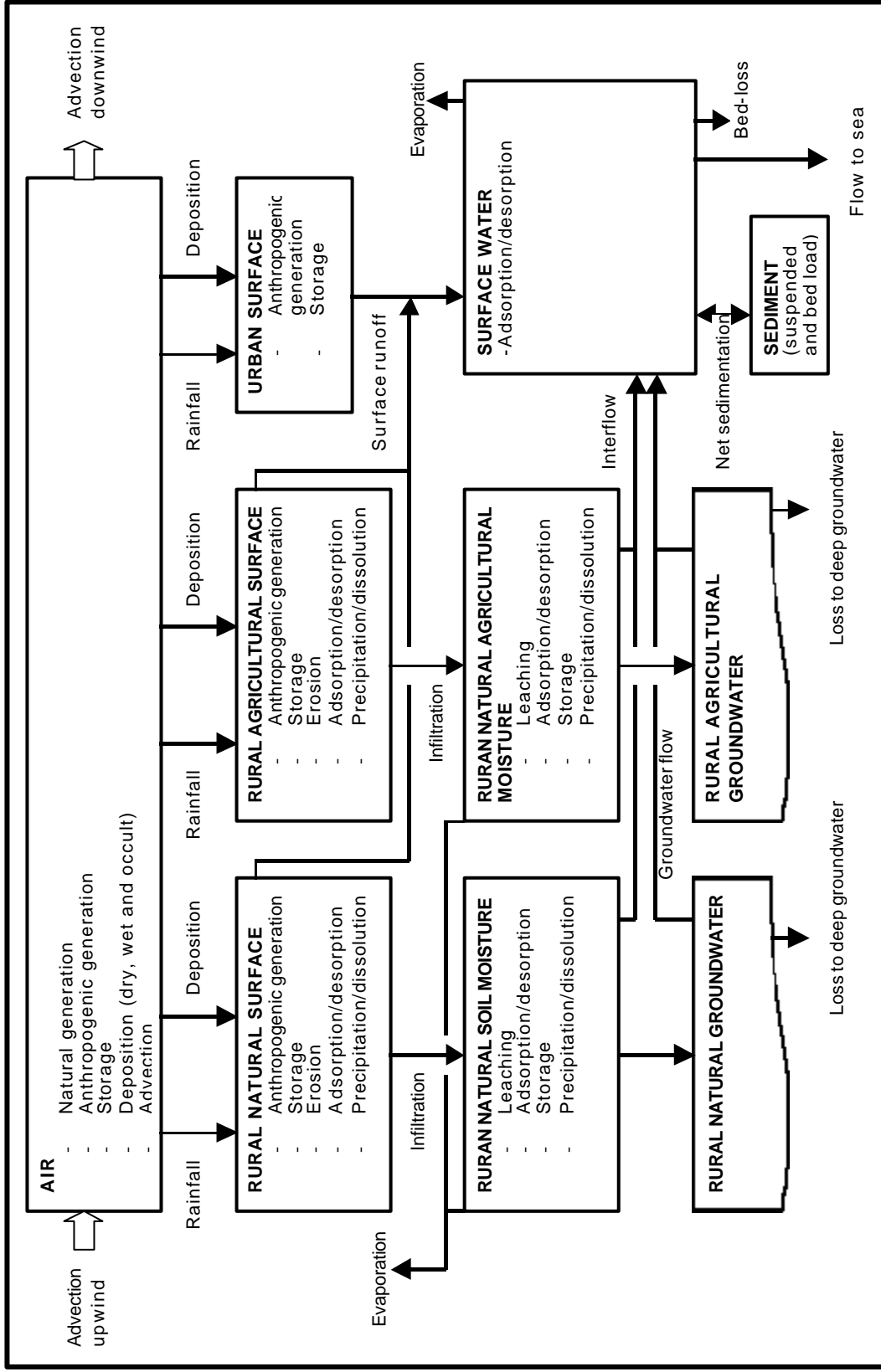
Figure 3.1: Schematic diagram of the conceptual fate model
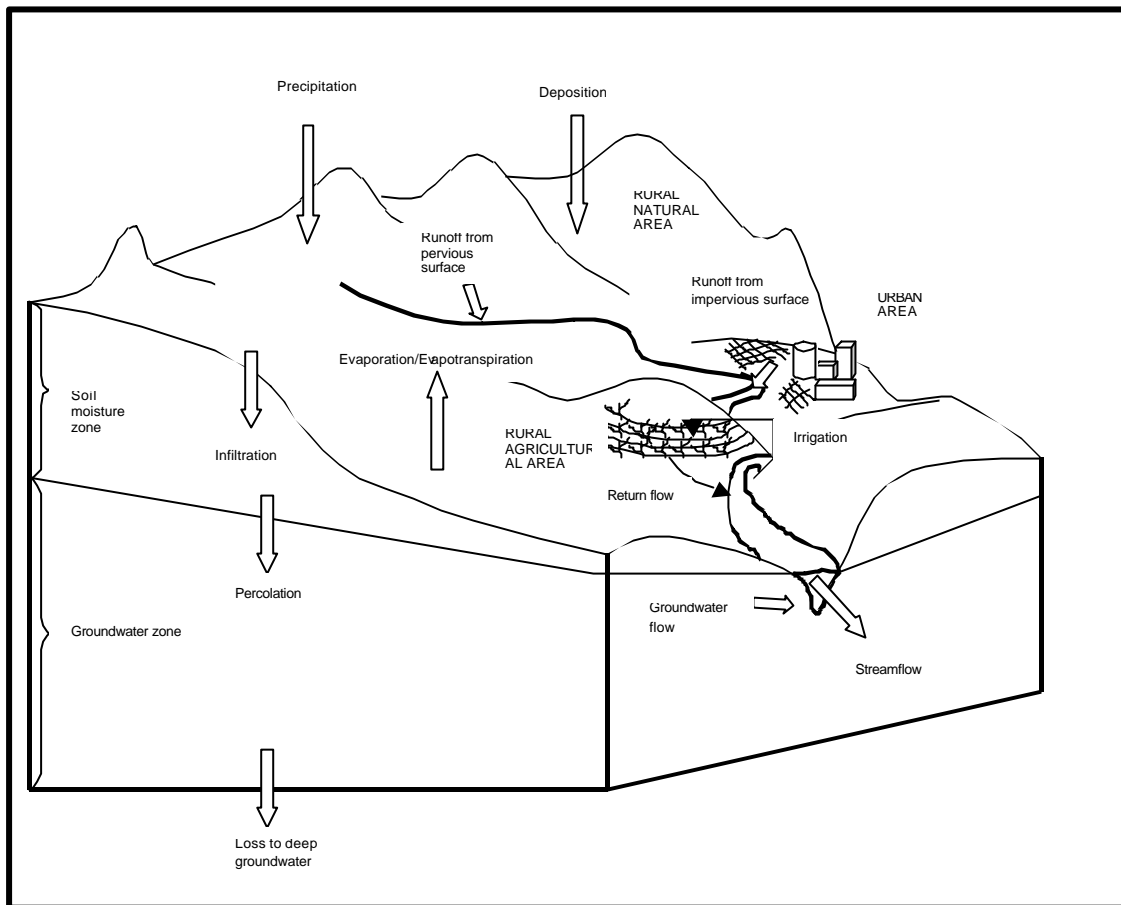
The rate at which these salts are removed from the atmosphere and deposited onto rural and urban surfaces, does however, have a significant influence on salinity impacts. The objectives of the model are therefore to:

- Improve on the methods used in available characterisation models for estimating atmospheric deposition. In the USES-LCA model (Huijbregts, 1999), for example, the volumetric airflow entering the regional air volume is calculated from an **annual average** wind velocity (3 m/s) and the regional air cross-sectional area. Total aerosol deposition is calculated as the sum of dry aerosol deposition and washout. Dry deposition is calculated by multiplying an annual average aerosol deposition rate (0.1 cm/s) with the assumed fraction of chemical associated with the aerosol. Washout is calculated by multiplying the average annual rainfall (700 mm/year) with a scavenger ratio (100 000).

- Calculate salt deposition rates on rural and urban surfaces at a daily time-step.

- Calculated deposition rates should be in the same order of magnitude as published values.

- Incorporate the maj or transport processes occurring in the atmosphere, particularly with regard to processes that influence the fate of salts in other compartments.

Conceptually, a simple box model could be developed that uses average wind speeds to advect aerosols over the catchment (de Nevers, 1995). The movement of aerosols over Southern Africa has been well researched, and some data are available to validate such a model (Swap et al., 1996). Simple models have also been developed to estimate aerosol removal processes (wet, dry and occult deposition), and some model parameters are available for South African conditions (Herold et al., 2001).

3.2.3 Hydrosalinity model

Potential salinity effects are discussed in **Section 2.2**. In order to calculate salinity equivalency factors, the hydrosalinity model must be able to predict the salt concentrations in the soil and surface water compartments. In order to do this, a rainfall-runoff model is required that can predict the soil moisture and groundwater profiles as well as the surface water flow.

As discussed in **Section 3.1.4**, it is proposed that a hydro-salinity model be developed based on the rainfall-runoff model originally developed by Pitman (1973) and later expanded to include salinity by Herold (1981). The Pitman model has become the most widely used rainfall-runoff model in South Africa. The current official version is referred to as WRSM90, and was used to model rainfall-runoff in all catchments within South Africa to the quaternary level. Monthly rainfall and evaporation data as well as simulated river flows and model parameters are therefore available for all catchments in the country (Midgely et al., 1994). It is proposed that the WRSM90 model be used to simulate rainfall-runoff relationships in the "unit South African catchment" that the salinity component, as proposed by Herold (1981) be used to model salt transport. The following modifications to the models are, however, proposed:

- Aerosol (and associated salt) deposition rates calculated using the atmospheric deposition model described above are used instead of average constant deposition rates.

- The pervious (rural) surface is divided into a rural agricultural area (on which irrigation takes place) and a natural area (on which no irrigation takes place). This will allow more accurate estimation of the salt concentration in soils supporting crops, and therefore more accurate estimation of potential salinity effects.

- An erosion and sediment transport component be added to account for the transport of adsorbed salt. It is proposed that the model presented by Paling et al (1989) be used as a starting point.
- Allowance is made in the model to impose a pulse or continuous emission into any environmental compartment, at any point during the simulation, at any magnitude and for any duration.

The objective of the hydrosalinity model is therefore to calculate the dissolved salt concentration in soil moisture and surface water at a daily time-step, taking all possible mechanisms that influence the distribution of dissolved salts between the various environmental compartments into account.

The objective of the environmental fate model as a whole must be seen in light of the discussion on the calculation of effects potentials given in **Section 3.3**.

3.3 CONCEPTUAL CHARACTERISATION MODEL

It is proposed that the effects potentials (or equivalency factors) be calculated in a similar manner to that of Huijbregts (1999) discussed in **Section 2.5.1**, however, since a non steady-state model is proposed, the effects potentials are in different units.

3.3.1 Effects potentials

In Figure 3.3 a schematic representation of the predicted environmental concentration profile in a compartment with (PEC_i) and without (PEC_i^0) an imposed impulse emission is shown. It is proposed that the same approach be adopted in calculating the equivalency factor, as discussed in **Section 2.4.4**, however, since the proposed model is not a steady-state model is it proposed that the following general equation be used to calculate the equivalency factor:

$$Effects\,Potential = \frac{\sum_{i=1}^{N}[PEC_i - PEC_i^0]\Delta t}{PNECM} \quad \text{(d/kg)} \quad\quad [3\text{-}1]$$

Where:

PEC_i = predicted environmental concentration (kg/m^3) in the compartment during day i after an emission of total mass M (kg).

PEC_i^0 = predicted environmental concentration (kg/m^3) in the compartment during day i without an emission into the compartment.

$PNEC$ = predicted no-effect concentration (kg/m^3)

Δt = time interval at which concentrations are calculated (d)

N = total number of days in the simulation

M = mass of impulse emission (kg)

The term "effects potential" is used rather than "equivalency factor", since the equivalency factor for salinity is made up of a number of effects potentials.
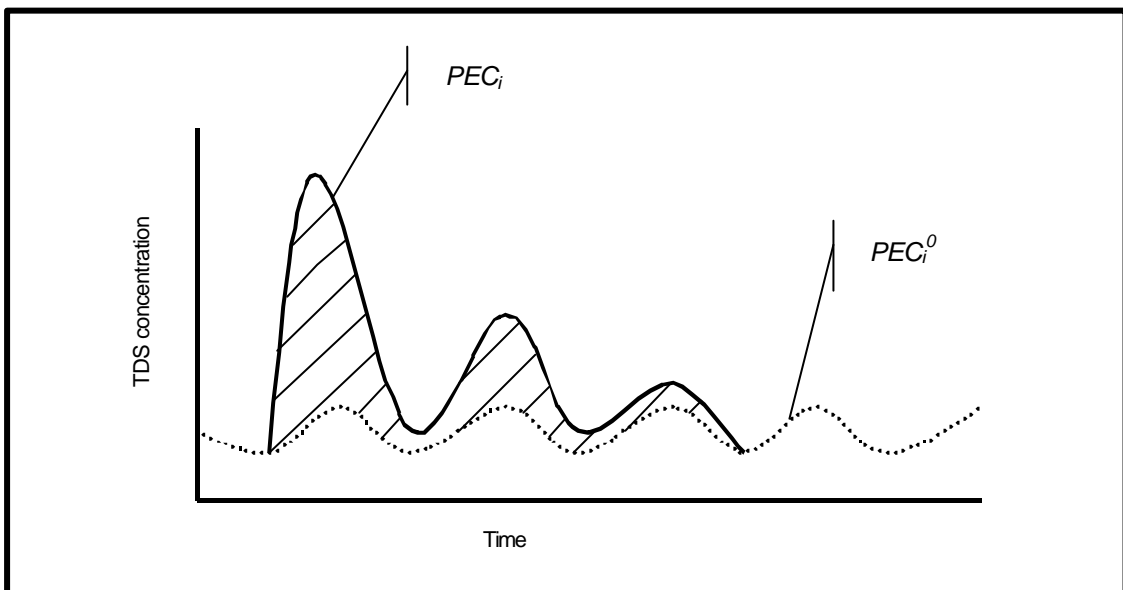
Figure 3.3: Schematic representation of the predicted environmental concentration profile in a compartment with (PEC_i) and without (PEC_i^0) an imposed impulse emission.

The numerator of Equation [3-1] is therefore the shaded area indicated in Figure 3.3. Several key principles should be mentioned regarding the results obtained from the environmental fate model and the calculation of the effects potentials:

- As the population in South Africa increases, land use practices change and urbanisation and industrialisation increase, it is likely that the concentration of dissolved salts in the water resources of South Africa will increase. It is however not necessary to include a salinity growth factor in the model, since it is logical to assume that the rate of increase in salination will be the same with and without the imposed impulse emission, and therefore the difference will be zero.

- The simulation length (N) should be selected so that at the end of the simulation the difference in concentration in each environmental compartment with and without an imposed emission impulse is at or close to zero. This in effect means that the salinity potentials are derived for an infinite time-horizon.

In terms of the potential salinity impacts discussed in **Section 2.2**, the following effects potentials are defined for a release of salt into an initial release compartment (irc):

$$AEEP_{irc} = \frac{\sum_{i=1}^{N}[PEC_i^R - PEC_i^{R,0}]\Delta t}{PNEC_{AE}\, M^R} \qquad\qquad [3\text{-}2]$$

Where:

$AEEP_{irc}$ = Aquatic ecotoxicity effects potential for the release of salt into an initial release compartment irc (d/kg)

$$AeEP_{irc} = \frac{\sum_{i=1}^{N}[PEC_i^R - PEC_i^{R,0}]\Delta t}{PNEC_{Ae}\, M^R} \qquad\qquad [3\text{-}3]$$

Where:

$AeEP_{irc}$ = Aesthetic effects potential for the release of salt into an initial release compartment irc (d/kg)

$$MDP_{irc} = \frac{\sum_{i=1}^{N}[PEC_i^R - PEC_i^{R,0}]\Delta t}{PNEC_{MD}\, M^R} \qquad\qquad [3\text{-}4]$$

Where:

MDP_{irc} =   Materials damage effects potential for the release of salt into an initial release compartment irc (d/kg)

$$NWEP_{irc} = \frac{\sum_{i=1}^{N}[PEC_i^R - PEC_i^{R,0}]\Delta t}{PNEC_{NW}\, M^R}$$ [3-5]

Where:

$NWEP_{irc}$ =   Natural wildlife effects potential for the release of salt into an initial release compartment irc (d/kg)

$$LEP_{irc} = \frac{\sum_{i=1}^{N}[PEC_i^R - PEC_i^{R,0}]\Delta t}{PNEC_L\, M^R}$$ [3-6]

Where:

LEP_{irc} =   Livestock effects potential for the release of salt into an initial release compartment irc (d/kg)

$$NVEP_{irc} = \frac{\sum_{i=1}^{N}[PEC_i^{rns} - PEC_i^{rnsR,0}]\Delta t}{PNEC_{NV}\, M^{rns}}$$ [3-7]

Where:

$NVEP_{irc}$ =   Natural vegetation effects potential for the release of salt into an initial release compartment irc (d/kg)

$$ACEP_{irc} = \frac{\sum_{i=1}^{N}[PEC_i^{ras} - PEC_i^{ras,0}]\Delta t}{PNEC_{AC}\, M^{ras}}$$ [3-8]

Where:

$ACEP_{irc}$ =   Agricultural crop effects potential for the release of salt into an initial release compartment irc (d/kg)

And:

3-14

PEC_i^R = predicted concentration of salt in the river during day i with an emission of total mass M^R (kg) into the river (kg/m^3)

$PEC_i^{R,0}$ = predicted concentration of salt in the river during day i without an emission into the river (kg/m^3)

PEC_i^{rns} = predicted salt concentration in rural natural soil moisture during day i with an emission of total mass M^{rns} (kg) onto the rural natural surface (kg/m^3)

$PEC_i^{rns,0}$ = predicted salt concentration in rural natural soil moisture without an emission onto the rural natural surface (kg/m^3)

PEC_i^{ras} = predicted concentration of salt in the rural agricultural soil moisture during day i with an emission of total mass M_{ras} (kg) onto the rural agricultural surface (kg/m^3)

$PEC_i^{ras,0}$ = predicted salt concentration in rural agricultural soil moisture without an emission onto the rural agricultural surface (kg/m^3)

$PNEC_{Ae}$ = predicted no-effect salt concentration for aesthetic effects (kg/m^3)

$PNEC_{AE}$ = predicted no-effect salt concentration for aquatic ecotoxicity effects (kg/m^3)

$PNEC_{MD}$ = predicted no-effect salt concentration for material damage effects (kg/m^3)

$PNEC_{NW}$ = predicted no-effect salt concentration for effects on natural wildlife (kg/m^3)

$PNEC_L$ = predicted no-effect salt concentration for effects an agricultural livestock (kg/m^3)

$PNEC_{NV}$ = predicted no-effect salt concentration for effects on natural vegetation (kg/m^3)

$PNEC_{AC}$ = predicted no-effect salt concentration for effects on agricultural crops (kg/m^3)

N = total number of days in the simulation

It can be seen from Equations [3-2] to [3-8] that the salt concentration in the river is used in the calculation of the aesthetic, damage, natural wildlife and agricultural livestock effects potentials. The inherent assumption is that only river water is used for domestic consumption, industrial activities, livestock watering, and by natural wildlife. In South Africa, approximately 13% of all water used is obtained from groundwater (DWAF, 1986). The agricultural sector is the biggest user of groundwater. It is estimated that 78% of all groundwater abstracted is used for irrigation, 7% for rural purposes and 6% for stock watering. Only 4% of the groundwater abstracted is used in the urban environment (Conrad et al., 1999).

3.3.2 Total salinity potential

The total salinity potential (or equivalency factor) for the release of salts into an initial release compartment (irc), can be calculated by the general formula:

$$
\begin{aligned}
TSP_{irc} = {} & AEEP_{irc}\,W_{AEE} + AeEP_{irc}\,W_{AeE} + MDP_{irc}\,W_{MD} \\
& + NWEP_{irc}\,W_{NWE} + LEP_{irc}\,W_{LE} + NVEP_{irc}\,W_{NVE} \\
& + ACEP_{irc}\,W_{ACE}
\end{aligned}
$$

[3-9]

Where:

TSP_{irc}	=	Total salinity potential for the release of salt into an initial release compartment irc (d/kg)
W_{AEE}	=	weighting factor for aquatic ecotoxicity effects (-)
W_{AeE}	=	weighting factor for aesthetic effects (-)
W_{MD}	=	weighting factor for material damage effects (-)
W_{NWE}	=	weighting factor for natural wildlife effects (-)
W_{LE}	=	weighting factor for livestock effects (-)
W_{NVE}	=	weighting factor for natural vegetation effects (-)
W_{ACE}	=	weighting factor for agricultural crop effects (-)

It is furthermore proposed that one reference emission compartment be chosen in a manner similar to that proposed by Huijbregts (2001), and that the compartment with the highest total

salinity potential be chosen as the reference emission compartment (in this case, the agricultural soil compartment). The effects potentials, and total salinity potentials are normalised using the total salinity potential for the reference compartment. This results in effects potentials and total salinity potentials that are expressed as kg TDS equivalents/kg TDS.

Weighting factors (W) have been included in the calculation of effects potentials in order to determine the relative importance (or value) of the salinity sub-impacts listed above. For example, the calculated value of the aesthetic effects potential may be larger than the calculated value of the aquatic ecosystem effects potential, which would imply that aesthetic impacts have more environmental "value" than aquatic ecosystem effects. The value that individuals place on toxicity effects may well be higher that the value they place on aesthetic effects, and therefore allowance has been made for including weighting factors. By sub-categorising the salinity impact category, therefore, value judgements would have to be made regarding the relative weighting between sub-categories. This is beyond ISO, but not in conflict with ISO (Udo de Haes, 1999).

Human toxic effects are excluded from the above conceptual methodology for defining a salinity impact category for the following reasons:

- Toxic effects in humans due to common ions occur only at very high concentrations. Humans will, by nature, avoid the intake of highly saline water or will treat the water to acceptable salinity levels before ingestion. This is not usually the case with aquatic and terrestrial ecosystems.
- Toxic effects by other ionic species are already accounted for in the calculation of human toxicity potentials using existing characterisation models.

3.4 CONCLUSIONS

In this chapter a conceptual characterisation model is proposed. The same approach is adopted as was adopted in the USES-LCA model where a "unit environment" was defined. The difference, however, is that a "unit South African catchment" is defined. A simple atmospheric deposition model is developed conceptually, and it is proposed that existing hydrosalinity models be used to determine the fate of salts in the aquatic and terrestrial environment. It is proposed that the effects potentials (or equivalency factors) be calculated in a similar manner to that of Huijbregts (1999) In **Chapter 4**, the conceptual characterisation model, consisting of an atmospheric deposition component and a hydrosalinity component is developed in more detail. Existing atmospheric deposition models are not used in this study and a simple atmospheric deposition

model is therefore developed. The hydrosalinity model is, however, based on existing models and the detailed equations are discussed in **Chapter 4**.

CHAPTER 4

DETAILED ENVIRONMENTAL FATE MODEL DEVELOPMENT

In this chapter, the conceptual environmental fate model proposed in Chapter 3 is developed in more detail. The chapter is sub-divided into two sections; Section 4.1 deals with the atmospheric deposition model, and Section 4.2 deals with the hydrosalinity model. Existing atmospheric deposition models were not used in this study. A simple atmospheric deposition model was developed to meet the objectives stated in Section 3.2.2, and therefore a detailed review of the literature relating to the generation, removal and transport mechanisms of aerosols over South Africa is presented in Section 4.1.1. The modelling approach and model development is presented in Section 4.1.2. The hydrosalinity model is, however, based on existing models and a detailed literature review is not given. The approach adopted in developing the hydrosalinity model is given in Section 4.2.1, and the development of the model itself is given in Section 4.2.2.

4.1 ATMOSPHERIC DEPOSITION MODEL

Existing hydrosalinity models are available, and can be used to calculate salt concentrations in the various terrestrial and aquatic compartments. No models are, however, available for calculating aerosol (and associated salt) depositions for a "unit catchment", and therefore a simple model was developed.

4.1.1 Literature review

The objective of this literature review is to gain sufficient understanding of the processes involved in the generation and movement of aerosols over South Africa, and the mechanisms by which aerosols are removed from the atmosphere, in order to allow the development of a simple atmospheric deposition model.

Generation and composition of aerosols over southern Africa

Aerosols refer to small solid and liquid matter in the atmosphere. Aerosols are distinguished from dust, which are larger pieces of solid material (approximately 20 μm diameter and greater) that settle out of the atmosphere by gravitation after short periods of suspension. Dust is generally a local problem, but aerosols can be transported long distances and may affect air quality and climate on a regional and global scale.

Aerosols originate from two main source regions. *Primary* aerosols directly injected into the atmosphere from the earth's surface mainly come from volcanism, the ocean surface, forest fires, re-suspension of soil material in rural areas, biological processes (pollen, bacteria, fungi), meteoric debris and anthropogenic processes. Ninety percent of these emissions occur in the troposphere. Secondary aerosols are formed after chemical conversion in the atmosphere, which usually involves gases, other aerosols, and atmospheric components, particularly moisture. Secondary aerosols are almost always confined to the fine size range, and grow rapidly from nucleation mode (< 0.1 μm) at initial formation to the accumulation mode (up to 2 μm). A large fraction of the fine aerosols comprise sulphate, with at least half the source in the northern hemisphere being anthropogenic in origin (Bridgman, 1990). Table 4.1 shows estimates of annual global aerosol generation.

Table 4.1: Range of estimates of aerosol generation from natural and anthropogenic sources (Hewitt and Sturges, 1993)

Sources	Global Aerosol Production (10^{15} g/y)
Natural – Primary Production	
Sea salt	0.2 - 2.0
Mineral dust	0.1 - 1.8
Volcanic emissions	0.0 - 0.1
Forest fires	0.0 - 0.2
Natural – Secondary Production	
Converted sulphate	0.3 - 2.4
Converted nitrate	0.1 - 0.7
Converted hydrocarbon	0.1 - 1.1
Anthropogenic – Primary Production	
Direct	0.0 - 0.1
Anthropogenic – Secondary Production	
Conversions	0.2 - 0.4
TOTAL	**1.0 - 8.7**

Aerosols derived from the crust of the earth and biomass burning, as well as sulphates and elemental material from industrial sources, frequently remain in the haze layer for periods of a week, and on occasions for as long as three, while they recirculate anticyclonically over South Africa before offshore export occurs. Particles surviving this long in the lower layers of the atmosphere typically have diameters less than 2 μm (Tyson and Gatebe, 2001).

Measurements made at a high-altitude site on the top of the 3 000 m Ben MacDhui mountain on the south-eastern edge of the Lesotho massif effectively sample mean maximum outflow within the haze layer in the transport plume to the Indian Ocean over South Africa. They reveal that in the coarse aerosol fraction (which makes up approximately 56% of the total load) 85% of the particulate matter being transported out to sea is aeolian, surface-derived, mineral dust. The second largest contribution to total plume loading is industrially derived sulphur at 23%. By contrast, in the fine fraction, industrial sulphur constitutes 59%, aeolian dust 36% and particulates from biomass burning only 6%. South of around 20°S, biomass burning produces only a small fraction of the aerosol loading of the lower troposphere over South Africa. North of 20°S the contribution from biomass burning is greater. The sulphur being transported, as a patchy coating of precipitated sulphur products on small dust nuclei, is at a maximum in warmer, moister summer air when oxidation of SOx is at its maximum (Tyson and Gatebe, 2001).

Results from the Ben MacDhui High Altitude Aerosol and Trace Gas Transport Experiment (BHATTEX) identified four sources in the coarse and fine particulate fractions: soil, industrial, biomass burning, and marine. In the coarse fraction, the soil and marine components are most prominent, contributing 40 to 60% of the total detected inorganic aerosol. In the fine fraction, fine sulphur and iron comprise the industrial components; fine potassium, related to biomass burning emissions; and fine silicon and aluminium from the soil, were most abundant. The industrial component was by far the largest contributor (47%) to the fine aerosol load. The total mass fraction of the fine fraction was in some instances equal and even greater than the course fraction. It is expected that most of the particulate sulphate occurs over the continent as ammonium sulphate. Ammonia acts as a neutralising agent of the sulphuric acid. Sulphate and ammonium concentrations at BenMacDhui measured during March 1996 varied between close to zero and 1 700 and 4 000 ppbv respectively. (Piketh et al., 1999).

Aerosol lifetimes in the troposphere are particle-size dependent and are typically a few hours for particles >10 μm aerodynamic diameter to several days for accumulation-mode particles (< 2.5 μmad). This leads to large regional variability of aerosol concentrations (Kirkman et al., 2000).

At surface remote rural sites north of 30°S, aerosol median mass concentrations determined during SAFARI at Etosha National Park, Victoria Falls, Palmer and Skukuza ranged from 26 to 33 μg/m^3. At rural background sites over north-eastern South Africa, contributions of industrial sulphur constitute 18 to 37% of the total aerosol load annually. The highest backgound sulphur loading is recorded at 3 000 m, high altitude Ben MacDhui site in summer when industrial sulphur constitutes 43% of the detected aerosol loading. Biomass burning contributes least to the total inorganic component of aerosol loading over South Africa.

Maenhaut et al, (1996) analysed fine and coarse aerosol fractions from samples taken in the Kruger National Park. Unfortunately, samples were not analysed for ammonium. Assuming, however, that all sulphur present is as ammonium sulphate (Piketh et al., 1999), the total inorganic fraction of the fine and course aerosol fractions is estimated at 0.8 and 0.4 respectively. The inorganic fraction of the combined sample is estimated at 0.6. The fraction of common ions (magnesium, calcium, chloride and sulphate) is estimated at 0.3 for the fine fraction, and 0.17 for the coarse fraction, with a value of 0.23 for the combined sample (carbonate was not measured).

Tyson et al, (1996) report average aerosol concentrations over the Johannesburg/Vereeneging area of 20 μg/m^3 (with a maximum of 120 μg/m^3), 15 μg/m^3 (with a maximum of 140 μg/m^3) over the Eastern Transvaal Highveld, 10 μg/m^3 (with a maximum of 60 μg/m^3) over the rural eastern part of South Africa, and 29 to 55 μg/m^3 over the Kruger National Park.

Movement of aerosols over South Africa

The mean circulation over the African sub-continent is anticyclonic throughout the troposphere for most of the year. The major outflow duct for aerosols and trace gases from the subcontinent south of Zambia is to the Indian Ocean over South Africa (Figure 4.1). The locus of the mean annual plume is at 31°S over southern Lesotho. More than 75% of all air circulating over South Africa and countries adjacent to the north, and material within, exits the subcontinent at this point. Annual mass fluxes of aerosols transported over southern Africa were estimated from trajectory-swarm determination of the volume of air being transported in mean plumes and from the measurements of background ambient aerosol loading. Over the central subcontinent, 12 Mt/y is transported over Zimbabwe and Botswana in the direction of the Atlantic Ocean. Over Botswana and Namibia the transport field diverges into a major plume recurving to the south with a minor plume moving westward. By the time the latter exits the continent to the ocean off Namibia, the mass load has increased 20 to 29 Mt/y. Recurving anticyclonically towards the east and the

Indian Ocean at 30 to 32°S, the mass load in the main transport plume has reached approximately 39 Mt/year over central South Africa. By the time the plume has reached 35°E off the southeast coast of South Africa, the mass load is estimated at approximately 45 Mt/year. The estimated mass loads out of South Africa do not take into account possible wet and dry deposition once air has exited South African airspace. The mass loads appear to be about half those reported for transport westward out of the Sahara from northern Africa (Tyson and Gatebe, 2001).
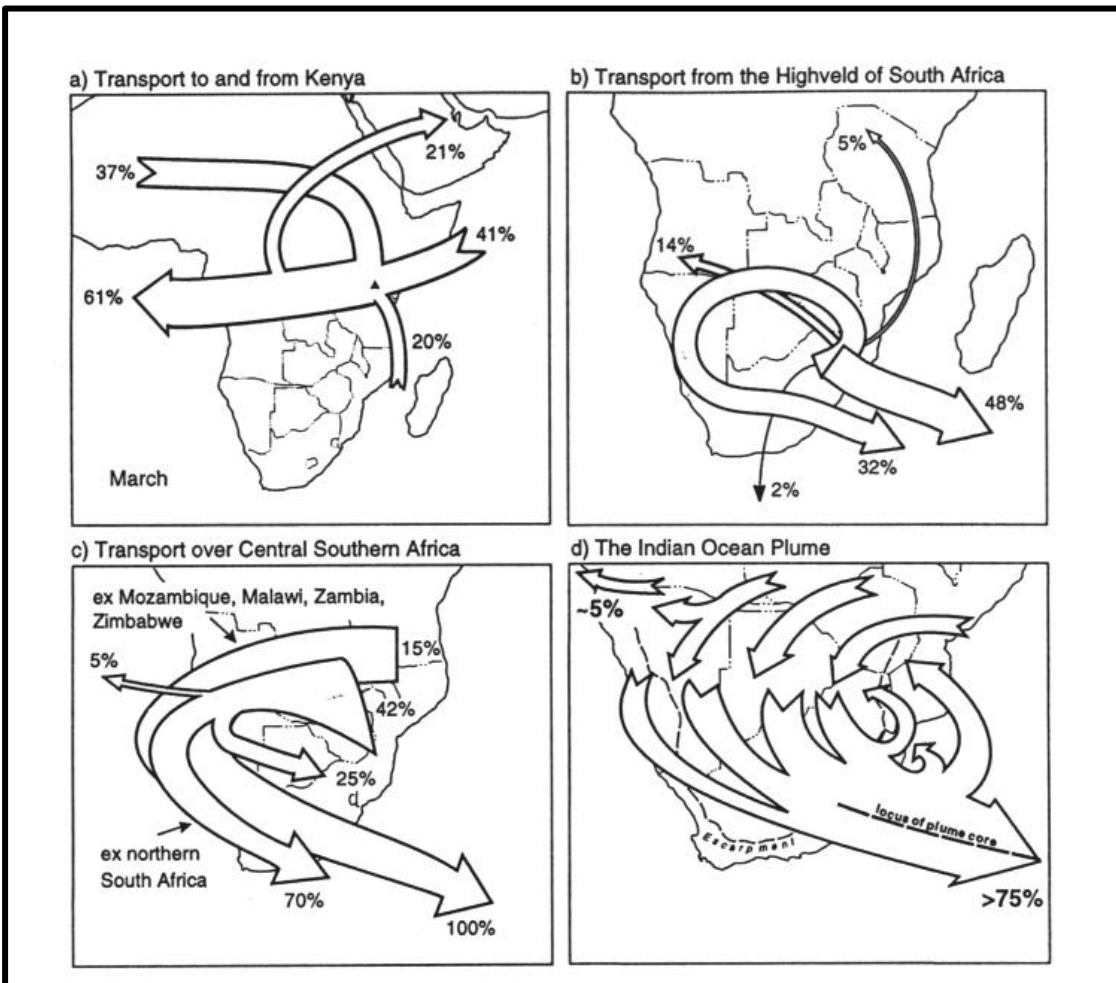
Figure 4.1: Aerosol and trace gas horizontal transport patterns over Southern Africa (Tyson and Gatebe, 2001).

A striking feature of the transport of aerosols and trace gases over South Africa is the degree of recirculation that takes place. Air trapped between the 700 and 500 hPa stable discontinuities may circulate for more than three weeks. Approximately 44% of all circulating air over South

Africa on fine (no-rain) days was recirculated on a sub continental scale at least once. The annual average flux of aerosols being recirculated to the west over northern South Africa and southern Zimbabwe is estimated at around 11.5 Mt/y; that being recirculated to the west over South Africa at about 17.3 Mt/y. Recirculation occurs at a variety of temporal and spatial scales extending from hours to weeks and from tens to thousands of kilometre (Tyson and Gatebe, 2001).

Tyson et al, (1996) identified five dominant circulation types over southern Africa. Volume fluxes were estimated for the five circulation types, and using average aerosol concentrations, monthly aerosol mass fluxes exported from South Africa into the Indian and Atlantic Oceans were estimated. The total zonal mass load into both oceans from southern Africa is approximately 74 Mt/year. Of this amount about 26 Mt/y is recirculated mass. Over the continent approximately 60.5 Mt/y of mass is recirculated with export. The total mass over the continent is thus about 134 Mt/y.

In a study of the long-range transport of southern African aerosols to the tropical south Atlantic, chemical tracers measured at Etosha Park were detected 6 to 7 d later at Ascension Island. The aerosol transport speed ranged from 6.6 to 7.7 m/s with an average of 7.1 m/s over the 4 000 km distance. These speeds are consistent with wind speeds in the mixed (~ 500 m) and cloud   (500 to 3 000 m) layers of the south tropical Atlantic (Swap et al., 1996).

Elevated, absolutely stable layers, inhibit free upward air motion. Over southern Africa the layers play an essential role not only in anthropogenic and biogenic product accumulation at specific altitudes, but also in water vapour, aerosol and trace gas transport and recirculation on a regional to sub-continental scale. The effects of accumulation are evident to the naked eye at approximately 700 hPa (approximately 3 000 m altitude) and 500 hPa (5 500 m altitude), as shown in Figure 4.2. These stable layers occur over the plateau at frequencies of 74% and 91% for the 700 hPa and 500 hPa stable layers respectively. Over the coast, comparable mean frequencies are about 80% and 87% respectively. Periodic merging of layers on singular days or even over several days may occur. Merging of the 500 hPa and 300 hPa layers has been noted on average 6% of the time (Piketh et al., 1999)

The stable layers are sufficiently stable to inhibit the vertical transport of aerosols and trace gases. The bulk of pollutants are transported below the first two capped atmospheric layers of absolute stability (Piketh 1999).

Figure 4.3 demonstrates the variability of wind speed with altitude during the Ben MacDhui experiment (Piketh et al., 1999).
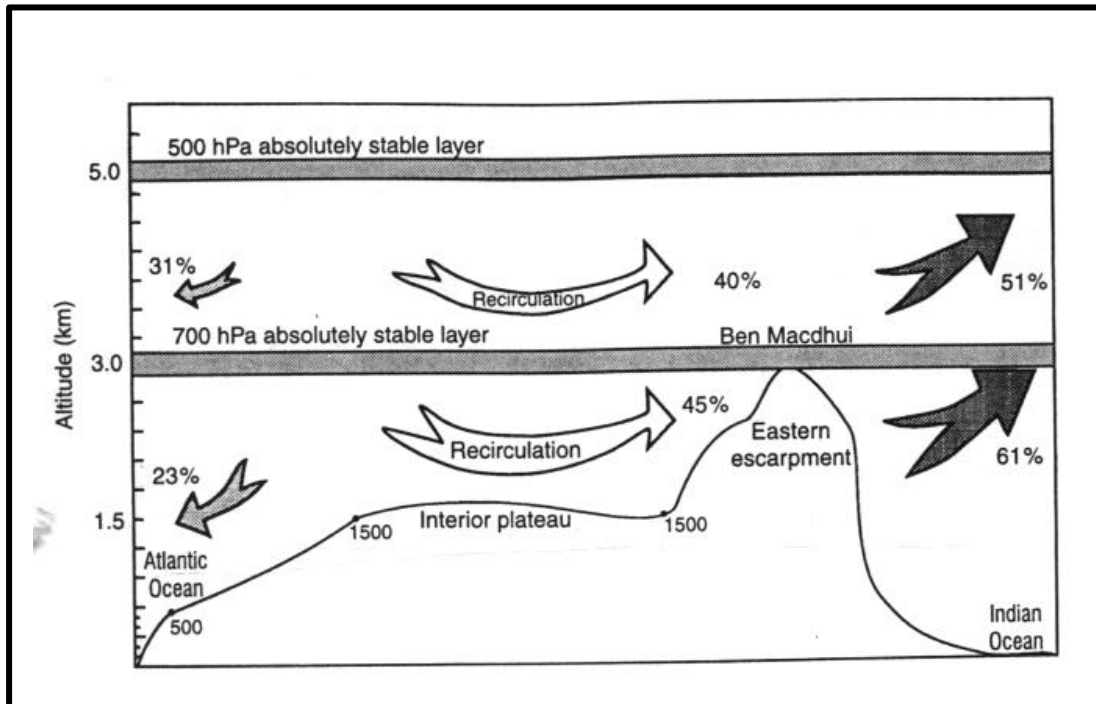
Figure 4.2: Variation with height of average transport from Southern African interior to the two adjacent oceans (Piketh et al, 1999).
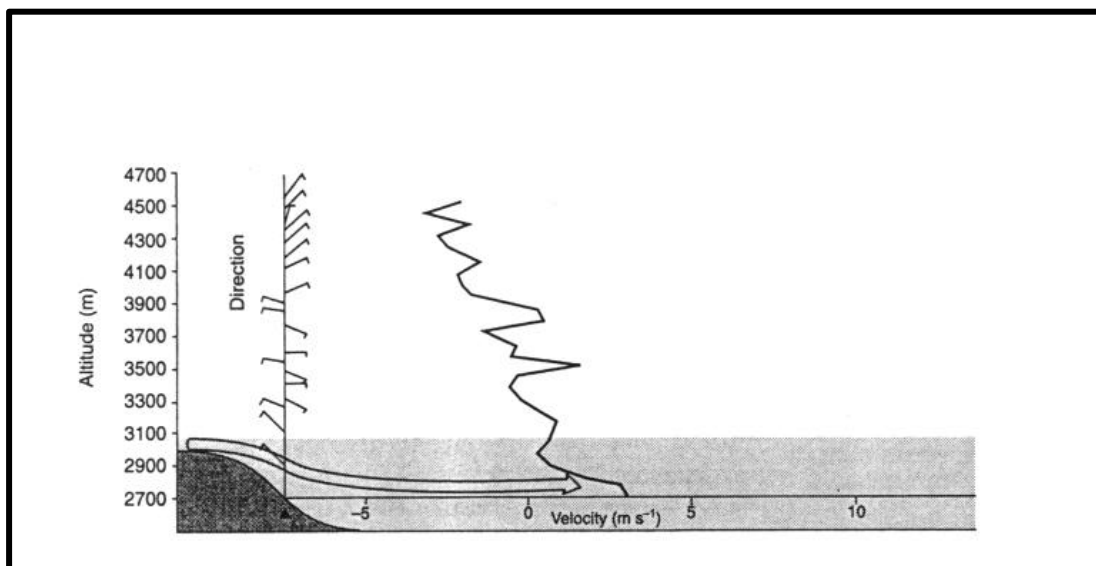
Figure 4.3: Example of variability of wind speed with altitude during the Ben MacDhui experiment. The example shows a stable layer with no flow separation in off-plateau flow (Piketh et al., 1996).

Low-level jets over various regions of southern Africa result in wind speeds in excess of 10 m/s in the jet core, which is typically located between 200 and 300 m above ground level. The Natal mountain-plain winds may exceed 10 m/s in a layer up to 1 000 m deep. Typical low-level jets persist for more than 12 h during which time wind speeds in excess of 10 m/s may transport products in excess of 400 km in a single night (Zunkel et al., 1996). Wind speeds in the range 6.6 to 7.7 m/s are consistent with wind speeds in the mixed (~500 m) and cloud (200 to 3 000 m) layers of South Africa (Swap et al., 1996).

Deposition processes

Aerosols are removed from the atmosphere by three main methods: dry deposition, wet deposition, and fog/cloud water capture (also known as occult deposition).

Dry deposition

Dry deposition is the deposition of gases and particles from the atmosphere by processes other than dissolution in rain, cloud or fog. It is governed by the concentration of pollutants in the air, by turbulent transport processes in the boundary layer, by the chemical and physical nature of the depositing species and by the efficiency of the surface in capturing and adsorbing gases and particles. The theory describing dry deposition processes is complex, requiring a large number of model parameters. A general indication of dry deposition rate is often estimated by calculating the product of the pollutant concentration and the pollutants deposition velocity (Bridgman, 1990).

Wet deposition

Removal by precipitation, called wet deposition, includes both in-cloud (rain-out) and below cloud scavenging (wash-out). Wet deposition is strongly dependent on the amount of rain, the distance from sources of pollution and the topography of the receptor area. Wet deposition is enhanced at high altitude as a result of the incorporation of particles into orographic clouds over hills and scavenging of the cloud droplets by rain droplets falling from higher-level cloud (Herold et al., 2001). There are several models available for estimating wet deposition, however, removal by rain is often expressed using the washout ratio, defined as the ratio of the concentration of the pollutant in rain water to the concentration of the pollutant in the air (Hewitt and Sturges, 1993). The composition of rainfall unaffected by anthropogenic activities is shown in Table 4.2.

Table 4.2: Volume weighted mean composition of background rainfall (adapted from Bridgman, 1990).

Ion	Concentration range (■eq/L)
Hydrogen	11.0 - 18.3
Calcium	0.1 - 9.7
Ammonium	1.1 - 7.4
Sulphate	2.7 - 18.3
Nitrate	1.7 - 5.5

Rainfall composition was studied over a one-year period on a small (32.5 ha) catchment at the Suikerbosrand Nature Reserve (Skoroszewski, 1999). The results of this study are shown in Table 4.3.

Table 4.3. Rainfall composition (adapted from Skoroszewski, 1999)

Parameter (mg/L, except pH)	Minimum	Average	Maximum	Average of total measured %
pH	2.3		7.3	
Nitrate	0.1	2.6	16.5	25.3
Chloride	0.1	0.6	3.8	5.4
Sulphate	0.3	3.8	12.4	36.6
Sodium	0.1	0.5	6.5	5.2
Potassium	0.1	0.8	9.1	7.6
Calcium	0.1	0.8	5.1	8.1
Magnesium	0.1	0.2	1.2	1.9
Ammonium	0.0	1.0	6.6	10.0
Total of measured parameters	0.9	10.3	61.2	100.0

Rainfall total dissolved solids concentration in an urban catchment varied between 3 and 104 mg/L. Wet total dissolved solids deposition rates varied between 0 and 824 $mg/m^2/day$ (Coleman, 1993)

4.1.2 Model approach and development

The objectives of the atmospheric deposition model are stated in **Section 3.2.2**. The approach adopted was to develop a simple "fixed-box" (de Nevers, 1995) atmospheric deposition model that could estimate salt deposition rates at a daily time step, without resorting to complex air dispersion modelling, with its associated data demand.

The conceptual atmospheric model is shown schematically in Figure 4.4. The total air volume is divided into a rural air volume, and an urban air volume that is totally bounded by the rural air volume.

Assumptions

The major simplifying assumptions made include:

1. Atmospheric turbulence in both the urban and rural air volumes produces complete mixing up to the mixing height (H).
2. The density of the atmosphere up to the mixing height (H) is constant, and the mixing height is constant.
3. All matter entering the air volumes and/or generated within the volumes is contained below the mixing height, and no matter leaves through the sides that are parallel to the direction of the wind.
4. The aerosol soluble inorganic mass fraction remains constant and is the same for the urban and rural air volumes.
5. The emission of pollutant into the air occurs into the urban air volume.
6. Wind does not change direction, and is independent of location and elevation.

The above assumptions are clearly a great simplification of what really occurs in nature. The worst assumption is that the air volumes are completely mixed (de Nevers, 1995). In reality, concentration gradients will exist that depend on very many variables, including local meteorological conditions and topography. The desired output from the atmospheric deposition model, in terms of the overall fate model, is the total daily salt deposition rate. This is the only output from the atmospheric deposition model that is used as input by the hydrosalinity model. More complicated air dispersion models exist that have a very high model parameter demand, and can generally only be applied to limited geographical scales, for which the topography and meteorological conditions are known. The simplifying assumptions made, although not ideal,

allow estimates to be made of deposition rates at a daily time step using comparatively few parameters.
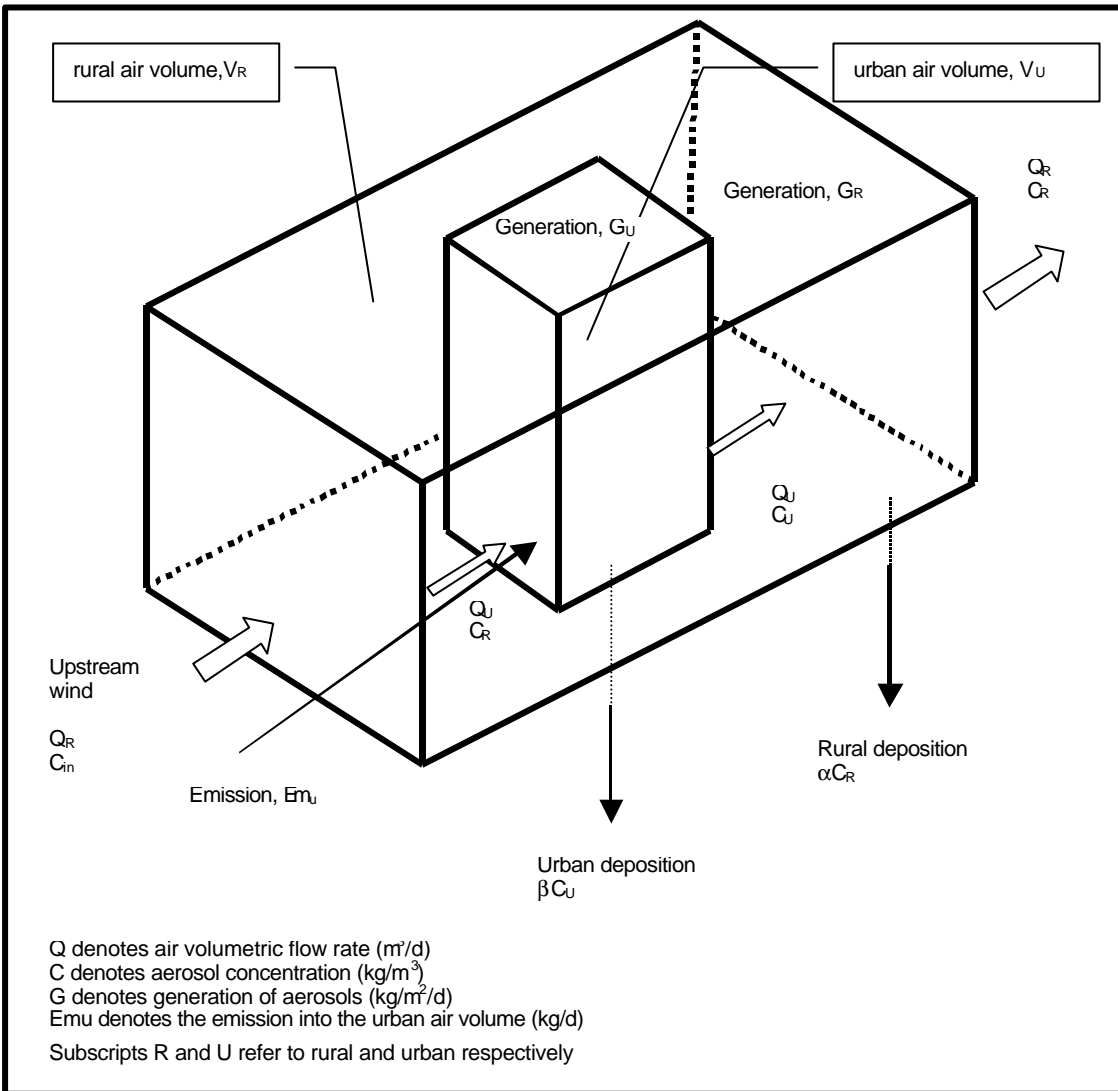
Figure 4.4: Schematic diagram of the conceptual atmospheric deposition model.

Referring to Figure 4.4, an aerosol mass balance over the total air volume over a time interval of 1 d yields:

$$M_T = M_T^0 + Q_R C_{in} + Em_u - \boldsymbol{a} C_R - \boldsymbol{b} C_U - Q_R C_R + G_R + G_U \qquad \text{[4-1]}$$

Where:

M_T =   total mass of aerosol in air volume at the end of the day (kg)

M_T^0 =   total mass of aerosol at the beginning of the day (kg)

a   =   a coefficient describing the deposition of aerosols from the rural air volume (m^3/d)(see below).

b   =   a coefficient describing the deposition of aerosols from the urban air volume (m^3/d)(see below).

Em_a =   emission into urban air (kg/d)

An aerosol mass balance over the urban air volume over a time interval of one day yields:

$$V_U\, C_U = M_U = M_U^0 + Q_U\, C_R + G_U + Em_a - Q_U\, C_U - \boldsymbol{b}\, C_U \qquad [4\text{-}2]$$

Where:

M_U =   total aerosol mass in the urban air volume at the end of the day (kg)

M_U^0 =   total aerosol mass in the urban air volume at the beginning of the day (kg)

An aerosol mass balance over the rural air volume over a time interval of one day yields:

$$V_R\, C_R = M_R = M_R^0 + Q_U\, C_U + G_R + Q_R\, C_{in} - Q_U\, C_R - \boldsymbol{a} C_R - Q_R\, C_R \qquad [4\text{-}3]$$

Where:

M_R =   total aerosol mass in the rural air volume at the end of the day (kg)

M_R^0 =   total aerosol mass in the rural air volume at the beginning the day (kg)

Rearranging Equation [4-3] yields:

$$C_R = \frac{M_R^0 + G_R + Q_R\,C_{in} + Q_U\,C_U}{V_R + \boldsymbol{a} + Q_R + Q_U}$$ [4-4]

Substitution of Equation [4-4] into Equation [4-2] yields:

$$C_U = \frac{\left[M_U^0 + G_U + Em_a\right]\left[V_R + \boldsymbol{a} + Q_R + Q_U\right] + Q_U\left[M_R^0 + G_R + Q_R\,C_{in}\right]}{\left[V_U + Q_U + \boldsymbol{b}\right]\left[V_R + \boldsymbol{a} + Q_R + Q_U\right] - Q_U^2}$$ [4-5]

Equations [4-4] and [4-5] are used to calculate the aerosol concentrations at the end of each successive day, based on the total aerosol mass at the start of the day.

The volumetric flow rate (in m³/d) of the air entering the rural area (Q_R) in one day is given by:

$$Q_R = \boldsymbol{u}W_T\,H$$ [4-6]

Where:

$\boldsymbol{u}$	=	wind speed (m/d)
W_T	=	width of the rural air volume (m)
H	=	atmospheric mixing height (m)

Average monthly wind speeds are input into the model, and are assumed to remain constant throughout the month.

The volumetric air flow rate (in m³/d) entering the urban air volume from the rural air volume (and hence the flow rate into the rural air volume from the urban air volume (Q_U) is given by:

$$Q_U = \boldsymbol{u}\,W_U\,H$$ [4-7]

Where:

W_U	=	width of the urban air volume (m)

The generation of aerosols (in kg/d) in the urban and rural air volumes comprises a natural component, and an anthropogenic component:

$$G_U = A_T \, AI(G_N + G_A^U)$$ [4-8a]

$$G_R = A_T(1 - AI)(G_N + G_A^R)$$ [4-8b]

Where:

A_T = total area (m^2)

G_N = natural aerosol generation rate (kg/m^2/d)

G_A^U = urban anthropogenic aerosol generation rate (kg/m^2/d)

G_A^R = rural anthropogenic aerosol generation rate (kg/m^2/d)

AI = fraction urban area (-)

Deposition mechanisms are modelled in a similar way to Herold et al. (2001). Total dry deposition is calculated as the product of the salt concentration in the atmosphere and the deposition velocity. The total dry deposition rate is then calculated as a factor of the total dry deposition. The total dry plus occult deposition is assumed to be F_o times the estimated dry deposition.

Dry, occult and wet aerosol deposition in the urban air volume is given by Equations [4-9] to [4-11].

$$D_U^d = F_d \, C_U \, V_d \, AI \, A_T$$ [4-9]

$$D_U^o = F_o \, F_d \, C_U \, V_d \, AI \, A_T$$ [4-10]

$$D_U^w = C_U \, R_d \, WR \, AI \, A_T \, 10^{-3}$$ [4-11]

Where:

D_U^d = dry aerosol deposition rate on the urban area (kg/d)

D_U^o = occult aerosol deposition rate on the urban area (kg/d)

D_U^w = wet aerosol deposition rate on the urban area (kg/d)

F_d = dry deposition factor (-)

V_d = deposition velocity (m/d)

F_o = occult deposition factor (-)

R_d = rainfall (mm/d)

WR = wash ratio (-)

Dry, occult and wet aerosol deposition in the rural air volume is given by Equations [4-12] to [4-14].

$$D_R^d = F_d \, C_R \, V_d \, (1 - AI) \, A_T \qquad\qquad\qquad [4\text{-}12]$$

$$D_R^o = F_o \, F_d \, C_R \, V_d \, (1 - AI) \, A_T \qquad\qquad\qquad [4\text{-}13]$$

$$D_R^w = C_R \, R_d \, WR \, (1 - AI) \, A_T \, 10^{-3} \qquad\qquad\qquad [4\text{-}14]$$

Where:

D_R^d = dry aerosol deposition rate on the rural area (kg/d)

D_R^o = occult aerosol deposition rate on the rural area (kg/d)

D_R^w = wet aerosol deposition rate on the rural area (kg/d)

The value of a and b used in Equations [4-1] to [4-5] are thus given by:

$$\boldsymbol{a} = (1 - AI) \, A_T \, [F_d \, V_d + F_o \, F_d \, V_d + R_d \, WR] \qquad\qquad [4\text{-}15]$$

$$\boldsymbol{b} = AI \, A_T \, [F_d \, V_d + F_o \, F_d \, V_d + R_d \, WR] \qquad\qquad [4\text{-}16]$$

The methodology for calculating the daily distribution of rainfall is given in **Section 4.2.2**. Summer and winter dry deposition factors are input into the model, and are considered constant throughout these periods. Winter months are from April to September. Summer and winter aerosol deposition velocities are input into the model. Summer deposition velocity remains constant for the months January to March and October to December. Winter deposition velocity remains constant for the months June to July. For the months April, May, August and September, the deposition velocity is calculated proportionately between the summer and winter values.

The value of a and b are calculated from Equations [4-15] and [4-16]. These values are then substituted into Equations [4-4] and [4-5] to calculate the aerosol concentrations in the rural and urban air volumes respectively. The concentrations are then substituted into Equations [4-9] to [4-14] to calculate the daily aerosol deposition rates. The salt associated with the aerosol deposited is calculated from the fraction of salt that is assumed to be soluble, which is input into the model.

4.2 HYDROSALINITY MODEL

The hydrosalinity model is based on existing models that have been applied to selected catchments throughout South Africa. The approach adopted in developing the hydosalinity model is discussed in **Section 4.2.1**, and the model itself is presented in **Section 4.2.2**

4.2.1 Introduction and modelling approach

Numerous hydrosalinity models have been developed and applied to various studies of South African catchments. These models range from simple models requiring very few input parameters to complex three-dimensional groundwater and solute-transport models that require a large number of input parameters (Hughes, 1997).

It has been shown (refer to **Section 2.5.2**) that the simple methodology used in the USES-LCA model is inadequate to describe salinity effects. At the other extreme, however, more complex models would require many more parameters, which are often not known for particular catchments within the country, and are certainly not known for a "regionalised catchment". A compromise was therefore sought between these two extremes; that would meet the objective of the model (discussed in **Section 3.2.3**), with the emphasis placed on the inclusivity of processes governing the fate of dissolved salts.

The hydrosalinity model developed by Herold (1981), based on the work by Pitman (Pitman 1973 and Pitman 1976) is deemed to be the best compromise. The Pitman model has become the most widely used monthly time-step, rainfall-runoff model within southern Africa. The current official version of the model is referred to as WRSM90, and was used to model rainfall-runoff in all catchments within South Africa to the quaternary catchment level (Midgely et al., 1994). Monthly simulated natural river flow data are therefore available for all catchments in the country, as are the model parameters used.

The rainfall-runoff component of the model initially developed by Pitman (1973) and later modified by Herold (1981) is essentially used as presented by Herold (1981). Only minor simplifications are made to the model, and these are highlighted in **Section 4.2.2** Several modifications are, however, made to the solute transport component of the model. These modifications are highlighted in **Section 4.2.2,** but the most notable are:

- The inclusion of salt adsorption algorithms, based on the Langmuir adsorption model.
- A sediment transport component is added to the model, including the generation of sediment through erosion and the transport of sediment in surface water as suspended sediment and as bed load. The sediment transport component of the model is based on the work done by Paling et al. (1989). Salt transport by means of adsorbed salt on sediment is also taken into account.
- The manner in which the precipitation and dissolution of salt is dealt with.

The hydrosalinity model is developed based on existing models that are accepted and are in general use in South Africa. The assumptions made in the development of these models can be found in the references, and are therefore not examined in detail. Where modifications to the models are made, these are highlighted.

4.2.2 Model development

Development of the hydrosalinity model is presented below. The model developed is based on the hydrosalinity model developed by Herold (1981). The differences between the model developed in this work, and that of Herold (1981) are highlighted.

Rainfall

Figure 4.5 is a typical plot of cumulative rainfall for a given month. Using daily rainfall data at several widely spread locations throughout South Africa, Pitman (1973) showed that the value of W (shown in Figure 4.5) could be described by:

$$W = -2 + 1.3732 \, (P_m + 1.6)^{0.8} \qquad\qquad [4\text{-}17]$$

Where:

P_m =   monthly rainfall (mm)
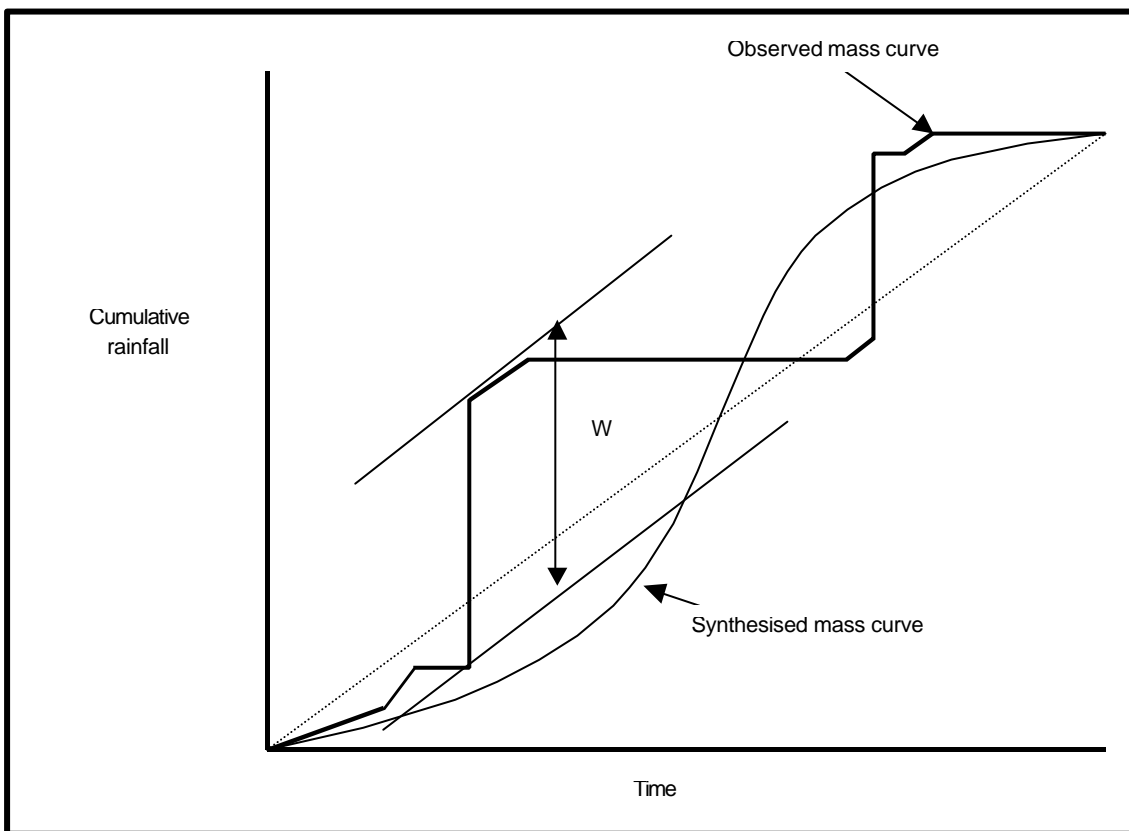
Figure 4.5: Typical rainfall mass curve (after Pitman, 1973)

Monthly rainfall is input into the model, and monthly W values are calculated using Equation [4-17]. Cumulative rainfall can be described by a sigmoid-shaped function of the form:

$$y = \frac{x^n}{x^n + (1 - x^n)}$$ [4-18]

Where:

y = cumulative rainfall/total rainfall (mm/mm)

x = cumulative time/total time (h/h)

n = exponent related to W (mm)

The relationship between W and n has been shown (empirically) to be (Pitman 1973):

$$n = \frac{1.28}{(1.02 - \frac{W}{P_m})^{1.49}}$$ [4-19]

Subtraction of successive cumulative rainfall values from each other yields daily rainfall values.

Rainfall duration ($DURS$) is calculated by the expression:

$$DURS = AA + BB\, x$$ [4-20]

Where AA and BB are empirical constants. After the rainfall duration has been calculated, the daily rainfall total is further disaggregated into hourly rainfall. The assumption is made that the onset of rain coincides with the beginning of the day. Each day is divided into 24 one-hour time intervals, regardless of the duration of rainfall. The distribution of rainfall is calculated assuming a sigmoid-shaped curve (Equation 4-18, with n set equal to 2, derived empirically). The rainfall occurring on the rural agricultural area includes irrigated water.

Interception

Interception by vegetation and soil surfaces is assumed to occur at a constant value (PI) when rainfall occurs. Infiltration and runoff will only occur if rainfall in excess of PI occurs. Intercepted storage is depleted at the potential evapotranspiration rate.

Infiltration, interflow and surface runoff

Permeability, and hence infiltration rate vary spatially, even in the most uniform of catchments. A triangular distribution of infiltration rates, identical to that adopted by Pitman (1976) is used. Hourly surface runoff (R_h) from rural (pervious) areas is calculated as follows:

$$R_h = \frac{2(P_h - Z1)^3}{3(Z3 - Z1)^2} \qquad\qquad [4\text{-}21]$$

For $Z1 \leq P_h \leq Z2$:

$$R_h = P_h - Z2 + \frac{2(Z3 - P_h)^3}{3(Z3 - Z1)^2} \qquad\qquad [4\text{-}22]$$

For $Z2 \leq P_h \leq Z3$:

$$R_h = P_h - Z2 \qquad\qquad [4\text{-}23]$$

For $P_h \geq Z3$:

Where;

$$Z3 = \frac{4 Z_{max}}{2^{\frac{2S}{ST}}} \qquad\qquad [4\text{-}24]$$

$$Z1 = \frac{Z_{\min} \; Z3}{Z_{\max}} \qquad\qquad\qquad\qquad\qquad\qquad [4\text{-}25]$$

$$Z2 = \frac{(Z1 + Z3)}{2} \qquad\qquad\qquad\qquad\qquad\qquad [4\text{-}26]$$

Where:

R_h	=	surface runoff (mm/h)
P_h	=	hourly rainfall (mm)
$Z_{\min}$	=	nominal minimum infiltration rate (mm/h)
$Z_{\max}$	=	nominal maximum infiltration rate (mm/h)
S	=	soil moisture (mm)
ST	=	soil moisture capacity (mm)

It is assumed that when the soil moisture storage is at full storage capacity, the interflow component is equal to a maximum portion of the surface runoff, and that the interflow component decreases linearly to zero when soil moisture storage is empty. Interflow is calculated from the following relationship:

$$T_h = \frac{PINTM \; R_h \; S}{ST} \qquad\qquad\qquad\qquad\qquad\qquad [4\text{-}27]$$

Where:

T_h	=	interflow (mm/h)
$PINTM$	=	maximum proportion of surface runoff derived from interflow (-)

On rural (pervious) areas all rainfall in excess of interception storage that does not give rise to surface runoff and interflow enters the soil moisture through infiltration. On urban (impervious) areas, all rainfall in excess of interception storage gives rise to surface runoff. Surface runoff and interflow is calculated separately for the rural natural surface and the rural agricultural surface.

Surface sediment generation

The erosion and sediment transport model is based on the work done by Paling et al (1989). The catchment is considered to consist of a layer of loose soil (immediately available for transport) underlain by a layer of erodible, but not loose, soil (available for detachment and thus conversion to loose soil). Initial depths for loose and erodible soil are input, and adjusted for addition and removal at each time step during the simulation. During each time step the depth of loose soil is reduced by the sediment discharged from the catchment. The removed sediment is therefore assumed to be derived uniformly from the catchment. The depth of loose soil is constrained to be positive. If the depth of erodible soil is positive then some of it is transferred to loose soil to account for raindrop detachment. The rate of detachment is given by:

$$D_r = K_D K_S \, i^2 \, (1 - \frac{Z_w}{Z_m})(1 - C_g)$$ [4-28]

The raindrop penetration depth (Z_m) is given by:

$$Z_m = 3(2.23 \, i^{0.187})$$ [4-29]

Where:

D_r = sediment detachment rate (kg/m^2/h)

K_D = detachment coefficient (0,0138 N/mm^2)

K_S = soil erosivity (kg/N/m^2)

i = effective rainfall intensity (mm/h)

Z_w = combined depth of water and loose soil (mm)

Z_m = raindrop penetration depth (mm)

C_g = catchment cover density (-)

In addition, during each time step an amount of erodible soil is converted to loose soil at a prescribed rate to account for sediment generation by fragmentation.

The mass of soil detached is calculated by multiplying the detachment rate by the area. Provision is made in the model to calculate separate detachment rates for the rural natural surface and the rural agricultural surface.

Surface salt

The daily urban and rural salt deposition rates, comprising dry, wet and occult deposition components is calculated from the atmospheric deposition model (refer to **Section 4.1.2**) and is used as input into the hydrosalinity model.

Salt is deposited onto the surface by deposition, is generated on the surface by anthropogenic activities, is stored on the surface and is removed from the surface via surface runoff.

Urban (impervious) surface

It is assumed that the salt load picked up and removed from the urban area within a time interval is proportional to the instantaneous mass of salt stored on the surface. This gives rise to the following first order differential equation (Herold, 1981):

$$-\frac{dM_{Us}}{dt} = K_U \, M_{Us}$$
[4-30]

Where:

M_{Us} =   Mass of salt stored on urban surface (kg)

K_U =   constant (1/h)

The wash-off parameter, K_U, in Equation [4-30] is assumed to be proportional to the surface runoff from the urban surface, which in turn is equal to the net rainfall on the surface. The proportionality constant is termed the impervious (urban) surface wash-off parameter ($ISWP$), and thus:

$$K_U = ISWP\,R_h \tag{4-31}$$

Integrating Equation [4-30] (from $M_U = M_U^1$ at $t=t_1$ to $M_U = M_U^2$ at $t=t_2$) and substitution of Equation [4-31] yields:

$$M_{Us}^2 = M_{Us}^1 e^{-ISWPR_h \, \Delta t} \tag{4-32}$$

A mass balance over the urban surface over the time interval Δt yields:

$$\Delta M_{Us} = M_{Us}^2 - M_{Us}^1 = T_{dep}^U + G_{Us} - L_{runoff}^U \tag{4-33}$$

Where:

T_{dep}^U = total aerosol salt deposited on the urban surface during time interval Δt (kg)

G_{Us} = anthropogenic salt generation on urban surface during time interval Δt (kg)

L_{runoff}^U = salt load in surface runoff (kg)

Noting that the concentration of salt in the surface runoff is given by the salt load in the runoff divided by the runoff volumetric flow, Equation [4-31] is substituted into Equation [4-33] and rearranged to calculate the concentration of salt in the urban surface runoff as follows:

$$C_{Us} = \frac{T_{dep}^U + G_{Us} - M_U^1 \left[e^{-ISWPR_h} - 1 \right]}{R_{Us}\,AI\,A_T\,10^3} \tag{4-34}$$

Where:

C_{Us} = salt concentration in urban surface runoff (kg/m3)

R_{Us} = urban surface runoff (m^3/d)

An initial salt storage mass on the urban surface is specified. During time intervals in which no rainfall occurs, successive salt storage is calculated using Equation [4-33], with L^U_{runoff} set to zero. During time intervals in which rainfall occurs, the concentration of salt in the runoff is calculated using Equation [4-34], which in turn is used to calculate the total salt mass at the end of the time interval, using Equation [4-32]. The urban surface runoff salt load is then calculated using Equation [4-33]. Initially, allowance was made in the model to check the concentration of salt in the runoff, and if it exceeded the solubility limit, restrict the concentration to this limit, and store the precipitated salt on the surface. This however led to unrealistically high surface salt storage values. The implicit assumption in the above equations is therefore that salt stored on urban surfaces may be removed by wash-off of solid salts.

Rural (pervious) surface

The generation, storage and transport of salt on pervious surfaces are calculated in a similar manner to urban surfaces. For rural surfaces, however, the change in storage mass is assumed proportional to the surface runoff and the infiltration flows. Over the time interval Δt:

$$M^2_{Rns} = M^1_{Rns} e^{-PSWP_n \Theta_n \Delta t}$$ [4-35a]

$$M^2_{Ras} = M^1_{Ras} e^{-PSWP_a \Theta_a \Delta t}$$ [4-35b]

Where:

$$\Theta_n = R_{hrn} - I_{hrn} - T_{hrn}$$

$$\Theta_a = R_{hra} - I_{hra} - T_{hra}$$

M^1_{Rns}	=	salt mass stored on rural natural surface at the start of Δt (kg)
M^2_{Rns}	=	salt mass stored on rural natural surface at the end of Δt (kg)
M^1_{Ras}	=	salt mass stored on rural agricultural surface at the start of Δt (kg)
M^2_{Ras}	=	salt mass stored on rural agricultural surface at the end of Δt (kg)
$PSWP_n$	=	rural natural surface wash-off parameter (1/mm)

$$PSWP_a = \qquad\qquad \text{rural agricultural surface wash-off parameter (1/mm)}$$

$$R_{hrn} = \qquad\qquad \text{rural natural surface runoff (mm/h)}$$

$$I_{hrn} = \qquad\qquad \text{rural natural surface infiltration (mm/h)}$$

$$T_{hrn} = \qquad\qquad \text{rural natural surface interflow (mm/h)}$$

$$R_{hra} = \qquad\qquad \text{rural agricultural surface runoff (mm/h)}$$

$$I_{hra} = \qquad\qquad \text{rural agricultural infiltration (mm/h)}$$

$$T_{hra} = \qquad\qquad \text{rural agricultural interflow (mm/h)}$$

In addition, salt is adsorbed onto the sediment generated on the surface and transported to the river. The adsorption of salt onto sediment is assumed to follow the Langmuir adsorption model (since some published values for the Langmuir constants are available, Fey and Guy, 1993) . Adsorption of salt is not taken into account in the Herold (1981) model. The mass of salt adsorbed onto sediment is given by:

$$M_{ads}^{rn} = \frac{A\,C_{Rns}\,M_{det}^{rn}}{B + C_{Rns}} \qquad\qquad\qquad \text{[4-36a]}$$

$$M_{ads}^{ra} = \frac{A\,C_{Ras}\,M_{det}^{ra}}{B + C_{Ras}} \qquad\qquad\qquad \text{[4-36b]}$$

Where:

$$M_{ads}^{rn} = \qquad\qquad \text{mass of salt adsorbed onto rural natural surface sediment (kg)}$$

$$A = \qquad\qquad \text{first Langmuir constant (kg adsorbed/kg sediment)}$$

$$B = \qquad\qquad \text{second Langmuir constant (kg salt/m3 solution)}$$

$$C_{Rns} = \qquad\qquad \text{salt concentration in rural natural surface runoff (kg/m3)}$$

$$M_{det}^{rn} = \qquad\qquad \text{mass of sediment detached from rural natural surface (kg)}$$

$$M_{ads}^{ra} = \qquad\qquad \text{mass of salt adsorbed onto rural agricultural surface sediment (kg)}$$

$$C_{Ras} = \qquad\qquad \text{salt concentration in rural agricultural surface runoff (kg/m3)}$$

$$M_{\text{det}}^{ra} \quad = \quad \text{mass of sediment detached from rural agricultural surface (kg)}$$

A mass balance for rural natural surface salt over the time interval Δt yields the following equations:

$$\Delta M_{Rns} = M_{Rns}^2 - M_{Rns}^1 = T_{dep}^{Rn} + G_{Rns} - L_{\text{inf}}^{Rn} - L_{runoff}^{Rn} - M_{ads}^{rn} \qquad \text{[4-37]}$$

Where:

$$T_{dep}^{Rn} \quad = \quad \text{total salt deposition onto rural natural surface (kg)}$$

$$L_{\text{inf}}^{Rn} \quad = \quad \text{salt load in rural natural infiltration (kg)}$$

$$L_{runoff}^{Rn} \quad = \quad \text{salt load in rural natural surface runoff (kg)}$$

$$G_{Rns} \quad = \quad \text{anthropogenic generation of salt on the rural natural surface (kg)}$$

Substitution of Equation [4-36a] into Equation [4-37] and noting that the salt load in the runoff and infiltration streams is calculated by multiplying the respective volumetric flow rates with the soluble salt concentration (assumed equal in the runoff and infiltration streams), the following quadratic equation is obtained, which can be solved for C_{Rns}, the soluble salt concentration in the rural natural surface runoff and infiltration (assumed equal):

$$a_{rn} C_{Rns}^2 + b_{rn} C_{Rns} + c_{rn} = 0 \qquad \text{[4-38a]}$$

Where:

$$a_{rn} = (1 - FI)(1 - AI) A_T \Theta_n 10_3 \qquad \text{[4-38b]}$$

$$b_{rn} = B A_{rn} + M_{Rns}^1 e^{-\Theta_n PSW_n^P} - M_{Rns}^1 - T_{dep}^{Rn} - G_{Rns} + A M_{\text{det}}^{rn} - E_{rns} \qquad \text{[4-38c]}$$

$$c_{rn} = B(M_{Rns}^1 e^{-\Theta_n PSW_n^P} - M_{Rns}^1 - T_{dep}^{Rn} - G_{Rns} - E_{rns}) \qquad \text{[4-38d]}$$

FI =   fraction of rural agricultural area under irrigation (-)

E_{rns} =   emission of salt onto the rural natural surface (kg)

An initial salt storage mass on the rural natural surface is specified. Successive salt storage is calculated using Equation [4-37]. During time intervals that no rainfall occurs, L_{runoff}^{Rn} and $L_{\inf}^{Rn}$ are set to zero. During time intervals that rainfall occurs, the concentration of salt in the urban surface runoff is calculated by solving equation [4-38] for C_{Rns}. If the concentration is less than the specified saturation concentration, then salt is removed at a rate equivalent to the concentration multiplied by the sum of the runoff and infiltration flows, and the storage mass at the end of the time interval (M_{Rns}^{2}) is calculated using Equation [4-35a]. If the concentration exceeds the saturation concentration, then the concentration is set equal to the saturation concentration, the surface runoff salt load and infiltration salt load are calculated as the product of the saturation concentration and the respective volumetric flow rates. The salt precipitated is added to the total salt storage mass, and the salt storage mass at the end of the time interval (M_{Rns}^{2}) is then calculated using equation [4-37]. The implicit assumption is that complete mixing of stored salt and surface runoff occurs, and that dissolution of salt is immediate.

For the rural agricultural surface, an additional term is included to account for irrigation. Crop water demand is assumed to be proportional to potential evaporation, in the same way as proposed by Herold (1989). The crop water demand is given by:

$$Q_{crop} = F_{irrig} A_{irrig} E_d \, 10^{-3} \qquad\qquad [4\text{-}39]$$

Where:

Q_{crop} =   crop water demand (m^3/d)

F_{irrig} =   monthly irrigation demand factor (-)

A_{irrig} =   area irrigated (m^2)

E_d =   daily evaporation (m^3/d)

The demand is met by rainfall and irrigation. The volumetric flow rate of water required for irrigation is thus given by:

$$Q_{irrig} = Q_{crop} - P_d \, A_{irrig} \qquad \text{[4-40]}$$

The salt load associated with the irrigated water (L_{irrig}) is calculated as the product of the volumetric flow rate and the salt concentration in the river.

A mass balance for rural agricultural surface salt over the time interval Δt yields the following equation:

$$\Delta M_{Ras} = M_{Ras}^2 - M_{Ras}^1 = T_{dep}^{Ra} + E_{ras} + L_{irrig} + G_{Ras} - L_{inf}^{Ra} - L_{runoff}^{Ra} - M_{ads}^{ra} \qquad \text{[4-41]}$$

T_{dep}^{Ra} = total salt deposition onto rural agricultural surface (kg)

L_{inf}^{Ra} = salt load in rural agricultural infiltration (kg)

L_{runoff}^{Ra} = salt load in rural agricultural surface runoff (kg)

E_{ras} = emission onto rural agricultural soil (kg)

Substitution of Equation [4-36b] into Equation [4-41] and noting that the salt load in the runoff and infiltration streams is calculated by multiplying the respective volumetric flow rates with the soluble salt concentration (assumed equal in the runoff and infiltration streams), the following quadratic equation is obtained, which can be solved for C_{Ras}, the soluble salt concentration in the rural agricultural surface runoff and infiltration (assumed equal):

$$a_{ra} \, C_{Ras}^2 + b_{ra} \, C_{Ras} + c_{ra} = 0 \qquad \text{[4-42a]}$$

Where:

$$a_{ra} = FI \, (1 - AI) \, A_T \, \Theta_a \, 10_3 \qquad \text{[4-42b]}$$

$$b_{ra} = M^1_{Rns}(e^{-\Theta_n PSWP^{ra}_n} - 1) + AM^{ra}_{det} + B\Theta_a(1 - AI)FIA_T 10^3 - T^{Ra}_{dep} - G_{Ras} - L_{irrig} - E_{ras}$$

[4-42c]

$$c_{rn} = BM^1_{Ras}(e^{-\Theta_a PSWP^{Ra}_a} - 1) - B(T^{Ra}_{dep} + G_{Ras} + E_{rns} + L_{irrig})$$

[4-42d]

The concentration of salt in the rural agricultural surface runoff and infiltration is calculated in the same way as for the rural natural surface.

Evaporation and percolation

Lake evaporation is calculated from Symons pan evaporation data. For the period July to October a pan coefficient of 0.8 is used, while for the period November to June, the coefficient is set to unity.

Pitman (1973) used the following generalised relationship between soil moisture and evaporation from soil moisture:

$$Ev = PE[1 - \frac{(1 - \frac{S}{ST})}{(1 - R(1 - \frac{PE}{PEMAX}))}]$$

[4-43]

Where:

Ev	=	evaporation from soil (mm)
PE	=	potential evaporation (mm)
R	=	evaporation coefficient (-)
$PEMAX$	=	maximum potential evaporation (mm)

Percolation is related to soil moisture by the following power curve:

$$Pe = FT\left[\frac{S - SL}{ST - SL}\right]^{POW} \qquad \text{[4-44]}$$

Where:

Pe	=	percolation flow rate (mm/d)
FT	=	percolation at soil moisture capacity (mm/d)
SL	=	soil moisture storage below which no percolation occurs (mm)
POW	=	power of soil moisture – percolation curve (-)

When the soil moisture capacity is exceeded, part or all of the excess is added to groundwater storage. The remainder of the excess is added to surface runoff.

Water balances around the rural natural and rural agricultural soil moisture storage over the time interval Δt yields the following:

$$\Delta S_{rn} = S_{rn}^2 - S_{rn}^1 = I_{rn} - T_{rn} - Pe_{rn} - Ev_{rn} \qquad \text{[4-45a]}$$

$$\Delta S_{ra} = S_{ra}^2 - S_{ra}^1 = I_{ra} - T_{ra} - Pe_{ra} - Ev_{ra} \qquad \text{[4-45b]}$$

Where (note that subscripts ra and rn refer to rural agricultural and rural natural respectively):

S^2	=	soil moisture at the end of time interval (mm)
S^1	=	soil moisture at the beginning of time interval (mm)

Substitution of Equations [4-43] and 4-44] into Equations [4-45a] and [4-45b] yields:

$$S_{rn}^2 - S_{rn}^1 - I_{rn} + T_{rn} + Ev_{rn}\left[1 - \frac{(1 - \dfrac{S}{ST})}{1 - R(1 - \dfrac{Ev_{rn}}{PEMAX})}\right] + FT\left[\frac{S_{rn}^2 - SL}{ST - SL}\right]^{POW} = 0 \qquad \text{[4-46a]}$$

$$S_{ra}^2 - S_{ra}^1 - I_{ra} + T_{ra} + Ev_{ra}\left[1 - \frac{(1 - \frac{S}{ST})}{1 - R(1 - \frac{Ev_{ra}}{PEMAX})}\right] + FT\left[\frac{S_{ra}^2 - SL}{ST - SL}\right]^{POW} = 0 \qquad [4\text{-}46b]$$

By specifying the soil moisture at the start of the time interval, the soil moisture at the end of the time interval (S^2) can be calculated by solving Equations [4-46a] and [4-46b] using the Newton-Raphson technique.

It is assumed that there is no lateral flow between the rural natural and rural agricultural soil moisture.

Soil moisture salt balance

It is assumed that salt enters the soil moisture storage via infiltration and through leaching, and leaves as percolation to groundwater and interflow. Allowance is made for precipitation/dissolution of salts as well as adsporption/desorption of salts. Complete mixing of the soil moisture is assumed.

Salt is assumed to leach out of the soil matrix at a constant rate per unit of soil moisture storage, as proposed by Herold (1989). The total salt load leached during time Δt, M_{leach}, is thus assumed to be directly proportional to the soil moisture storage, S:

$$M_{leach} = LeachRate(1 - AI)A_T\,S \qquad [4\text{-}47]$$

Where $LeachRate$ is the rate of leaching of salts from soil (kg/m^3 soil water/d).

The salt load entering the soil moisture via infiltration (M_{inf}) during time interval Δt is given by:

$$M_{inf}^{rn} = Q_{inf}^{rn}C_{Rns} \qquad [4\text{-}48a]$$

$$M_{inf}^{ra} = Q_{inf}^{ra}C_{Ras} \qquad [4\text{-}48b]$$

Where Q_{inf}^{rn} and Q_{inf}^{ra} are the volumetric flow rate of infiltration through the rural natural and rural agricultural surfaces respectively.

The salt load leaving the soil moisture via interflow (M_{int}) during time interval Δt is given by:

$$M_{\text{int}}^{rn} = Q_{\text{int}}^{rn} C_{soil}^{rn} \qquad\qquad \text{[4-49a]}$$

$$M_{\text{int}}^{ra} = Q_{\text{int}}^{ra} C_{soil}^{ra} \qquad\qquad \text{[4-49b]}$$

Where Q_{int}^{rn} and Q_{int}^{ra} are the volumetric flow rate of interflow through the rural natural and rural agricultural soils respectively. C_{soil}^{rn} and C_{soil}^{ra} are the corresponding soil moisture salt concentrations.

The salt load leaving the soil moisture via percolation (M_{perc}) during time interval Δt is given by:

$$M_{perc}^{rn} = Q_{perc}^{rn} C_{soil}^{rn} \qquad\qquad \text{[4-50a]}$$

$$M_{perc}^{ra} = Q_{perc}^{ra} C_{soil}^{ra} \qquad\qquad \text{[4-50b]}$$

Where Q_{perc}^{rn} and Q_{perc}^{ra} are the volumetric flow rate of percolation to the rural natural and rural agricultural groundwater respectively.

The salt load adsorbed onto the soil matrix (M_{ads}) during the time interval is given by:

$$M_{ads}^{rn} = \frac{A\,C_{soil}^{rn} M_{soil}^{rn}}{B + C_{soil}^{rn}} \qquad\qquad \text{[4-51a]}$$

$$M_{ads}^{ra} = \frac{A\,C_{soil}^{ra} M_{soil}^{ra}}{B + C_{soil}^{ra}} \qquad\qquad \text{[4-52a]}$$

Where M_{soil}^{rn} and M_{soil}^{ra} are the wetted soil mass (product of area, soil moisture storage and soil density) of the rural natural and rural agricultural areas respectively, and are given by.

$$M_{soil}^{rn} = S_{rn} A_T (1 - AI)(1 - FI)(1 - F_{void}) \, r_{soil} 10^{-3} / F_{void} \qquad \text{[4-53a]}$$

$$M_{soil}^{ra} = S_{ra} A_T (1 - AI) FI (1 - F_{void}) \, r_{soil} 10^{-3} / F_{void} \qquad \text{[4-53b]}$$

Where:

F_{void} = soil void fraction (-)

r_{soil} = soil density (kg/m^3)

Mass balances on the rural natural and rural agricultural soils yields:

$$\Delta M_T^{rn} = M_{Trn}^2 - M_{Trn}^1 = M_{\text{inf}}^{rn} + M_{leach}^{rn} - M_{perc}^{rn} - M_{\text{int}}^{rn} \qquad \text{[4-54a]}$$

$$\Delta M_T^{rn} = M_{Trn}^2 - M_{Trn}^1 = M_{\text{inf}}^{rn} + M_{leach}^{rn} - M_{perc}^{rn} - M_{\text{int}}^{rn} \qquad \text{[4-54b]}$$

At any time the total mass of salt in the soil is equal to the sum of the mass of salt present in solution, the mass of salt precipitated and the mass of salt adsorbed onto the soil. If the concentration of salt in solution is less than the saturation concentration, then the change in the total mass of salt during a time interval is sum of the salt adsorbed and the salt in solution at the end of the interval minus the sum of the salt adsorbed and the salt in solution at the start of the interval. ΔM_T in Equations [4-54] are therefore equivalent to:

$$\Delta M_T^{rn} = C_{soil}^{rn'} V_{rnw}^{'} + \frac{A \, C_{soil}^{rn'} M_{soil}^{rn'}}{B + C_{soil}^{'}} - C_{soil}^{rn0} V_{rnw}^0 - \frac{A \, C_{soil}^{rn0} M_{soil}^{rn0}}{B + C_{soil}^{rn0}} \qquad \text{[4-55a]}$$

$$\Delta M_T^{ra} = C_{soil}^{ra'} V_{raw}^{'} + \frac{A \, C_{soil}^{ra'} M_{soil}^{ra'}}{B + C_{soil}^{ra'}} - C_{soil}^{ra0} V_{raw}^0 - \frac{A \, C_{soil}^{ra0} M_{soil}^{ra'}}{B + C_{soil}^{ra0}} \qquad \text{[4-55b]}$$

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Where (note that the subscripts *rn* and *ra* refer to rural natural and rural agricultural respectively):

C'_{soil} = soil moisture salt concentration at the end of the time interval (kg/m^3)

C^0_{soil} = soil moisture salt concentration at the beginning of the time interval (kg/m^3)

V'_w = soil water volume at the end of the time interval (m^3)

V^0_w = soil water volume at the beginning of the time interval (m^3)

M'_{soil} = wetted soil mass at the end of the time interval (kg)

M^0_{soil} = wetted soil mass at the beginning of the time interval (kg)

Substitution of Equations [4-47] to [4-52] and [4-55] into Equations [4-54] yields the following quadratic equations, that can be solved for, C'_{soil}, the concentration of salt in solution in the soil moisture at the end of time the interval:

$$Con1_{rn}\, C^{rn'}_{soil}{}^2 + Con2_{rn}\, C^{rn'}_{soil} + Con3_{rn} = 0 \qquad \text{[4-56a]}$$

$$Con1_{ra}\, C^{ra'}_{soil}{}^2 + Con2_{ra}\, C^{ra'}_{soil} + Con3_{ra} = 0 \qquad \text{[4-56b]}$$

Where:

$$Con1_{rn} = V^0_{rnw} + Q^{rn}_{perc} + Q^{rn}_{\text{int}} \qquad \text{[4-56c]}$$

$$Con1_{ra} = V^0_{raw} + Q^{ra}_{perc} + Q^{ra}_{\text{int}} \qquad \text{[4-56d]}$$

$$Con2_{rn} = A M^{rn'}_{soil} + B V'_{rnw} - C^{rn^0}_{soil} V^0_{rnw} - (M^{rn}_{\text{inf}} + M^{rn}_{leach}) + B Q^{rn}_{perc} + B Q^{rn}_{\text{int}} - \frac{A M^{rn^0}_{soil} C^{rn^0}_{soil}}{B + C^{rn^0}_{soil}}$$

$$\text{[4-56e]}$$

$$Con2_{ra} = A M_{soil}^{ra^{'}} + B V_{raw}^{'} - C_{soil}^{ra^0} V_{raw}^0 - (M_{inf}^{ra} + M_{leach}^{ra}) + B Q_{perc}^{ra} + B Q_{int}^{ra} - \frac{A M_{soil}^{ra^0} C_{soil}^{ra^0}}{B + C_{soil}^{ra^0}}$$

[4-56f]

$$Con3_{rn} = B \left[M_{inf}^{rn} + M_{leach}^{rn} - \frac{A C_{soil}^{rn^0}}{B + C_{soil}^{rn^0}} - C_{soil}^{rn^0} V_{rnw}^0 \right]$$

[4-56g]

$$Con3_{rn} = B \left[M_{inf}^{rn} + M_{leach}^{rn} - \frac{A C_{soil}^{rn^0}}{B + C_{soil}^{rn^0}} - C_{soil}^{rn^0} V_{rnw}^0 \right]$$

[4-56h]

If the salt concentration exceeds the solubility limit (C_{sat}) then the mass of salt precipitated during the time interval ($Mppt$) is calculated as follows:

$$Mppt_{rn} = (C_{soil}^{rn^{'}} - C_{sat}) V_{rnw}^{'}$$

[4-57a]

$$Mppt_{ra} = (C_{soil}^{ra^{'}} - C_{sat}) V_{raw}^{'}$$

[4-57b]

Salt that is precipitated during the time interval is added to the total salt storage mass and may re-dissolve during the next time interval or may accumulate if the concentration remains above the solubility limit.

Groundwater discharge and losses to deep groundwater

The total groundwater flow is calculated from the following relationship (Pitman, 1973):

$$GWFT = \frac{W_G^{\frac{2}{3}}}{GL\sqrt{ST}}$$

[4-58]

Where:

$GWFT$ = groundwater flow (mm/d)

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W_G = groundwater storage (mm)

GL = groundwater constant (d)

Allowance is made for loss of water to deep-seated groundwater in the same manner as proposed by Herold (1981), by using the parameter DGL. DGL is the proportion of total groundwater flow that enters deep groundwater. The deep-seated groundwater discharge is regarded as having been lost from the system.

The average groundwater flow over the time interval Δt is given by:

$$W_{Gave} = W_G^0 + \frac{1}{2}(W_G^{'} - W_G^0)$$ [4-59]

Where:

W_{Gave} = average groundwater flow over time interval (mm/d)

W_G^0 = groundwater flow at the beginning of the time interval (mm/d)

$W_G^{'}$ = groundwater flow at the end of the time interval (mm/d)

The groundwater storage over the time interval is given by:

$$S_{Gv}^{'} - S_{Gv}^0 = Pe - W_{Gave}$$ [4-60]

Where:

$S_{Gv}^{'}$ = groundwater storage volume at the end of the time interval (mm)

S_{Gv}^0 = groundwater storage volume at the beginning of the time interval (mm)

Substitution of Equations [4-58] and [4-59] into Equation [4-60] (for rural natural groundwater and rural agricultural groundwater) yields:

$$S_{Gv}^{rn^{'}} + \frac{GW}{2\sqrt{ST}}(S_{Gv}^{rn^{'}})^{1.5} = S_{Gv}^{rn^0} - \frac{GW}{2\sqrt{ST}}(S_{Gv}^{rn^0})^{1.5} + Pe_{perc}^{rn}$$ [4-61a]

$$S_{Gv}^{ra'} + \frac{GW}{2\sqrt{ST}} (S_{Gv}^{ra'})^{1.5} = S_{Gv}^{ra^0} - \frac{GW}{2\sqrt{ST}} (S_{Gv}^{ra^0})^{1.5} + Pe_{perc}^{ra} \qquad \text{[4-61b]}$$

Equation [4-61] can be solved for $S_{Gv}^{'}$ using the Newton-Raphson technique. The total groundwater flow is calculated using Equation [4-58]. The groundwater flow entering the river is calculated using the parameter DGL, and the groundwater loss to deep-seated groundwater is the difference between the total flow and the flow to the river.

Groundwater salt balance

A mass balance of salt in the (rural natural and rural agricultural) groundwater yields:

$$M_{gw}^{rn'} - M_{gw}^{rn^0} = M_{perc}^{rn} + LeachRate\,(1-AI)\,A_T\,S_{Gv}^{rn} - Q_{TGWF}^{rn}\,C_{Gw}^{rn'} \qquad \text{[4-62a]}$$

$$M_{gw}^{ra'} - M_{gw}^{ra^0} = M_{perc}^{ra} + LeachRate\,(1-AI)\,A_T\,S_{Gv}^{ra} - Q_{TGWF}^{ra}\,C_{Gw}^{ra'} \qquad \text{[4-62b]}$$

Where:

$M_{gw}^{'}$ =   mass of salt in groundwater at the end of the time interval (kg)

M_{gw}^{0} =   mass of salt in the groundwater at the beginning of the time interval (kg)

$C_{Gw}^{'}$ =   salt concentration in the groundwater at the end of the time interval (kg/m^3)

Noting that the total mass of salt in the groundwater is the product of the groundwater volume and the salt concentration, Equations [4-62] are solved for $C_{Gw}^{'}$, the concentrations of salt in the groundwater at the end of the time interval. The salt concentration at the end of the time interval is used to calculate the salt load entering discharged into the river and the salt load entering the deep-seated groundwater.

Mixing, time delay and attenuation of runoff

The surface runoff from the urban and rural areas, containing salt in solution and salt adsorbed onto the sediment load is assumed to mix completely with the interflow stream. A salt mass balance yields:

$$M_{Rns} + M_{ads}^{rn} + M_{Ras} + M_{ads}^{ra} + M_{Us} + M_{int}^{rn} + M_{int}^{ra} = Q_{totalrunoff} \, C_{sr} + \frac{A C_{sr} M_{sed}}{B + C_{sr}} \qquad \text{[4-63]}$$

Where:

$Q_{totalrunoff}$ =   total surface runoff flow (m^3/d)

C_{sr} =   salt concentration in combined surface runoff flow (kg/m^3)

M_{sed} =   total mass of surface sediment (kg)

Equation [4-63] is quadratic, and is solved for C_{sr}, the salt concentration in the un-routed total surface runoff and interflow stream.

The calculated instantaneous runoff is lagged by means of the parameter LAG, which has units of days. Attenuation of surface runoff is achieved by means of the Muskingum equation, which can be written as (Herold, 1981):

$$O_2 = C_0 \, O_1 + C_1 \, I_1 + C_2 \, I_2 \qquad \text{[4-64a]}$$

Where:

O_2 =   surface runoff at catchment outlet during current day (mm)

O_1 =   surface runoff at catchment outlet during previous day (mm)

I_1 =   surface runoff input during previous day (mm)

I_2 =   surface runoff input during current day (mm)

$$C_0 = \frac{TL - \dfrac{\Delta t}{2}}{TL + \dfrac{\Delta t}{2}} \qquad \text{[4-64b]}$$

$$C_1 = C_2 = \frac{\frac{\Delta t}{2}}{TL + \frac{\Delta t}{2}} \qquad \text{[4-64c]}$$

TL = routing constant (d)

Equation [4-64] is only used to route runoff as far as the main river channel. Routing in the river channel is accomplished by means of a channel routing model.

Equation [4-64] is used in a similar manner to route the salt load associated with the total runoff and interflow streams.

$$C'_{routed} = \frac{C_0 \, Q^0_{routed} C^0_{routed} + C_1 \, Q_{totalrunoff} C^0_{unrouted} + Q_{totalrunoff} C'_{unrouted}}{Q'_{routed}} \qquad \text{[4-65]}$$

Where:

C'_{routed} = routed salt concentration at the end of the current day (kg/m^3)

Q'_{routed} = routed surface runoff at the end of the current day (m^3/d)

Q^0_{routed} = routed surface runoff at the end of the previous day (m^3/d)

$C^0_{unrouted}$ = unrouted salt concentration at the end of the previous day (kg/m^3)

$C'_{unrouted}$ = unrouted salt concentration at the end of the current day (kg/m^3)

The routed salt load is calculated by multiplying the routed salt concentration with the surface runoff flow. An equation similar to Equation [4-63] is used to calculate the salt concentration of the total surface and groundwater flow after mixing.

River flow and salt routing

The method used to route the river flow and salt load in the river is the same as that used by Herold (1989). A schematic diagram of the streams entering and leaving the river is shown in Figure 4.6. The river is sub-divided into N_{step} cells of equal volume. The catchment runoff entering the river at its upstream end during time step, Δt, is given by:

$$Q_{upstream} = F_{head}\, Q_{totalrunoff} / N_{step} \qquad\qquad [4\text{-}66]$$

Where:

$Q_{upstream}$ =   upstream river flow (m^3/d)

F_{head} =   fraction of the catchment draining to the upstream end of the river reach (-)

The flow entering the river laterally during time step, Δt, is thus given by:

$$Q_{lateral} = (1 - F_{head})Q_{routed} / N_{step} \qquad\qquad [4\text{-}67]$$

Net evaporation losses are calculated on a daily basis from the mean monthly potential evaporation and daily rainfall. The potential evaporation is multiplied by an evaporation factor in order to account for the reduction or increase in evaporation. The daily evaporation from the river (Q_{evap}) is calculated as follows:

$$Q_{evap} = [PE\, F_{evap} - P_d]W_R\, L_R /1000 / N_{step} \qquad\qquad [4\text{-}68]$$

Where:

F_{evap} =   river evaporation factor (-)

W_R =   river width (m)

L_R =   river length (m)
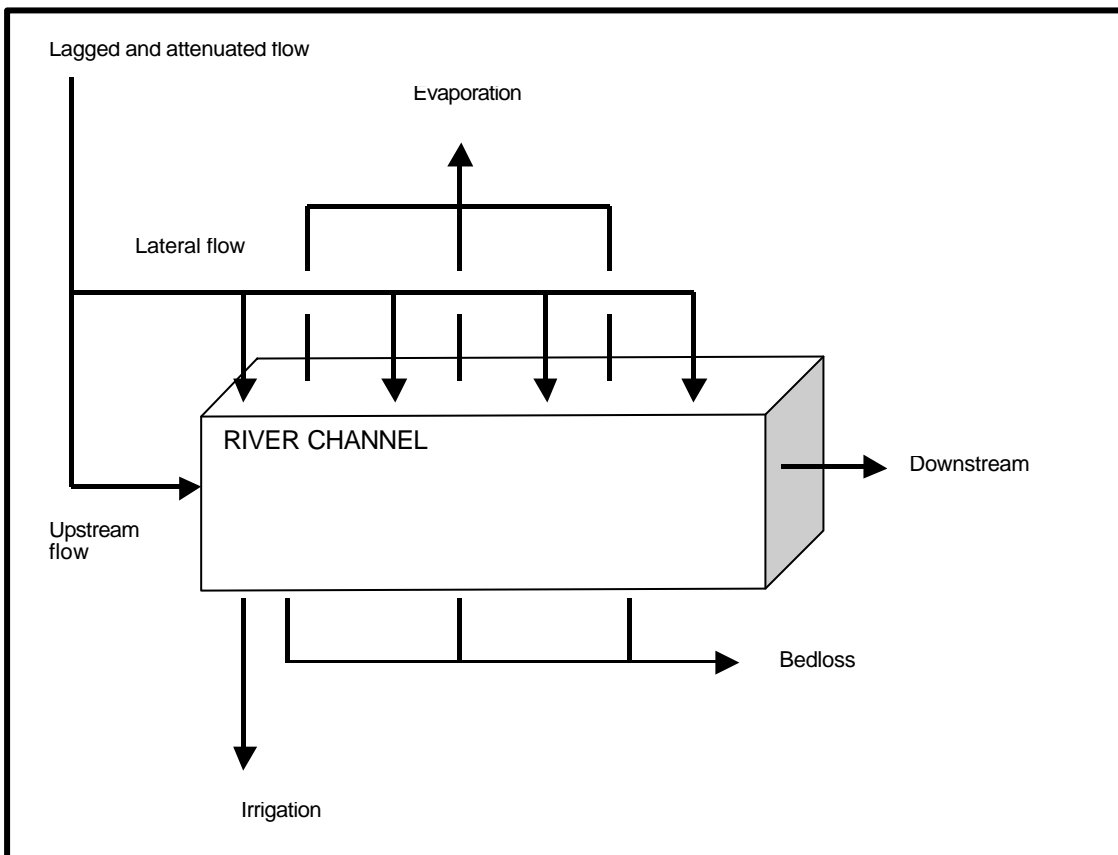
Figure 4.6: Schematic diagram of the river routing model

The river is assumed to have a simple rectangular shape, and does not include wetlands. The model developed by Herold (1989) assumes a more complex river geometry, and makes allowance for wetlands.

Bedloss from the river is calculated from a constant bedloss factor ($F_{bedloss}$) as follows:

$$Q_{bedloss} = F_{bedloss} W_R L_R / 1000 / N_{step}$$ [4-69]

The flow at the downstream end of the river is calculated N_{step} times in the time interval Δt using the following:

$$Q_{downstream} = \frac{W_R h}{M_F} \left(\frac{W_R h}{W_R + h} \right)^{\frac{2}{3}} (slope)^{0.5} \qquad\qquad [4\text{-}70]$$

Where:

h =   water depth in river (m)

M_F =   Manning factor for river (-)

$slope$ =   river slope (m/m)

A water balance over the river during time interval Δt yields:

$$V_R^{'} = V_R^0 + Q_{upstream} + Q_{lateral} - Q_{evap} - Q_{bedloss} - Q_{downstream} - Q_{irrig} \qquad [4\text{-}71]$$

Where V_R^0 and $V_R^{'}$ are the volume of the river at the start and end of the time interval.

Noting that $V_R^{'} = h^{'} W_R L_R$, substitution of Equations [4-67] to [4-70] into [4-71] yields:

$$ConA^{'} - W_R L_R h^{'} - ConB h^{'} \left[\frac{W_R h^{'}}{W_R + 0.5 h^{'}} \right]^{\frac{3}{2}} = 0 \qquad\qquad [4\text{-}72a]$$

Where

$$ConA^{'} = V_R^0 + Q_{upstream} + Q_{lateral} - Q_{evap} - Q_{bedloss} - Q_{irrig} \qquad\qquad [4\text{-}72b]$$

$$ConB = W_R (slope)^{0.5} \, 86400 \, / \, M_F \qquad\qquad [4\text{-}72c]$$

Equation [4-72] is solved (N_{step} times per time interval) for $h^{'}$, the water depth in the river at the end on the time interval, by using the Newton-Raphson technique.

The river depth is used to calculate the downstream river flow at the end of the time interval, by using Equation [4-70], and the river volume is calculated by substitution of the downstream river flow into Equation [4-71]

River salt is routed in a similar manner, according to the following equation:

$$C_R^{'} = \frac{C_R^0 V_R^0 + Q_{upstream} C_{routed}^{'} + Q_{lateral} C_{routed}^{'} + E_R}{V_R^{'} + Q_{downstream} + Q_{irrig}}$$

[4-73]

Where E_R is the emission directly into the river (kg/d).

River sediment

The river sediment bed load is calculated according to the method given by Paling et al (1989):

$$Q_S = 0.041 W_R (t_o - t_c)^{1.5}$$

[4-74]

Where:

Q_S	=	river sediment bed load (kg/s)
t_o	=	boundary shear stress (N/m^2)
	=	$9810\, h\, slope$
t_c	=	critical shear stress for sediment motion (N/m^2)
	=	$0.047 (S_s - 1) D_S$
S_s	=	relative sediment density (-)
D_S	=	sediment particle diameter (m)

The suspended sediment load is calculated from the simple relationship given by Pye (1994):

$$C_{ss} = a Q_R^b$$

[4-75]

Where:

$$C_{ss} \quad = \quad \text{concentration of suspended solids in the river (mg/L)}$$

$$Q_R \quad = \quad \text{river flow (m}^3\text{/s)}$$

$$a, b \quad = \quad \text{constants}$$

The suspended solids load in the river is the product of river flow and suspended solids concentration.

The concentration of salt in the river is adjusted to allow for adsorption onto suspended and bed sediment load.

The algorithms developed above were programmed using Visual Basic 6.0. The structure of the program and the program code is given in **Appendix D**.

CHAPTER 5

MODEL CALIBRATION AND PARAMETER SENSITIVITY

In this chapter the environmental fate model developed is calibrated, based on published data and calculated surface water flow and quality data for the "unit South African catchment". The chapter is divided into four sections. In Section 5.1, the approach adopted and the rationale for adopting the approach in validating the environmental fate model is presented. The environmental fate model essentially consists of two sub-models; an atmospheric deposition model, and a hydrosalinity model. These are sub-models are covered in Sections 5.2 and 5.3 respectively. The hydrosalinity model in turn consists of a catchment hydrology (or rainfall-runoff) component, and a salt transport component (which includes a sediment transport component). Each component of the fate model is addressed in the same way in this chapter. Firstly, the parameters used in the model component are presented, and as far as possible, published values are presented. Secondly, the calibration results, based on several indices correlating observed to predicted values are presented. A simple sensitivity analysis is conducted to determine the most sensitive parameters, and these parameters are adjusted in order to further refine the calibration of the model. The results of the calibrated model are then presented and discussed. In Section 5.4 the influence of the identified sensitive parameters on the difference in concentrations with and without an imposed impulse emission (upon which the calculation of salinity effects potentials are based) is evaluated. Concluding remarks are given in Section 5.5.

5.1 APPROACH

As discussed in Section **2.4.2**, in LCA, it is the **capacity** of causing harmful effects that forms the basis for the assessment, and not so much the extent to which this capacity has become **effective**. If we move away from full space and time integration to add more details with respect

to spatial and temporal characteristics of release and receiving environment, then we are entering the area of **actual** impacts, as opposed to **potential** impacts. In general, for an assessment in completely potential terms, it suffices to use a smaller number of model parameters. For an assessment in completely actual terms, a larger number of parameters are required. Practitioners of LCA are happy if simplifying assumptions are made so that modelling can be done with reasonable accuracy that include the total environmental interventions, integrated over all locations and infinite time in an assumed steady state. The omission of economic mechanisms and spatial detail leads to a great simplification, but it reduces the quality of the results of the analysis.

Model uncertainty is discussed in more detail in **Section 7.3**, however the following points are worth mentioning here:

- There is a large degree of uncertainty in some of the no-effect concentrations used to calculate equivalency factors.
- There are limited published data on model parameters in some cases, and where data are available, uncertainty is introduced due to the regionalisation of parameters.
- There is a lack of soil water and groundwater quality data. The only data available to calibrate the hydro-salinity model are average monthly surface water flows and average monthly TDS concentrations. The uncertainty associated with the monthly river flows used to calibrate the model is not known, and the monthly surface water quality values are based on limited data.

In order to calculate the salinity effects potentials (refer to **Section 3.3.1**), the difference in concentrations with and without an imposed impulse emission in the soil water and surface water compartments is required. The selection of the environmental fate model parameters will influence the value of this concentration differential (refer to **Section 5.4**). The implicit assumption is therefore that if the model parameters are chosen such that the best possible correlation between observed (or calculated values for the "unit catchment") values and predicted (modelled) values is obtained, then these parameters will also result in the correct concentration differential.

The approach used to calibrate the model and determine the sensitivity of the model outputs to the model parameters is shown schematically in Figure 5.1. The general approach adopted was to, as far as possible, use published or estimated values for the model parameters, and by varying the parameters individually, the sensitive parameters could be identified. The model was

then calibrated (based on several indices for best-fit) by refining the identified sensitive parameters.

The fate model developed consists of two distinct sub-models; the atmospheric deposition model is essentially a separate sub-model of the fate model, inasmuch as the output from the model is daily salt deposition rate, which is the only parameter that affects the salt concentrations in other compartments of the model. The second sub-model is termed the hydrosalinity model, which in turn consists of two components. The *catchment hydrology component* models the movement and storage of surface, soil and groundwater throughout the catchment, and the *salt transport component* models the movement and storage of salt throughout the catchment, including salt adsorption. The hydrological component can also be calibrated separately since the movement of water throughout the various compartments making up the catchment does not change from year to year, and observed surface water flows can be used to calibrate this component of the model. Each sub-model and components making up the sub-models are discussed separately under the same sub-titles:

a) **Model parameters**: The model parameters used in the model are presented and discussed individually. Published values for the parameters are cited, and where appropriate, the method used for estimating the parameters are given.

b) **Model calibration**: The methodology used to calibrate the sub-models, and calibration results are presented.

c) **Parameter sensitivity analysis** The sensitivity of the model outputs to the model parameters, around the calibration point, is presented, and the most sensitive parameters are identified and used to refine the calibration.

d) **Model results and discussion**: Mass balance results are presented to establish that mass has been conserved. Selected outputs from the model are presented and the effects of varying the most sensitive parameters to these outputs are presented and discussed. Results are examined to ensure that the behaviour of modelled outputs follow expected patterns.

In light of the uncertainty of some of the data used to calibrate the model, the simplistic approach to atmospheric deposition modelling, and the number of parameters required, it was decided that a detailed multi-variate parameter sensitivity and uncertainty analysis is not warranted at this point in the development of the method, and that this could be the subject for further research.
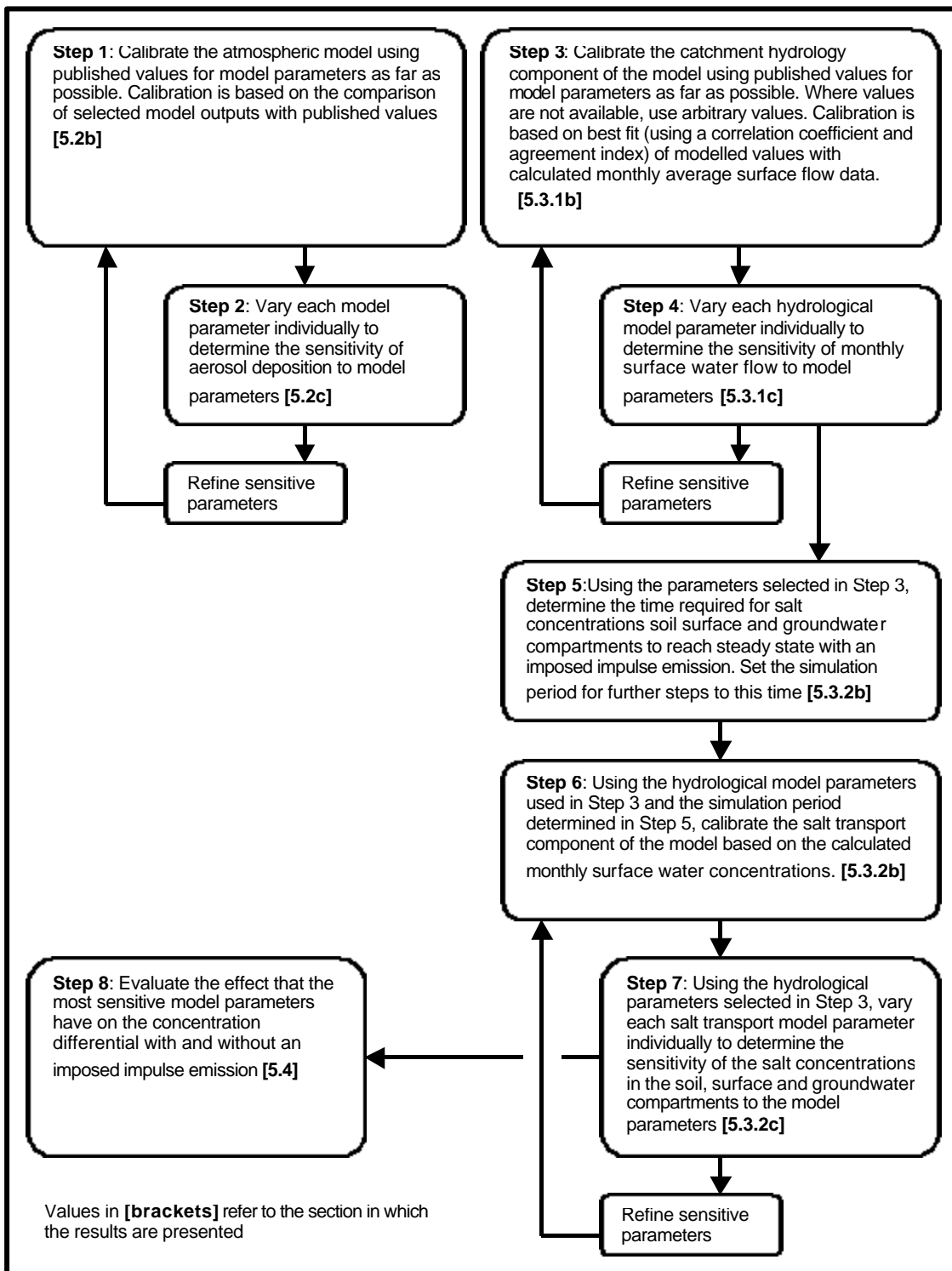
Figure 5.1: Schematic diagram showing the approach followed for model calibration and parameter sensitivity analysis.

5.2 ATMOSPHERIC DEPOSITION MODEL

The atmospheric deposition model parameters, calibration results, parameter sensitivity analysis results, and discussion of the results are presented in **Section 5.2a** to **5.2d**.

a) Model parameters

The atmospheric deposition model parameters are summarised in Table 5.1. Each model parameter is discussed in more detail. Catchment characteristics are given in Table 5.11.

Table 5.1: Atmospheric deposition model parameters

Model Parameter	Symbol	Units
Average monthly wind velocity	u	m/s
Aerosol deposition velocity (summer)	V_d	cm/s
Aerosol deposition velocity (winter)	V_d	cm/s
Dry deposition factor (summer)	F_d	-
Dry deposition factor (winter)	F_d	-
Occult deposition factor	F_O	-
Atmospheric mixing height	H	m
Wash ratio	WR	-
Fraction salt in aerosol	F_{salt}	-
Concentration of aerosol entering rural air volume from upstream	C_{in}	kg/m^3
Anthropogenic aerosol generation rate in urban area (reference year)	G_A^U	ton/km^2/d
Anthropogenic aerosol generation rate in rural area (reference year)	G_A^R	ton/km^2/d
Natural aerosol generation rate	G_N	kg/m^2/d

<u>Wind speed</u>

The volume flux of air through the defined air volumes (and hence the wind velocity, for constant air density and cross-sectional area) defines the aerosol carrying capacity (Tyson *et al*., 1996).

Wind speed is highly variable in all space dimensions. The average monthly wind velocities from 20 monitoring stations were used in the model (refer to **Appendix A**), and are shown in Table 5.2.

Table 5.2: Summary of wind speed statistics measured at 20 sites throughout South Africa (South African Weather Service, 2003).

Month	Wind speed (m/s)		
	Minimum	Average	Maximum
January	1.4	4.2	6.6
February	1.3	4.0	6.5
March	1.1	3.6	5.6
April	0.9	3.4	5.0
May	0.7	3.2	4.8
June	0.7	3.3	4.9
July	0.9	3.5	5.2
August	1.3	3.7	5.2
September	1.6	4.0	5.7
October	1.7	4.3	6.2
November	1.7	4.4	6.2
December	1.6	4.3	6.4

Deposition velocity

Deposition velocity is an experimentally derived parameter. It is highly variable and depends on the physical and chemical characteristics of the particular substance, the nature of the surface with which it is interacting and meteorological factors. In a review of the literature, Skoroszewski (1999) quotes typical values in the range from 0.3 to 2.3 cm/s for sulphur dioxide. Deposition velocities have been experimentally determined for several natural surfaces. These include values for grassland of 1.3 cm/s in summer and 0.3 cm/s in winter. An average value of 0.8 cm/s was assumed for the eastern Transvaal Highveld by Skoroszewski (1999).

In eastern Canada, the dry deposition velocity for sulphur dioxide ranges from 0.19 to 0.30 cm/s, for sulphate 0.25 to 0.37 cm/s and for nitrate 0.35 to 0.65 cm/s. Over eastern England a range of 0.11 to 0.22 cm/s and an average of 0.18±0.15 cm/s for continental aerosols, and a range of 0.54 to 0.63 cm/s with an average of 0.58±0.26 cm/s for marine aerosols is quoted. An overall deposition velocity of about 0.1 cm/s is the accepted approximation for accumulation mode

aerosols (Bridgman, 1990). Table 5.3 shows deposition velocities for selected elements over forests and urban gardens.

In a review undertaken by Herold et al. (2001), winter (April to September) maximum and average deposition velocities are 0.28 and 0.15 cm/s, while for summer they are 0.61 and 0.3 cm/s respectively.

Table 5.3: Representative examples of dry deposition velocities by elements for aerosols over a forest and urban garden location (Bridgman, 1990).

Element	Deposition Velocity (cm/s)	
	Forest	**Urban garden**
Sulphur	0.40	-
Chloride	1.80	-
Potassium	0.86	-
Calcium	1.60	-
Vanadium	0.45	0.46
Manganese	0.72	0.43
Iron	1.10	1.60
Nickel	0.56	1.00
Copper	0.53	1.40
Zink	0.48	0.2
Lead	0.41	0.46
Aluminium	-	2.0

<u>Deposition factors</u>

Particulate contribution to total dry deposition is reported to range between 7% in winter and 9% in summer for sulphate particles on the Mpumalanga Highveld (Herold et al., 2001). Skoroszewski (1999) reported the proportion of dry to total sulphate deposition in the range 39 to 91%.

The contribution of occult deposition to total deposition varies widely, from 1.5% at an English moor, to 100% in a forest in North America (Hewitt and Sturges, 1993). Herold et al. (2001) report that occult deposition contributes 25% of the total dry deposition. Skoroszewski (1999) reports that the total deposition of sulphate associated with dew over the three-month sampling period (August to October 1993) was 1.14 kg/ha. This was 12% of the total sulphate deposited in the rainfall over the same period.

Natural and anthropogenic aerosol generation

Very little data are available for the rate of generation of aerosols. Rough estimates reported by Hewitt and Sturges (1993) are shown in Table 4.1, estimated for the year 1988. Natural aerosol generation is reported in the range 0.015 to 0.151 ton/km^2/d, and anthropogenic aerosol generation in the range 0.0037 to 0.0092 ton/km^2/d (using a global surface area of 1.49×10^9 km^2).

Atmospheric mixing height

Aerosols were assumed to be contained below the 700 hPa (~3 000 m) stable layer (Piketh et al., 1999). With a mean surface altitude of South Africa of 1 050m, the mixing height is taken as 1 950 m.

Wash ratio

Wash ratios for ions are reported to vary between 1×10^5 and 1.4×10^6 (Hiujbregts, 2001). Using the data by Skoroszewski (1999) on deposition in the Suikerbos Nature Reserve, a wash ratio for sulphate of 2×10^5 was calculated, which falls within the range of other published values.

Soluble salt fraction of aerosols

Maenhaut et al (1996) analysed fine and course aerosol fractions from samples taken in the Kruger National Park. Unfortunately, samples were not analysed for ammonium. Assuming, however, that all sulphur present is as ammonium sulphate (Piketh et al., 1999), the total inorganic fraction of the fine and course aerosol fractions is estimated at 0.8 and 0.4 respectively. The inorganic fraction of the combined sample is estimated at 0.6. The fraction of common ions is estimated at 0.3 for the fine fraction, and 0.17 for the course fraction, with a value of 0.23 for the combined sample (carbonate was not measured).

In the work done by Coleman (1993), on urban catchments, the total inorganic fraction ranged between 0.79 and 0.82. The fraction of common ions ranged between 0.71 and 0.74.

<u>Concentration of aerosol in the upstream air</u>

A typical background aerosol concentrations of 13 $\mu g/m^3$ is reported by Hewitt and Sturges (1993). Maenhaut et al (1996) report background values ranging between 9 and 19 $\mu g/m^3$ in the Kruger National Park. Tyson et al (1997) report an average background value of 10 $\mu g/m^3$ in rural areas on the eastern side of South Africa. Anderson et al (1996) report values ranging between 0.4 and 9.3 $\mu g/m^3$, with an average of 2.2 $\mu g/m^3$ as African background concentration.

b) Atmospheric deposition model calibration

The atmospheric model is essentially a separate component of the fate model, inasmuch as the output from the model is daily salt deposition rate, which is the only parameter that affects the salt concentrations in other compartments of the model. Toxicity effects due to inhalation and dermal contact are not taken into account in the effect model (refer to **Section 3.3.2**) and therefore the concentration of aerosol/salt is not important. Furthermore, although deposition rates are calculated at a daily time-scale, it is not possible to calibrate the model on a daily time-scale, since daily data are not available. The approach adopted to "calibrate" the model was to use published values for the model parameters (shown in Table 5.4), and then to adjust the anthropogenic aerosol generation rate (this is the most sensitive parameter, refer to **Section 5.2c**) until the following model results were within the same order of magnitude as published values (usually isolated measurements).

- Total aerosol deposition.
- Aerosol concentration.
- Rainwater composition.

The anthropogenic aerosol generation rate was adjusted to give the model outputs shown in Table 5.5. Values of 0.04 and 0.4 ton/km^2/d for rural and urban anthropogenic aerosol generation rates respectively resulted in the outputs shown.

The model outputs fall within the ranges of the limited published data, except for the urban aerosol deposition rate, which the model appears to over predict. The deposition data reported by Tyson and Gatebe (2001) and DWAF (1995) for total aerosol deposition, and the data presented by Coleman (1993), appear to be contradictory, however. Based on the data presented by Coleman (1993), the total aerosol deposition rate would be expected to be significantly higher, considering that only a fraction (approximately 0.6) of the aerosol is soluble.

Table 5.4: Model parameters used in the atmospheric deposition model compared to published values

Parameter	Units	Published			Value used in model
		Value *	Comments	Reference	
Aerosol deposition velocity (summer)	cm/s	-(0.3)-6.61	For SO_2 Grasslands	Herold et al (2001)	**1.3**
		-(1.3)-		Skorosweski, 1999	
Aerosol deposition velocity (winter)	cm/s	-(0.28)-0.15	For SO_2 Grasslands	Herold et al (2001)	**0.3**
		-(0.3)-		Skorosweski, 1999	
Annual deposition velocity	cm/s	0.3-( )-2.3	For SO_2	Skorosweski, 1999	
		-(0.8)-	Eastern Transvaal	Skorosweski, 1999	
		0.11-(0.18)-0.22	England – continental aerosols	Bridgman, 1990	
		0.54-(0.58)-0.63	England-marine aerosols	Bridgman, 1990	
Dry deposition factor (summer)	-	-(1.09)-	For SO_2	Herold et al (2001)	**1.09**
Dry deposition factor (winter)	-	-(1.07)-	For SO_2	Herold et al (2001)	**1.07**
Occult deposition factor	-	-(0.025)-	For SO_2	Herold et al (2001)	**0.025**
Atmospheric mixing height	m	-(1950)-	700 hPa	Piketh et al., 1999	**1950**
Wash ratio	-	$1x10^5$-( )-$1.4x10^6$		Huijbregts, 1999	**$7.5x10^5$**
		-($2x10^5$)-	For sulphate	Skorosweski, 1999	
Fraction salt in aerosol	-	0.4-( )-0.8	Kruger National Park	Maenhaut et al ,1996	**0.6**
		0.71-( )-0.74	Urban area	Coleman, 1991	
Concentration of aerosol entering rural air volume from upstream	µg/m³	-(13)-		Hewitt and Sturges, 1993	**15**
		9-( )-19	Kruger National Park	Maenhaut et al,1996	
		-(10)-	Rural areas of eastern South Africa	Tyson et al, 1997	
		0.4-(2.2)-9.3	Africa	Anderson et al, 1996	
Natural aerosol generation rate	kg/km²/d	$1.5x10^{-5}$-( )-$1.5x10^{-4}$	Global average	Hewitt and Sturges, 1993	**$1.3x10^{-5}$**

* minimum-(average)-maximum

Table 5.5: Summary of atmospheric deposition model outputs compared to published values.

Parameter	Units	Published			Model outputs		
		Value *	Comments	Reference	Urban	Rural	Combined
Total aerosol deposition	kg/ha/y	-(208)-	South Africa	Tyson and Gatebe, 2001	773	267	273
		-(317)-	Urban (Pinetown, South Africa)	DWAF, 1995			
		-(215)-	Residential (Durban, South Africa)				
Total aerosol (soluble) salt deposition	kg/ha/yr	-(193)-	Urban (Pinetown, South Africa)		464	160	165
		0-(412)-1836	Urban (South Africa)	Coleman, 1993			
		16-(1059)-3011	Urban (South Africa)				
Rainfall TDS	mg/L	20-( )-104	Urban (South Africa)	Coleman, 1993	44	18	31
		0.9-(10)-61	Suikerbos Natural Reserve (South Africa): Winter	Skoroszewski, 1999			
Aerosol concentration	µg/L	20-( )-80	Ben MacDhui, 4 km stable layer (South Africa)	Tyson and Gatebe, 2001	97	39	68
		26-( )-33	Several locations throughout South Africa	Picketh et al, 1999			
		9-( )-19	Kruger National Park (South Africa)	Maenhaut et al, 1996			
		-(20)-120	Johannesburg (South Africa)	Tyson et al, 1997			
		-(15)-140	Eastern Transvaal Highveld (South Africa)				
		-(10)-60	Rural eastern South Africa				

* minimum-(average)-maximum

c) Atmospheric deposition model parameter sensitivity analysis

Model parameters were adjusted to –50% and +50% of the values presented in Table 5.4, and the resulting change to salt deposition rates are listed in Table 5.6.

Table 5.6: Atmospheric deposition model parameter sensitivity analysis results

Parameter	-50% change in model parameter			+50% change in model parameter		
	% change in salt deposition			% change in salt deposition		
	Rural	Urban	Combined	Rural	Urban	Combined
Deposition velocity (summer)	**-10.9**	**-17.0**	**-11.1**	**6.1**	**13.3**	**6.3**
Deposition velocity (winter)	-3.3	-3.4	-3.3	2.5	3.0	2.5
Dry deposition factor (summer)	**-0.3**	**-0.6**	**-0.3**	**0.3**	**0.6**	**0.3**
Dry deposition factor (winter)	-0.5	-0.7	-0.5	0.5	0.7	0.5
Occult deposition factor	-0.3	-0.4	-0.3	12.6	21.0	12.8
Mixing height	8.5	38.2	9.4	-5.8	-18.5	-6.2
Wash ratio	-3.1	-9.8	-3.3	1.8	7.3	2.0
Fraction salt	**-50**	**-50**	**-50**	**50**	**50**	**50**
Upstream aerosol concentration	-6.0	-1.5	-5.9	6.0	1.5	5.9
Natural aerosol generation rate	**-10.3**	**-3.8**	**-10.1**	**10.3**	**3.8**	**10.1**
Rural aerosol generation rate	**-31.4**	**-8.1**	**-30.7**	**31.4**	**8.1**	**30.7**
Urban aerosol generation rate	-2.4	-36.6	-3.3	2.4	36.6	3.3
Wind speed *	-8.8	-38.5	-9.7	6.2	18.6	6.5

* adjusted to ±50% of average wind speeds shown in Table 5.2

Daily aerosol deposition rates are calculated by the model, and the soluble salt associated with the aerosol is calculated by multiplying the aerosol deposition rate with the fraction of soluble salt (F_{salt}). There is therefore a direct correlation between this parameter and the salt deposition rate. The value of F_{salt} used is based on measurements made on South African aerosols, albeit using limited data.

The three model parameters (other than F_{salt}, the fraction of salt associated with the aerosol) that influence the salt deposition rate most are, in order of decreasing influence; rural anthropogenic aerosol generation rate, natural aerosol generation rate and summer deposition velocity. The influence that F_{salt} and the rural anthropogenic aerosol generation rate have on the

concentration differentials (with and without an imposed impulse emission) in the soil water and surface water compartments is discussed in **Section 5.4**.

d) Atmospheric model results and discussion

A simple block flow diagram showing the calculated aerosol loads (in Mton/y) over a one-year period is shown in Figure 5.2. Mass is conserved to an accuracy of 99.7%.
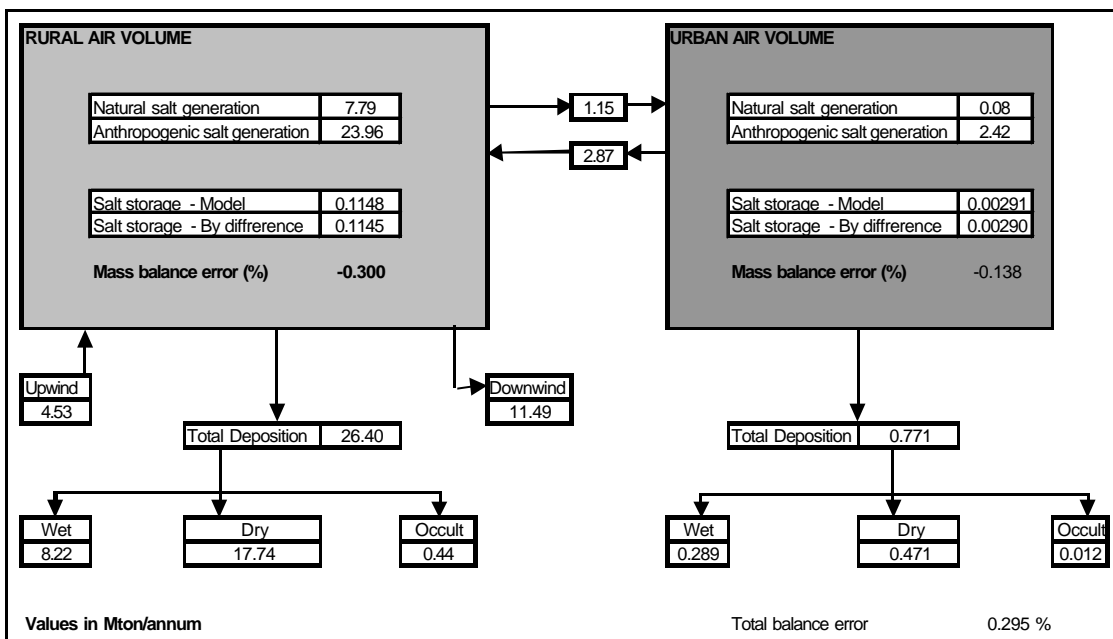

Figure 5.2: Atmospheric deposition model mass balance results

Selected model results are shown below in Figures 5.3 to 5.6 below. Figure 5.3 shows the daily variation of aerosol concentrations over a one-year period in the rural and urban air compartments. Figure 5.4 shows the variation of rainfall TDS concentration and the distribution of rainfall. Figures 5.5 and 5.6 show the aerosol deposition rates (comprising dry, wet and occult components) for the urban and rural air compartments respectively.

The following is evident from the Figures 5.3 to 5.6:

- The aerosol and rainfall TDS concentrations and the salt deposition rates are higher in the urban compartment than the rural compartment. This is in agreement with published findings (refer to Table 5.5).

- The method for calculating daily rainfall distribution is given in **Section 4.2.2**, and daily rainfall is plotted in Figure 5.4. As the rainfall intensity increases, the aerosol concentration decreases, wet deposition rate increases and dry deposition rate decreases. This behaviour is in agreement with published information. The dry deposition rate is a linear function of aerosol concentration and deposition velocity. As the aerosol concentration decreases due to wash-out by rain, the wet deposition rate increases and the dry deposition rate decreases accordingly.

- The aerosol and rainfall TDS concentrations are higher during the winter months than the summer months. The average total salt deposition is however slightly lower during the winter months. This is due to higher rainfall during summer months, which effectively cleans the air, and results in higher deposition rates.

- The ranges of published values for the model outputs (shown in Table 5.5) are generally large and modelled values fall within these ranges.
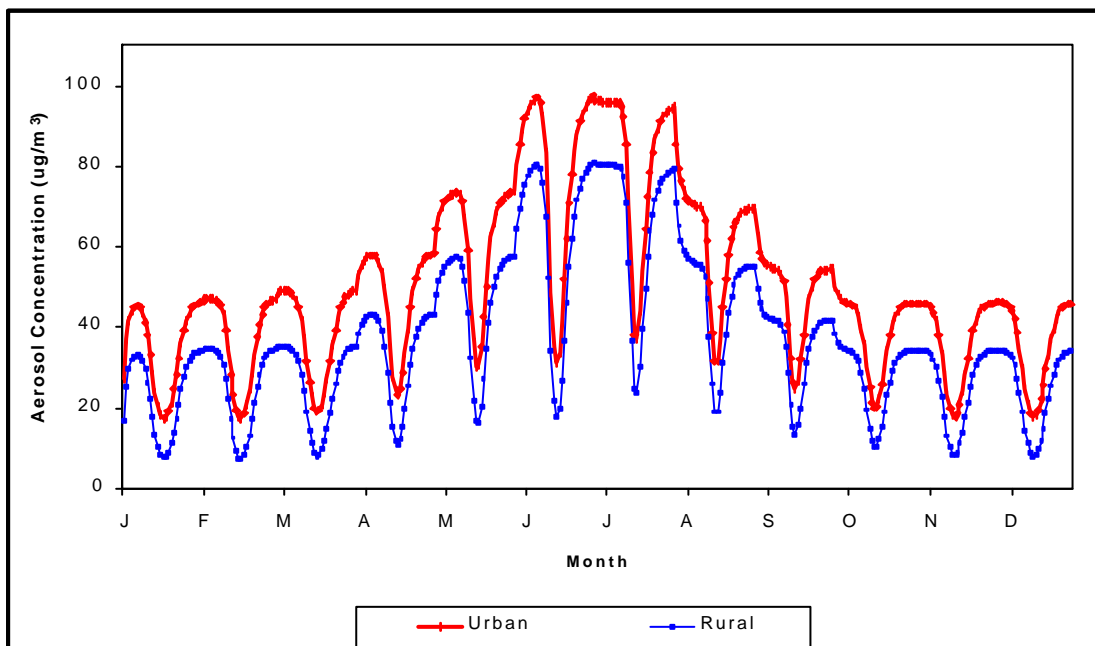

Figure 5.3: Modelled daily variation of aerosol concentration over a one-year period
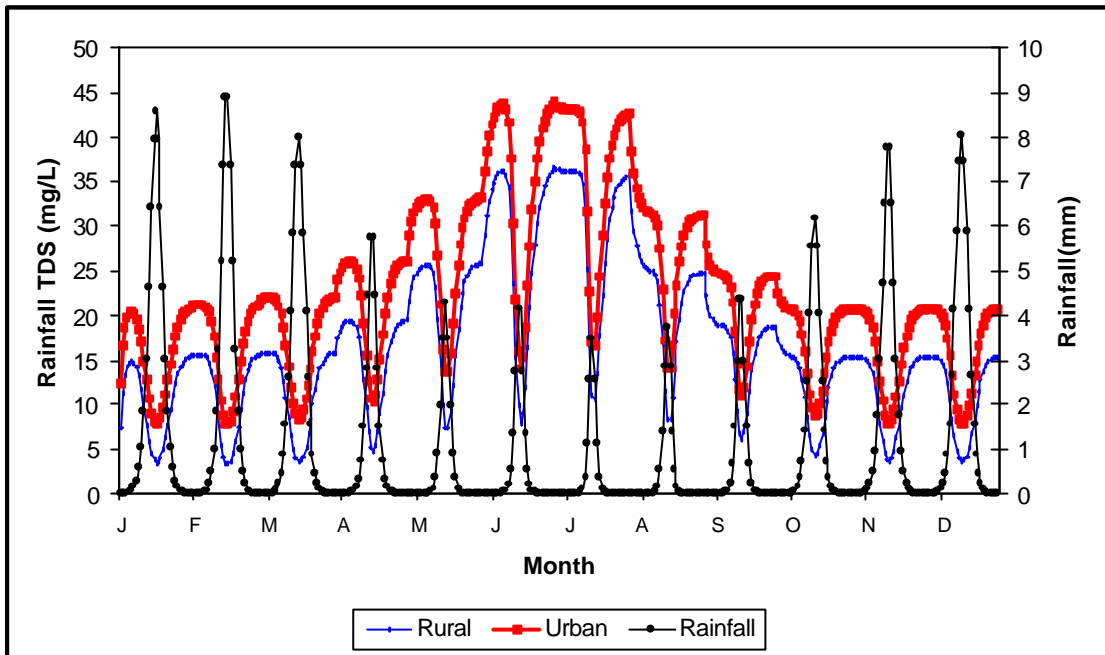
Figure 5.4: Modelled daily variation of rainfall TDS concentration over a one-year period
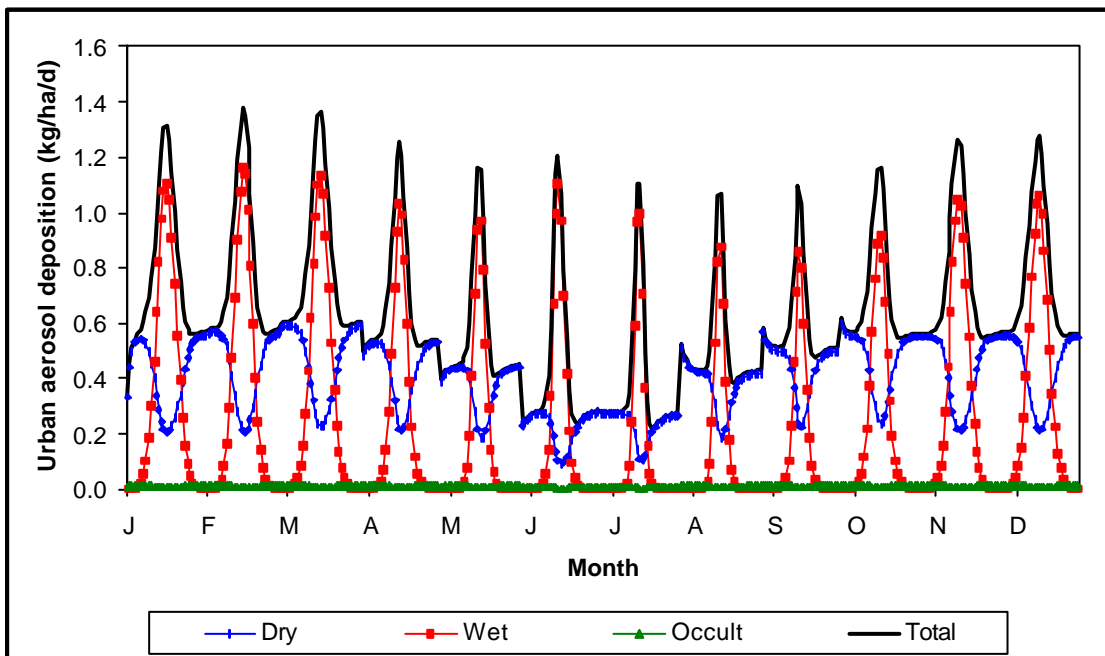

Figure 5.5: Modelled daily variation of dry, wet and occult aerosol deposition rate in the urban air compartment.
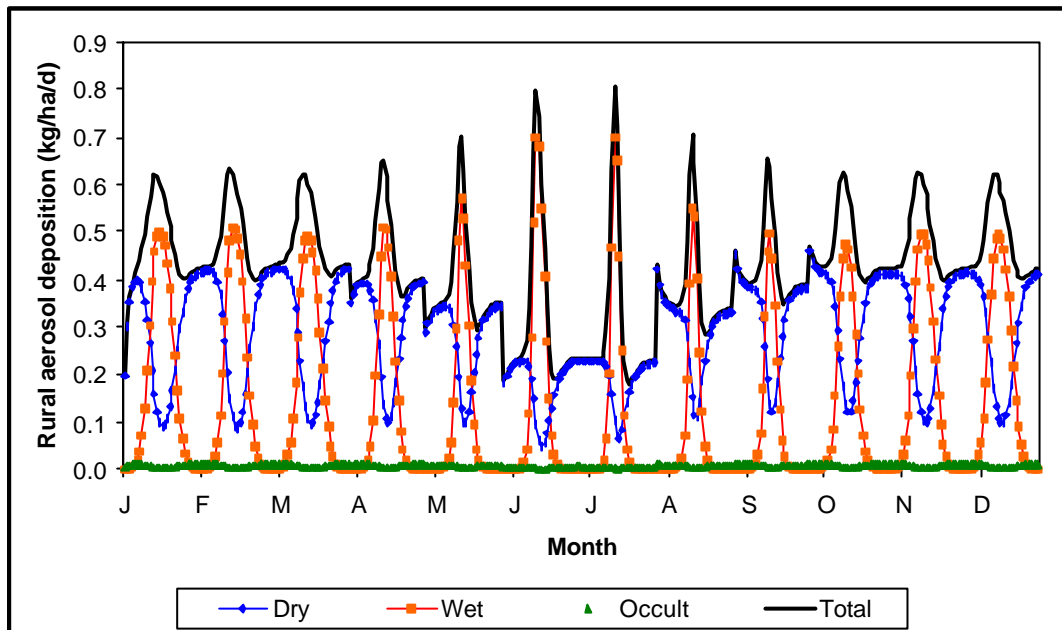
Figure 5.6: Modelled daily variation of dry, wet and occult aerosol deposition rate in the rural air compartment.

It was stated in **Section 3.3.1** that it is not necessary to specify the rate of growth of salination due to anthropogenic activities, either due to increased emissions to water, soil or the atmosphere. It is, however, necessary that the reference (or starting year) year of the simulation be the same for the atmospheric deposition model component and the hydrosalinity model component, and that the model parameters be chosen accordingly. For the hydrosalinity model, the year 2000 was chosen as the reference year (refer to **Appendix B**), and therefore, the atmospheric model parameters should be chosen to predict outputs that one would expect to measure in the year 2000. Unfortunately, these data are not always available. From the discussion on model parameters in **Section 5.2a**, the published model parameters shown in Table 5.4, and the published model outputs shown in Table 5.5, it can be seen that some of the data were published as far back as 1988 (natural and anthropogenic aerosol generation rates), and some data are current. Taking this into consideration, and the fact that the published data generally span very broad ranges, the atmospheric deposition model calibration results using parameters shown in Table 5.4 were taken as the reference year (2000) values.

The objectives set for the atmospheric model (refer to **Section 3.2.2**) have therefore been achieved. Daily salt deposition rates are calculated for rural and urban surfaces. Although it is not

possible to verify these values at a daily time-step, annual averages agree with published data. In this respect, the model is an improvement on other characterisation models, where single average parameter values are used to calculate the steady-state deposition rates. The model furthermore includes the major transport processes that influence the fate of salts in other compartments. The influence of salt deposition rate on salt concentrations in other compartments is discussed in **Section 5.4**.

5.3 HYDROSALINITY MODEL

The hydrosalinity model consists of two sub-components; namely a catchment hydrology component and a salt transport component. These are discussed in **Section 5.3.1** and **5.3.2** respectively.

5.3.1 Catchment hydrology component of hydrosalinity model

The catchment hydrology model parameters, model calibration results, model parameter sensitivity analysis and discussion are presented in **Section 5.3.1a** to **5.3.2d**.

a) Model parameters

The model parameters used in the catchment hydrology model are listed in Table 5.7, and are discussed individually below.

<u>Catchment and river geometry parameters</u>

The area of the unit catchment is calculated as the sum of areas of all catchments given by Midgley et al. (1994). The total area is 1.662×10^{12} m^2. A square catchment is assumed, giving a catchment width and length of 1.289×10^6 m. The river is assumed to be 1×10^6 m long (78% of catchment length). The slope of the river is calculated from the river length and an average altitude of 1 000 m above sea level, giving a slope of 0.001. The river width used in the model is back calculated from average river depth to give an average river flow velocity in the range reported by Chow et al. (1988) for natural channels with a slope ranging between 0 and 3 %.

The proportion of surface runoff draining to the upstream end of a river reach (F_{head}) varies from river to river in the range 0 to 1 (Herold ,1981). A value of 0.1 was assumed.

Table 5.7: Catchment hyrology model parameters

Model Parameter	Symbol	Units
Catchment area	A_T	m^2
Catchment length	L_C	m
Monthly rainfall	P_m	mm
Monthly evaporation	E_m	mm
Monthly irrigation demand factor	F_{irrig}	-
Fraction urban area	AI	-
Fraction rural area under irrigation	FI	-
Proportion of catchment runoff draining to the upstream end of the river	F_{head}	-
River width	W_R	m
River slope	$slope$	m/m
River length	L_R	m
River evaporation factor	F_{evap}	-
River bedloss	$F_{bedloss}$	mm/d
River Manning factor	M_F	-
First constant in rainfall duration relationship	AA	h
Second constant in rainfall duration relationship	BB	h/mm
Power of soil moisture-percolation relationship	POW	-
Soil moisture below which no percolation occurs	SL	mm
Soil moisture capacity	ST	mm
Percolation at soil moisture capacity	FT	mm/d
Nominal minimum infiltration rate	Z_{min}	mm/h
Nominal maximum infiltration rate	Z_{max}	mm/h
Interception loss	PI	mm
Routing constant for surface runoff	TL	d
Recession constant for groundwater depletion	GL	d
Coefficient of evaporation-soil moisture relationship	R	-
Soil moisture below which no evaporation occurs	SE	mm
Lag period for surface runoff	LAG	d
Proportion of groundwater entering deep groundwater	DGL	-
Maximum proportion of surface runoff from interflow	$PINTM$	-

<u>Land use parameters</u>

Data used to define the "unit South African catchment" and the methodology used in defining the catchment are summarised in **Appendix B**, and are mostly taken from Midgley et al. (1994). Of

the 1 662 020 km^2 of total land area, 568 km^2 (AI = 0.034%) is urban (impervious) surface and 6520 km^2 (0.39%) is normally under irrigation. A total land area of 1 654 932 (99.57%) is classified as rural natural land. The fraction of rural land irrigated (FI) is therefore also 0.034%. In terms of the model developed, agricultural land not irrigated is classified as natural land. In practice, only approximately 10.5% of the total land area is classified as conservation areas (which, in terms of the model developed would be classified as rural natural area), where anthropogenic influences are likely to be minimal. The remaining land (i.e. excluding urban areas, natural areas and irrigated areas) is classified as grazing land and potentially arable land, where some anthropogenic influences will be evident (NDA, 2002).

Rainfall, rainfall duration and evaporation

Monthly average rainfall and potential evaporation was calculated from data presented by Midgley (1994). A summary of the data, and the method of calculation is given in **Appendix B**. The rainfall and evaporation data used in the model are shown in Table 5.8.

Table 5.8: Monthly rainfall and evaporation used in model

Month	Rainfall (mm)	Potential Evaporation (mm)
January	60.7	195.6
February	56.9	157.1
March	54.3	142.7
April	31.8	103.1
May	18.2	79.2
June	12.8	63.1
July	11.9	69.3
August	13.8	93.7
September	19.8	124.9
October	36.0	159.0
November	51.5	175.5
December	54.9	197.2

Rainfall duration is estimated using Equation [4-20]. Pitman (1976) found, after analysing a plot of daily rainfall against duration for an autographic rainfall recorder at Pretoria, that values of 0.96 and 0,14 for AA and BB (Equation [4-20]) respectively fitted the observed data. Data for other

areas in South Africa were not available, and the values reported by Pitman (1976) were used initially, and their influence on model results evaluated by means of a sensitivity analysis.

<u>Irrigation demand factor</u>

The irrigation demand factor (F_{irrig}) is used in Equation [4-39] to calculate the crop irrigation demand. The irrigation demand factor was calculated (refer to **Appendix B** for method) using the monthly rainfall, evaporation and irrigation requirements published by Schulze (1997). Monthly irrigation demand factors are shown in Table 5.9.

Table 5.9: Monthly irrigation demand factors

Month	Irrigation Demand Factor
January	0.92
February	1.02
March	0.98
April	0.94
May	0.92
June	0.94
July	0.92
August	0.85
September	0.94
October	0.88
November	0.93
December	0.87

<u>River parameters</u>

Typical Manning roughness coefficients (M_F) for natural channels range between 0.03 for clean, straight streams to 0.1 for streams with heavy brush and timber (Chow et al., 1988). A value of 0.065 (midpoint of the range) was assumed.

Midgley et al (1994) report total losses from catchments, which include bedloss, losses due to wetlands and losses to aquifers. The total loss from all catchments is 1 349 million m^3 (refer to **Appendix B**). Using the river geometry above, the bedloss is calculated at 3.7 mm/d.

The choice of river evaporation factor depends on the aquatic vegetation. For most rivers a value of 1.0 is recommended. For rivers with large stands of reeds or other vegetation, a lower value is recommended (Herold, 1981). Data presented by McKenzie and Craig (1999) for the Orange River indicates an evaporation rate in the order of 1.8×10^{-5} mm/m^2 of river surface. An evaporation factor of 0.9 is used in the model, to account for some degree of vegetation.

Pitman model parameters

Parameters for the model originally developed by Pitman (1973) are published for all quaternary catchments of South Africa in Midgley et at (1994). These model parameters were derived from the calibration process, and were overlayed on maps showing features such as topography, rainfall, soil type, geology and vegetation. Parameters were first averaged on this basis for groups of hydrologically similar catchments and were then transposed to un-gauged areas. The WRSM90 model (an updated version of the original Pitman model, used by Midgley and co-workers) was then run with virgin land-use conditions and with the regionalised parameter set. The simulated flows were compared with naturalised flow records and all significant discrepancies noted. The regionalised parameters were then adjusted to bring the simulated virgin flows more closely into line with the naturalised records.

The methodology used to calculate the regionalised parameters for the "unit South African **Appendix B** but essentially they are calculated as area weighted averages from the quaternary level data presented by Midgley et al. (1994).

The minimum, average, maximum model parameters for the entire data set of parameters presented by Midgley et al. (1994) are summarised in Table 5.10. The area weighted averages are also shown.

Midgley et al (1994) warn that one should not read too much physical relevance into the values of the parameters. For instance, the recommended value for the parameter Z_{min} over much of the more humid areas of the country is 999 mm/m (1.37 mm/h). This figure is obviously way above what can be considered realistic. However, when used in conjunction with the other recommended parameters, a Z_{min} of 999 mm/m yields realistic flows.

Table 5.10: Pitman model parameters

Parameter	Units	Minimum	Average	Maximum	Area weighted average
Power of soil moisture-percolation relationship	-	0.10	1.63	3.20	0.71
Soil moisture below which no percolation occurs	mm	0.00	0.00	0.10	0.004
Soil moisture capacity	mm	0	166	600	107
Percolation at soil moisture capacity	mm/d	0.00	0.45	3.22	0.11
Nominal minimum infiltration rate	mm/h	0.00	0.35	1.37	0.21
Nominal maximum infiltration rate	mm/h	0.00	0.87	1.37	0.67
Interception loss	Mm	0.00	1.54	4.00	1.05
Routing constant for surface runoff	d	0.00	0.26	1.50	0.18
Recession constant for groundwater depletion	d	0.00	0.16	10.00	0.09
Coefficient of evaporation-soil moisture relationship	-	0.00	0.25	1.26	0.14

In the Pitman (1973) model, evaporation is assumed to cease when the soil moisture storage is at or near zero. Herold (1981) recommends that an initial value of the soil moisture below which no evaporation occurs (SE) can be estimated by subtracting 400 mm from the soil moisture capacity. A value of 107 mm was used for the soil moisture capacity, and the value of SE was set to zero.

Herold (1981) recommends that unless there is positive evidence of a substantial loss to deep groundwater, the proportion of groundwater entering deep groundwater (DGL) should be set to zero. A value of zero was found to be most appropriate even in the case of the southern Witwatersrand, where underlying dolomitic compartments have been dewatered to great depths by gold mining activities. The value of DGL was therefore set to zero.

The interflow through the soil moisture storage will depend upon catchment slopes, lateral and vertical permeabilities and other geographical features. $PINTM$ values calibrated for southern PWV catchments varied between 0.6 and 0,9 with an average of 0.8 (Herold, 1981).

b) Model calibration

The catchment hydrology component of the model was calibrated against the observed average monthly river flows. The methodology used to calculate the observed monthly river flows is given in **Appendix B** The model parameters discussed above were used as initial values, and were then adjusted to give the best correlation with observed values. The criteria used to measure correlation were the correlation coefficient (r^2) and the Agreement Index. The Agreement Index is given by the following equation (Moolman, 1993):

$$d = 1 - \frac{\sum_{i=1}^{N}(P_i - O_i)^2}{\sum_{i=1}^{N}[|P_i'| + |O_i'|]^2}$$

[5-1]

Where:

d = Agreement Index

P_i = i'th predicted value

O_i = i'th observed value

$P_i' = P_i - O^-$

$O_i' = O_i - O^-$

O^- = arithmetic mean of the observed values

High coefficients of determination (r^2) do not necessarily indicate good correlation between predicted and observed results. The Agreement Index (d) is recommended by Moolman (1993) as a better measure to use in validating model predictions. The Agreement Index is not a measure of correlation or association in the formal sense, but rather a measure of the degree to which a model's predictions are error free. The index varies between 0.0 and 1.0 where a value of 1.0 indicates perfect agreement between the observed and predicted observations. The index specifies the degree to which the observed deviations about the arithmetic mean correspond, both in magnitude and sign, to the predicted deviations about the arithmetic mean (Moolman, 1993).

Figure 5.7 shows the average monthly observed and predicted river flows. The hydrological model parameters used to obtain the results shown in Figure 5.7 are given in Table 5.11.

The monthly rainfall and evaporation rates used are shown in Table 5.8, and the monthly crop factors used are shown in Table 5.9.

The model parameters discussed in **Section 5.3.1a** above were used as initial values, and thereafter the parameters were adjusted to give the highest Agreement Index. The highest Agreement Index was obtained with the parameter values shown in Table 5.11. It can be seen that the only parameters that required adjustment (from published values) were POW, Z_{min}, and Z_{max}.

The value of the parameter POW determines the rate at which subsurface flow reduces as soil moisture is depleted (Equation [4-44]), and as the value of POW increases, the subsurface flow decreases more rapidly during periods between rainfall events.

The value of the parameter Z_{min} represents the minimum rainfall intensity that is required to initiate surface runoff (Equations [4-21] to [4-26]), and an increase in the value of Z_{min} will result in a reduction in the frequency and volume of surface runoff events.

The value of Z_{max} determines (in conjunction with Z_{min}) the average infiltration to soil moisture, and a reduction in the value of Z_{max} results in a reduction in the volume of surface runoff events.

The calibrated values of Z_{min} and Z_{max} are both higher than the calculated area weighted averages shown in Table 5.10, suggesting that using an area weighted average method to regionalize these parameters may lead to an overestimation in the volume of surface runoff. The value of the parameter POW is marginally (8.5%) below the area weighted average, but is well within the reported range for this parameter.
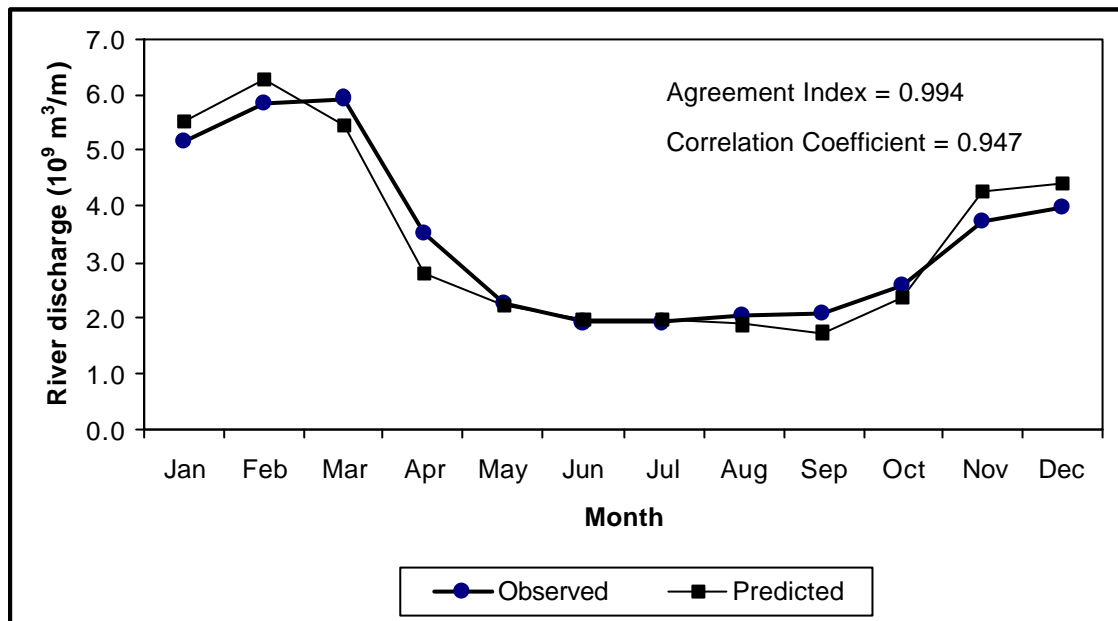
Figure 5.7: Predicted and observed monthly river flow

c) Model parameter sensitivity analysis

The model parameters shown in Table 5.11 were varied by ± 50%, and the effect on the Agreement Index and correlation coefficient determined. The results of this analysis are shown in Table 5.12.

It is evident from the parameter sensitivity analysis results that, in terms of the change in Agreement Index over the range in which the parameters were adjusted, the nominal maximum infiltration rate (Z_{max}) is the most sensitive parameter followed by the interception storage (PI) and percolation at soil moisture capacity (FT). More detailed sensitivity analyses of the hydrological component of the model parameters can be found in Herold (1981) and Moolman (1993). The influence that these parameters have on the concentration differential (with and without an imposed emission impulse) is presented in **Section 5.4**.

Table 5.11: Calibrated catchment hyrology model parameter values

Model Parameter	Symbol	Value	Units
Catchment area	A_T	1.66×10^{12}	m^2
Catchment length	L_C	1 289 194	m
Fraction urban area	AI	0.00034	-
Fraction rural area under irrigation	FI	0.00034	-
Proportion of catchment runoff draining to the upstream end of the river	F_{head}	0.1	-
River width	W_R	1000	m
River slope	$slope$	0.001	m/m
River length	L_R	1 000 000	m
River evaporation factor	F_{evap}	0.9	-
River bedloss	$F_{bedloss}$	3.7	mm/d
River Manning factor	M_F	0.065	-
First constant in rainfall duration relationship	AA	0.964	h
Second constant in rainfall duration relationship	BB	0.137	h/mm
Power of soil moisture-percolation relationship	POW	0.65	-
Soil moisture below which no percolation occurs	SL	0.004	mm
Soil moisture capacity	ST	107	mm
Percolation at soil moisture capacity	FT	0.11	mm/h
Nominal minimum infiltration rate	Z_{min}	0.31	mm/h
Nominal maximum infiltration rate	Z_{max}	3.30	mm/h
Interception loss	PI	1.05	mm
Routing constant for surface runoff	TL	0.183	d
Recession constant for groundwater depletion	GL	0.09	d
Coefficient of evaporation-soil moisture relationship	R	0.14	-
Soil moisture below which no evaporation occurs	SE	0	mm
Lag period for surface runoff	LAG	0	d
Proportion of groundwater entering deep groundwater	DGL	0	-
Maximum proportion of surface runoff from interflow	$PINTM$	0.8	-

Table 5.12: Catchment hydrology model parameter sensitivity analysis results

	Change to Agreement Index (%)		Change to correlation coefficient (%)	
	-50%	**+50%**	**-50%**	**+50%**
F_{head}	0.000	0.000	0.000	0.000
W_R	-0.066	-0.013	0.318	-0.339
$slope$	0.043	-0.017	-0.364	0.136
F_{evap}	-0.019	0.003	0.078	-0.083
$F_{bedloss}$	0.000	-0.027	0.004	-0.004
M_F	-0.039	0.052	0.306	-0.445
AA	-0.494 (1)	-0.910	0.910 (1)	2.442
BB	-0.494 (2)	-0.904	0.910 (2)	2.334
POW	-0.009 (3)	-2.844	0.004 (3)	0.160
SL	0.000	0.000	0.000	0.000
ST	-0.191 (4)	0.015	0.266 (4)	-0.025
FT	**-4.941**	**-1.407**	**1.217**	**-0.727**
Z_{min}	-1.461	-0.828	0.691	-0.617
Z_{max}	**-26.724**	**-8.797**	**4.070**	**-2.197**
PI	**-4.147**	**-2.215**	**0.868**	**-0.923**
TL	-0.001	0.001	0.010	-0.010
GL	-0.002	0.002	-0.001	-0.003
R	-0.302	-0.025	0.366	-0.169
SE (5)	0.000	0.000	0.000	0.000
DGL (6)	-0.238	-5.377	0.227	1.236
$PINTM$	0.004	-0.087 (7)	-0.116	0.061 (7)

Note: Some parameters could not be varied by ±50% as this resulted in unrealistic model results (for example; decreasing the rainfall duration constants by 50% resulted in periods of zero flow in the river). For these parameters the following changes were made:

(1) −17%	(5) Range 50-100
(2) −20%	(6) Range 0.1 to 0.8
(3) − 5%	(7) +25%
(4) −16%	

d) Model results and discussion

The water balance over a one-year period is shown in Figure 5.8. Small errors are introduced due to the structure of the program (given in **Appendix D**). An error of 3.4% in the conservation of mass over the rural agricultural surface is due to the fact that the surface runoff and infiltration of the current day is calculated using the previous day's irrigation flow. An error of 1.1% in the conservation of mass over the river is introduced due to the method in which channel routing is calculated in the program. The assumption is that the entire upstream inflow enters the reach at the beginning of the day, whereas in fact any cell grows from zero at the start of the day to its full volume at the end of the day. The lateral inflow to any cell will therefore be over-estimated. Similarly, at the downstream en of the reach, the lateral inflow to those cells leaving the reach will also be overestimated (Herold, 1981).

Selected outputs for the hydrological component of the hydrosalinity model (for the model parameters shown in Table 5.11) are shown in Figures 5.9 to 5.17. Figure 5.9 shows the daily rainfall and potential evaporation distribution over a one-year period. Average monthly rainfall and potential evaporation data is input into the model. Monthly rainfall is disaggregated into daily rainfall using the parameters AA and BB (Equation [4-20]), however, potential evaporation remains constant over any given month. The effect that these distributions have on the surface runoff and infiltration flow rates for the rural natural and rural agricultural surfaces are evident in Figures 5.10 and 5.11 respectively.
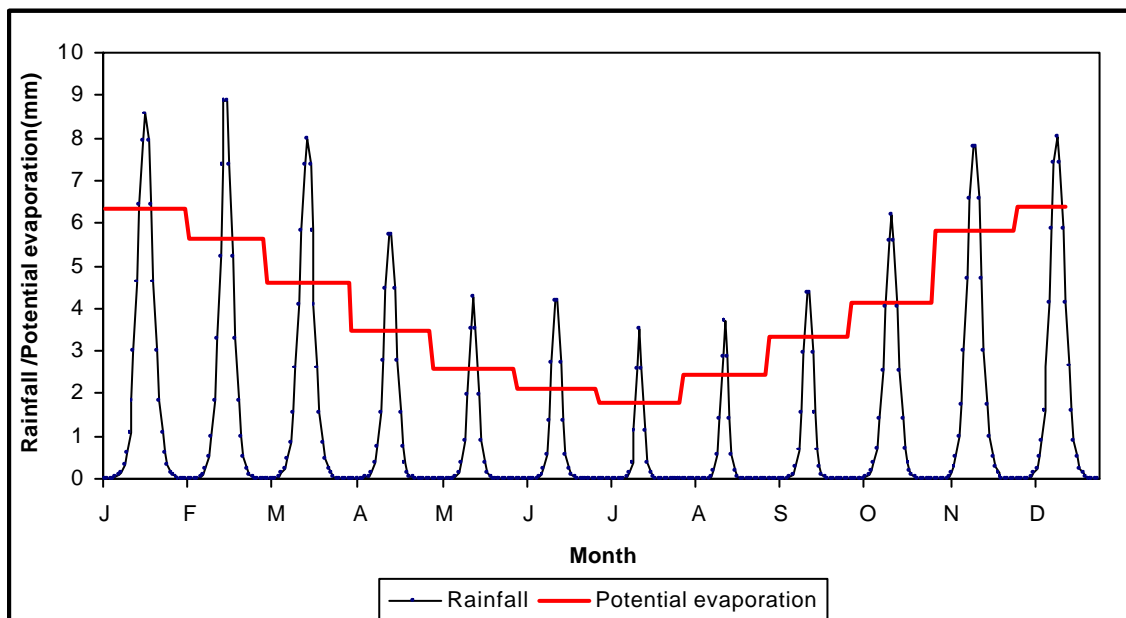

**Figure 5.9: Modelled daily rainfall and potential evaporation distribution over a one-year cycle**
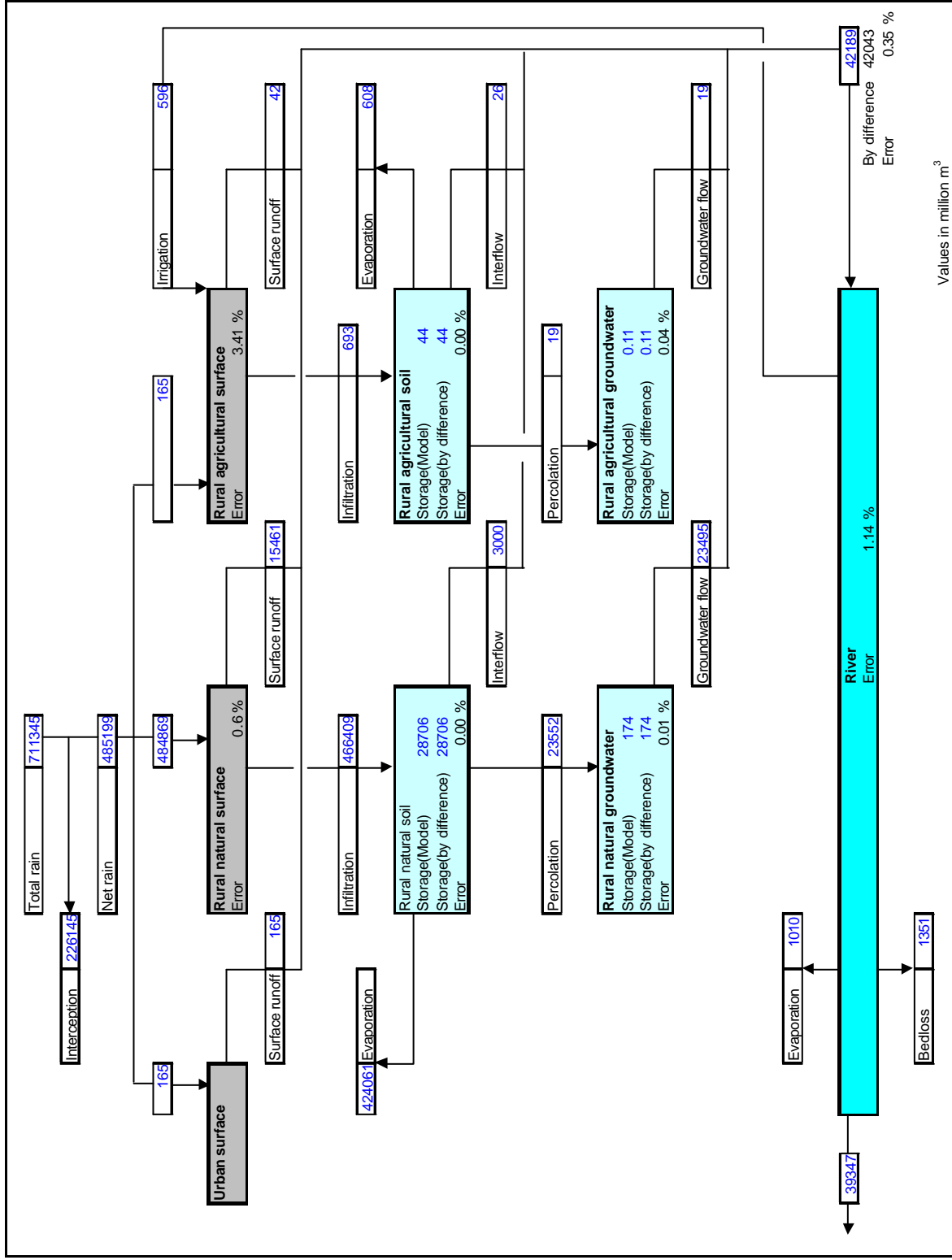
Figure 5.8: "Unit catchment" annual water balance
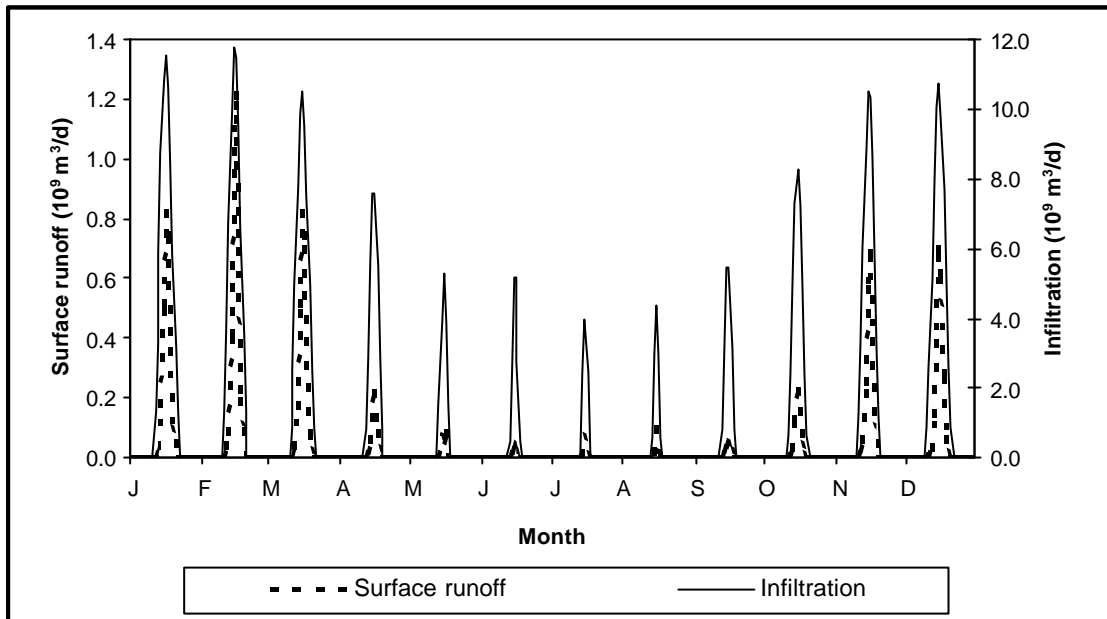
Figure 5.10: Modelled daily surface runoff and infiltration flows from the rural natural surface over a one-year cycle
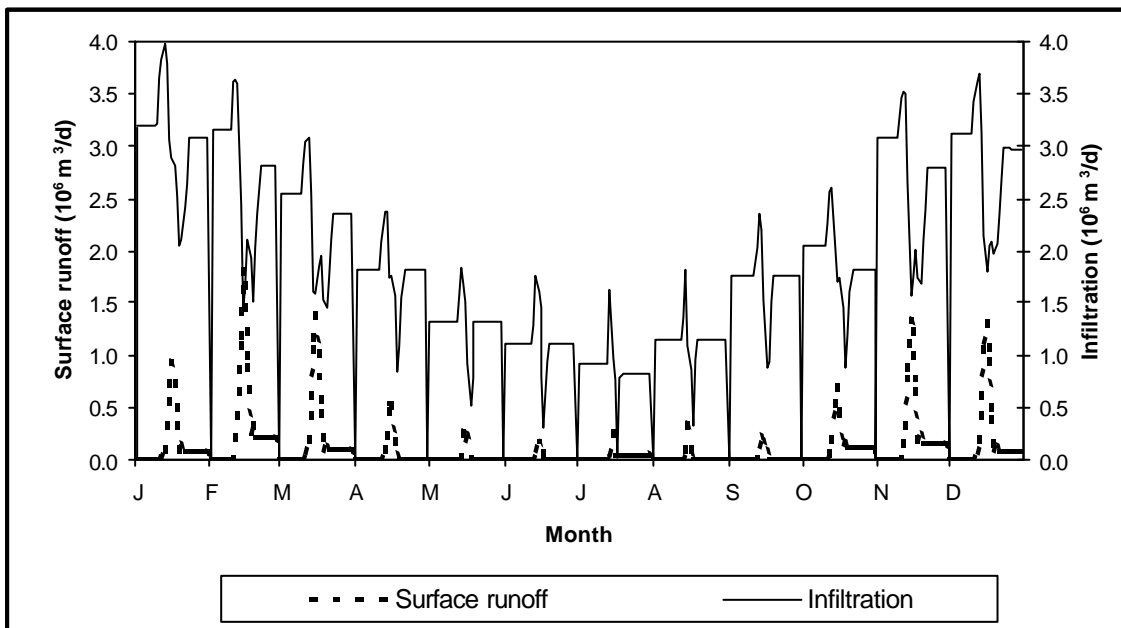

Figure 5.11: Modelled daily surface runoff and infiltration flows from the rural agricultural surface over a one-year cycle.

The daily irrigation demand is shown in Figure 5.12. The effect that irrigation has on the surface runoff and infiltration from the rural agricultural area is evident. During high rainfall days, irrigation demand is low and surface runoff and infiltration is governed by the rainfall and evaporation distributions, while during low rainfall days, the irrigation demand dominates.
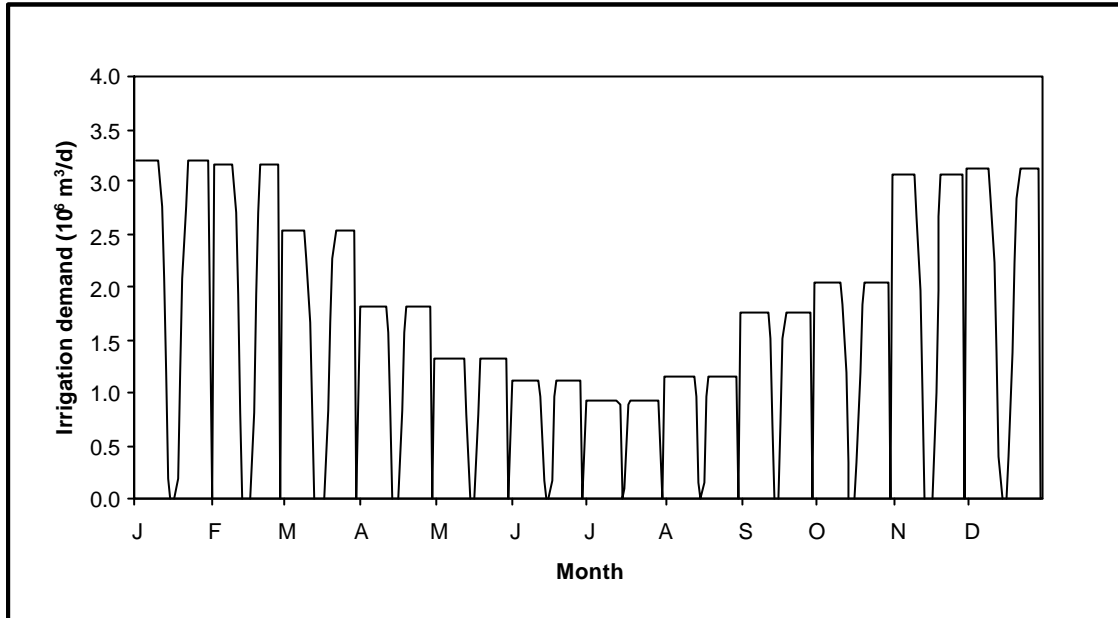
**Figure 5.12: Modelled daily irrigation demand over a one-year cycle**
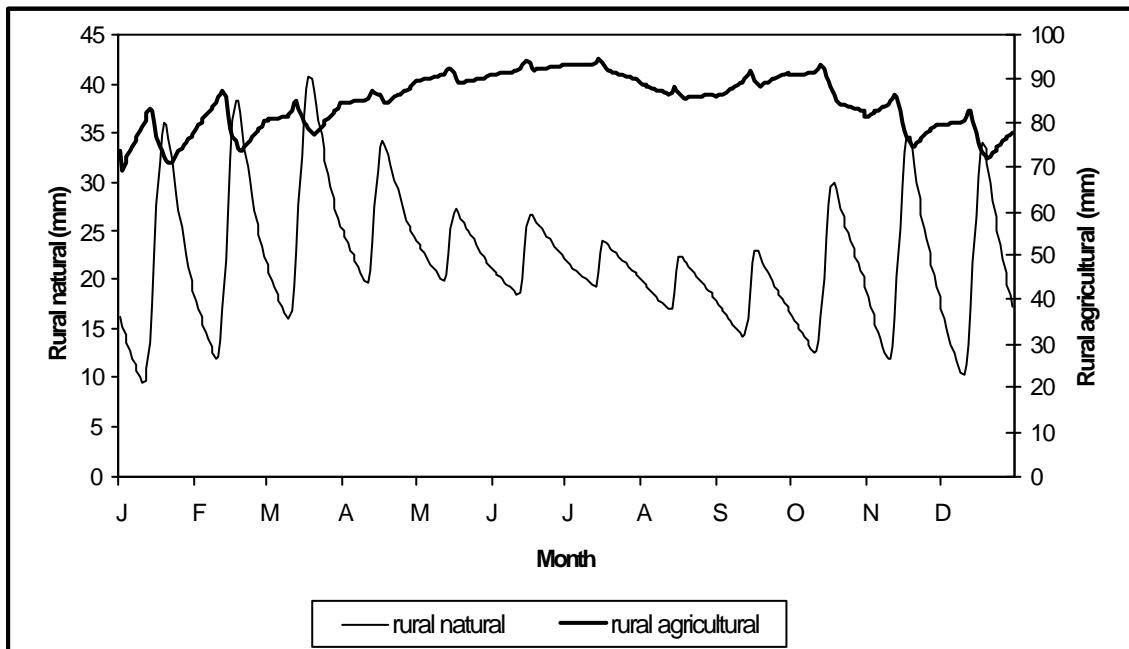
Figure 5.13: Modelled daily soil moisture over a one-year cycle

Figure 5.13 shows the soil moisture distribution in the rural natural and rural agricultural soils. It is evident that the soil moisture in the rural agricultural soil is higher than the rural natural soil, and the profile is modified due to the irrigation demand.
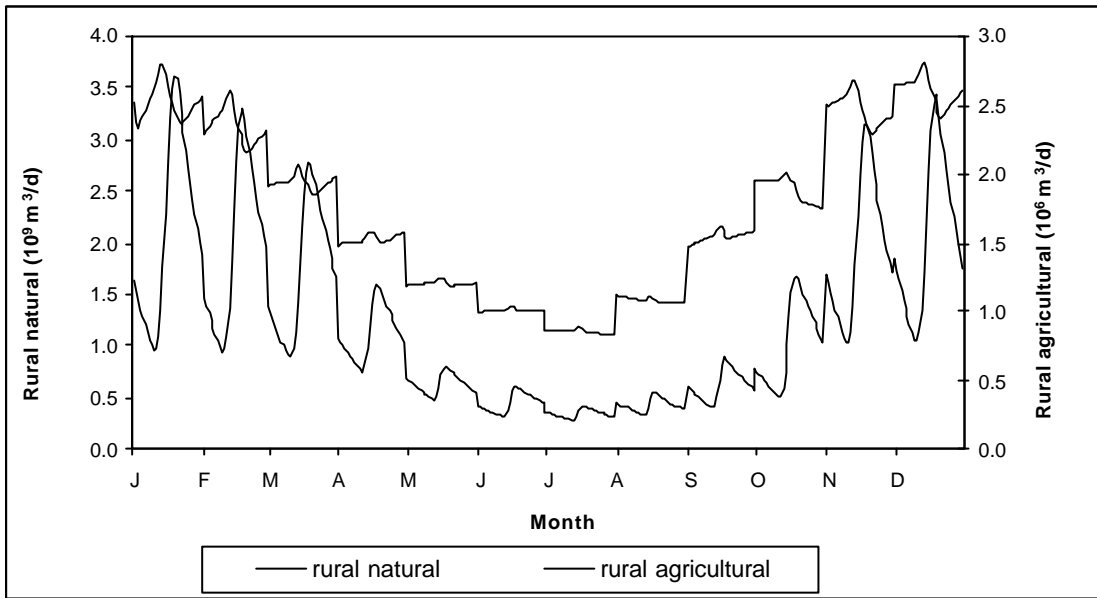

**Figure 5.14: Modelled daily soil moisture evaporation over a one-year cycle**
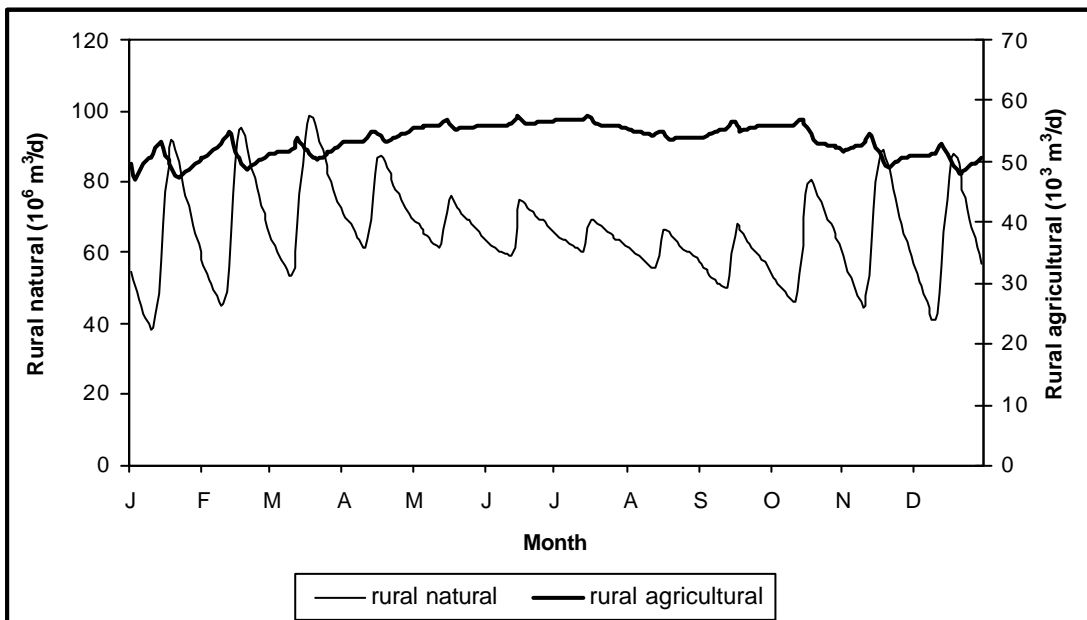
Figure 5.15: Modelled daily percolation flow over a one-year cycle

Figure 5.14 shows evaporation from rural natural and rural agricultural soils. Evaporation from soil moisture is calculated using Equation [4-43], and is linearly related to the soil moisture. Percolation of water from the root zone to groundwater (Figure 5.13) is governed by equation [4-44], and the profile is the same as for soil moisture. The soil moisture remains al relatively high levels during the winter months in the rural agricultural soils since the irrigation demand (in terms of the number of days in the month in which irrigation water is required) is high. The influence of irrigation is also evident in the groundwater flow entering the river (Figure 5.16).
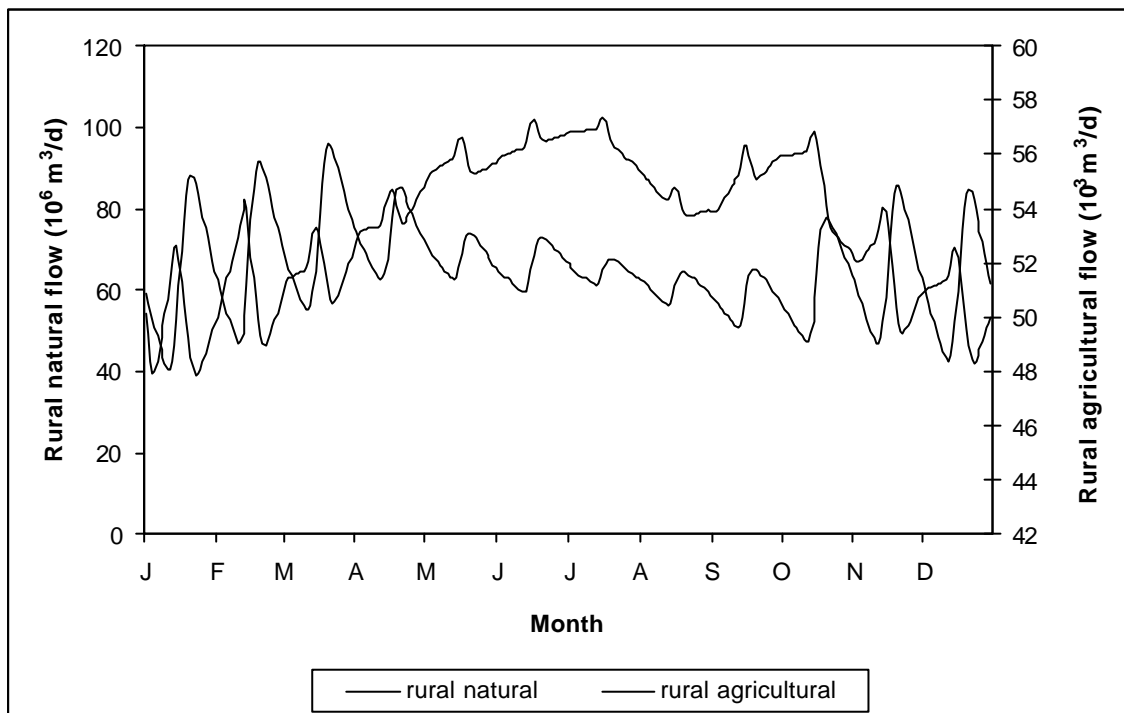

Figure 5.16: Modelled daily groundwater flow to surface water over a one-year cycle.

The surface water (river) flow (Figure 5.17) is the sum of the attenuated and lagged surface runoff, inteflow and groundwater flow. The daily values plotted in Figure 5.17 were used to calculate monthly average values, which were used to calibrate the catchment hydrology component of the model (Figure 5.7)

The effect that parameters Z_{max} (nominal maximum infiltration rate), PI (interception storage) and FT (maximum percolation rate at soil moisture capacity) have on the river flow distribution is shown in Figures 5.18 to 5.20.
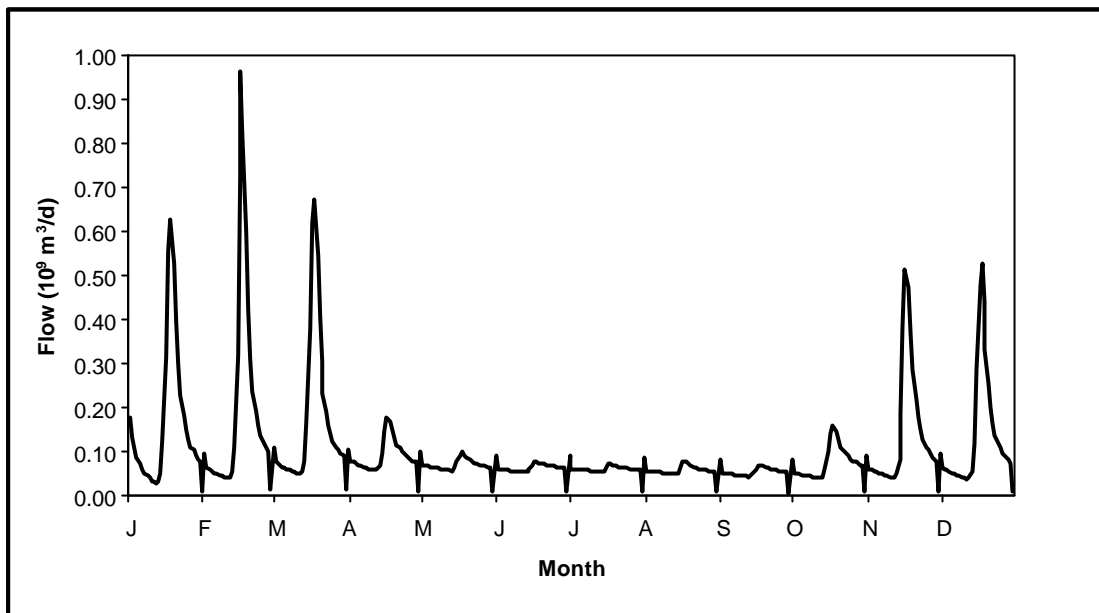
**Figure 5.17: Modelled daily river discharge over a one-year cycle.**
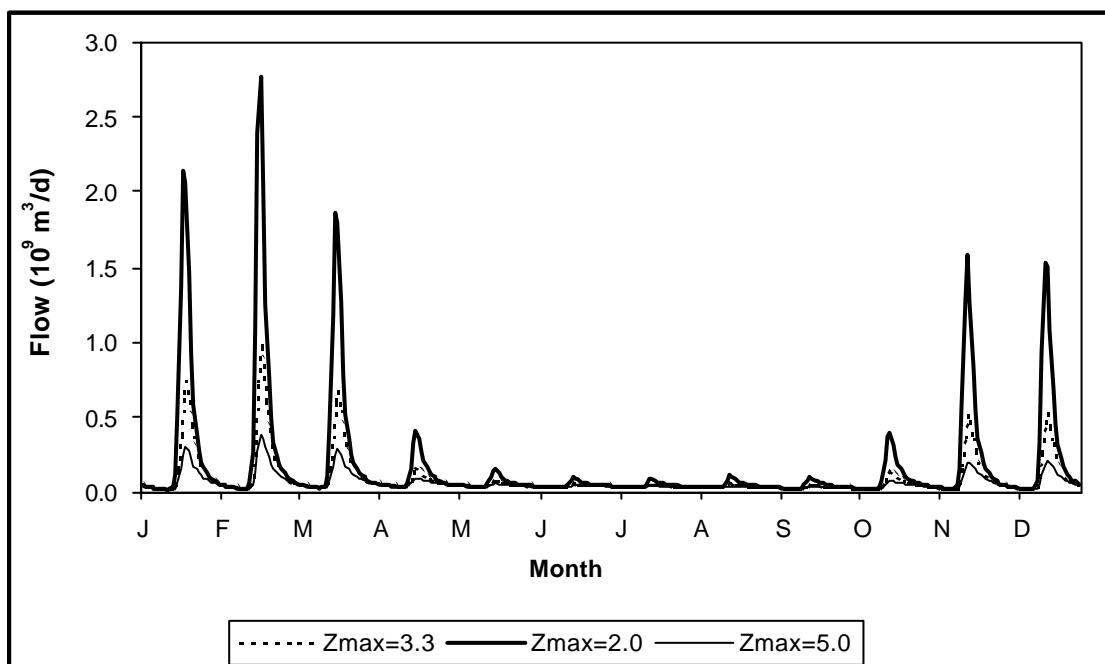
Figure 5.18: Sensitivity of modelled daily river discharge to the parameter $Z_{\max}$
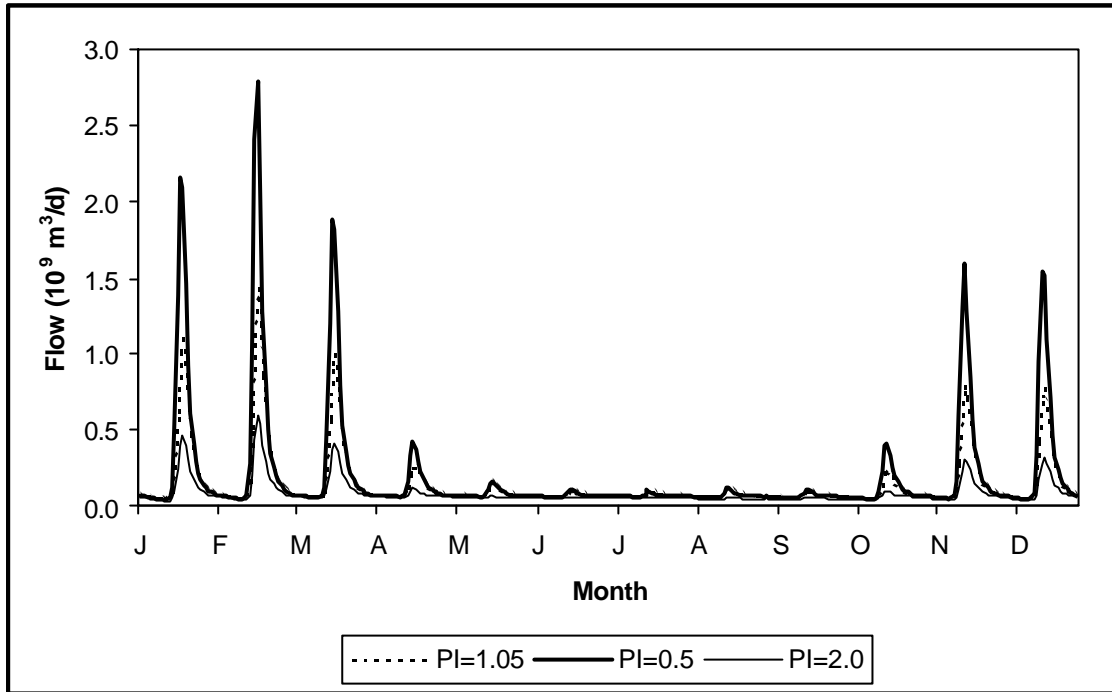
Figure 5.19: Sensitivity of modelled daily river discharge to the parameter PI
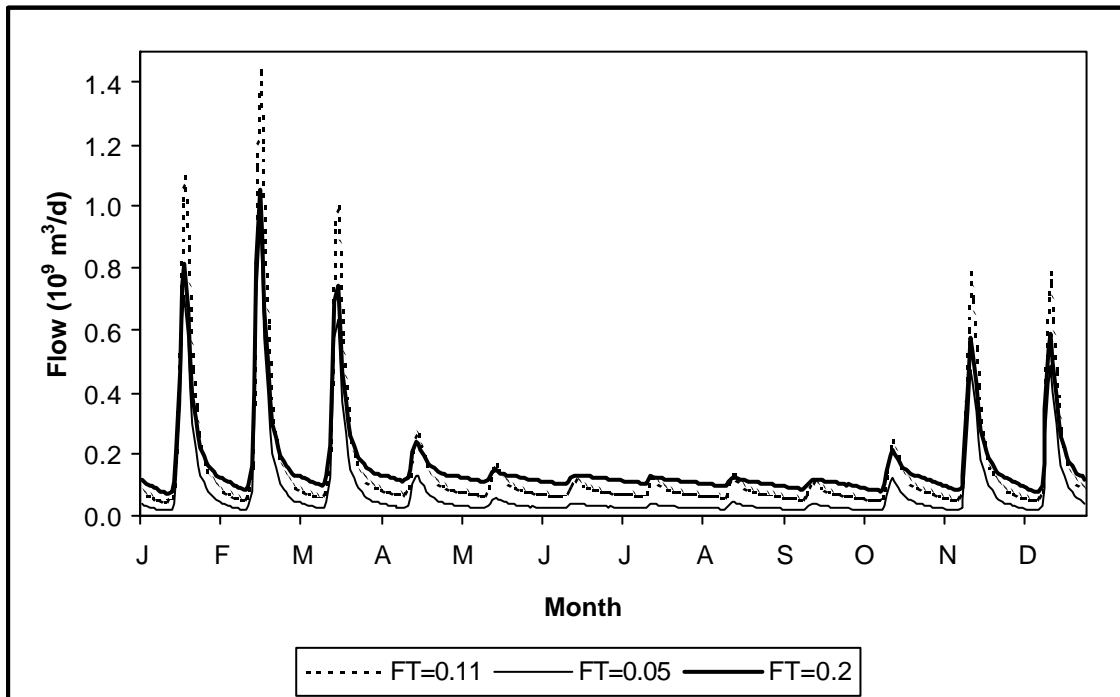

Figure 5.20: Sensitivity of modelled daily river discharge to the parameter FT

The nominal maximum infiltration rate determines (in conjunction with the nominal minimum infiltration rate) the average infiltration into soil moisture. An increase in $Z_{\max}$ results in a reduction in the volume of surface runoff and an increase in the volume of infiltration, particularly during high rainfall events.

The effect of interception storage is straightforward. An increase in PI results in a decrease in the amount of rainfall available for runoff and infiltration, and thus the flow increases.

An increase in FT results in a greater subsurface flow at the expense of evaporation and surface flow, particularly during dry periods.

The influence that $Z_{\max}$ and PI have on the concentration differential (with and without an imposed impulse emission) is discussed in **Section 5.4**.

5.3.2 Salt transport component of the hydrosalinity model

a) Model parameters

The model parameters used in the salt transport component of the hydrosalinity model are listed in Table 5.13.

Surface wash-off parameters

The method for calculating the removal of pollutants from surfaces is identical to that proposed by Herold (1981). It is assumed that the pollutant load removed per unit area is proportional to the instantaneous storage at any time. It is further assumed that the proportionality constant is proportional to the runoff from the surface (and infiltration for pervious areas). Surface wash-off parameters are defined in Equations [4-31] and [4-35]. Herold (1981) reports surface wash-off parameters in the range 0.0007 to 0.001/mm for pervious areas and 0.001 to 0.015/mm for impervious areas of the PWV area. The mid-point of these ranges were used as initial values.

Table 5.13: Salt transport model parameters

Model Parameter	Symbol	Units
Urban surface wash-off parameter	$ISWP$	1/mm
Rural natural surface wash-off parameter	$PSWP_n$	1/mm
Rural agricultural surface wash-off parameter	$PSWP_a$	1/mm
Solubility limit	C_{sat}	kg/m^3
Salt leach rate	$LeachRate$	kg/m^3/d
First Langmuir adsorption constant	A	kg/kg
Second Langmuir adsorption constant	B	kg/m^3
Soil void fraction	F_{void}	-
Soil density	r_{soil}	kg/m^3
Urban anthropogenic salt generation rate	G_{Us}	t/km^2/y
Rural natural anthropogenic salt generation rate	G_{Rns}	t/km^2/y
Rural agricultural anthropogenic salt generation rate	G_{Ras}	t/km^2/y

Salt solubility

Salts are modelled as a lumped parameter, and there is therefore no solubility limit for total dissolved salts *per se*. The solubility limits of several compounds containing the common ions are listed in Table 5.14.

Calcium carbonate is likely to precipitate first (as calcite or aragonite, which is often a precursor to calcite). Magnesium carbonate (brucite) and a mixture of calcite and brucite (dolomite) may form. The precipitation of calcite leads to cementation of soil particles and possibly to the formation of hardpans. The solubilities of many of the compounds are dependent on various factors such as pH, temperature, and partial pressures of gases such as oxygen and carbon dioxide (Eriksson, 1985). In the model developed, total dissolved salts are modelled as a lumped parameter. The approach adopted was to vary the "solubility limit" and evaluate the effect on the model results (refer to **Sections 5.3.2e** and **5.4**).

Table 5.14: Solubility limits of selected compounds containing common ions (*Handbook of Chemistry and Physics, 63rd Edition*)

Compound	Mineral	Solubility (g/L)	Temperature (°C)
Na_2SO_4	Thenardite	47.6	0
$Na_2SO_4.10H_2O$	Mirabilite	110	0
Na_2CO_3		71	0
$Na_2CO_3.H_2O$	Thermonatrite	330	0
NaCl	Halite	357	0
$CaCO_3$	Aragonite	0.0153	25
$CaCO_3$	Calcite	0.014	25
$CaCl_2$		745	20
$CaCO_3.MgCO_3$	Dolomite	0.32	18
$CaSO_4$		2.09	30
$CaSO_4.2H_2O$	Gypsum	3	Cold
$MgCO_3$	Magnesite	0.106	Cold
$MgCl_2$		542.5	20
$Mg(OH)_2$	Brucite	0.009	18
$MgCO_3.5H_2O$	Iansfordite	1.76	7
$MgCO_3.3H_2O$	Nesquehonite	1.79	16

<u>Salt leaching rates</u>

The mass of salt leached from soil is assumed to be proportional to the volume of water in the soil, and is characterised by the parameter $LeachRate$ in Equation [4-47]. Chemical weathering in the root zone does not contribute much to the concentration of dissolved components in soil water. Weathering rates of magnesium, calcium and sodium in the leached horizon of a podsol in the north of Sweden are reported as 46, 30 and 34 $mg/m^2/y$ respectively (Eriksson, 1985). Matthess et al. (1992) report calcium, magnesium and bicarbonate weathering rates of 4.5, 0.84 and 16.2 $g/m^2/y$ respectively. In a study reported by Matthess et al. (1992), a mass of 54 000 kg/y of sodium was released from a soil volume of $1.8X10^9$ m^3, giving a weathering rate for sodium of $8.2x10^{-8}$ kg/m^3 soil/d for combined saturated and unsaturated soil zones. Assuming that the soil moisture capacity was 100 mm, and that sodium comprises 21.4 % of the total dissolved solids (refer to **Appendix B**), a leach rate of $3.84x10^{-6}$ kg/m^3 water/d is derived.

<u>Langmuir adsorption constants</u>

The Langmuir adsorption isotherm has been used to describe adsorption of salts onto soil. The model is characterised by the two constants (A and B) in Equation [4-51]. Salts are modelled as a lumped parameter, total dissolved salts, and there is therefore no single set of Langmuir constants. In addition, very little data are available on the values of these constants for common ions adsorbed onto soils. Fey and Guy (1993) report values of A and B in the ranges 60 to 984 mg/kg and 90 to 1000 mg/L respectively, for adsorption of sulphate onto a number of different soil types found in South Africa.

The constant A determines the maximum amount of adsorption that occurs, while the constant B determines how rapidly the maximum concentration is reached. At steady state, sorption will have no effect on the anion composition of percolating soil water, other than sulphate. Common cations in soil solutions are in most cases in exchange equilibrium with large storages of exchangeable ions (Eriksson, 1985). Sulphate constitutes, on average, approximately 10% of the total dissolved salt concentration (refer to **Appendix B**). Assuming therefore that sulphate is the major ion involved in adsorption processes, the value of the parameter A used in the model initially was taken as one-tenth the value obtained by Fey and Guy (1993) for sulphate. The value of B was assumed to remain the same.

<u>Soil characteristics</u>

Mackay (1991) reports typical values for soil void fraction and soil density of 0.5 and 1 200 kg/m^3 respectively. These values were used in the model.

<u>Anthropogenic salt generation rates</u>

Herold (1981) found that salt generation rates in the range 0.4 to 1.2 t/km^2/y (for the year 1981) resulted in the best agreement with observed values for catchments in the southern Pretoria-Witwatersrand-Vereeneging area. The surface water salt concentration was found to be sensitive to the anthropogenic salt generation rates, particularly the rural natural generation rate, due to the large area (refer to **Section 5.3.2c**). The anthropogenic generation rates were therefore used as the primary calibration parameter.

b) Model calibration

The hydrosalinity component of the model was calibrated against the calculated average monthly river total dissolved salt concentrations. The methodology used to calculate the monthly river concentrations is given in **Appendix B** The model parameters discussed above were used as initial values, and were then adjusted to give the best correlation between predicted and calculated values. The criteria used to measure correlation were the correlation coefficient (r^2) and the Agreement Index (given by Equation [5-1]).

Figure 5.21 shows the average monthly observed and predicted salt concentrations in the "unit South African river". The hydrosalinity model parameters used to obtain the results shown in Figure 5.21 are given in Table 5.15. Depending on the initial conditions chosen, the model reached steady-state (identical cycles, in terms of salt concentrations) after approximately 15 years (refer to **Section 5.3.2e**), all subsequent simulations were therefore done for a 20-year simulation period.

Although the modelled values agree with the predicted values reasonably well (both the agreement index and correlation coefficient > 0.9), the fit is not as good as was achieved with the river flows. Further adjustment of the parameters did not yield better results, and it is likely that this is partly due to the lack of surface water quality data in some catchments (refer to **Appendix B**).
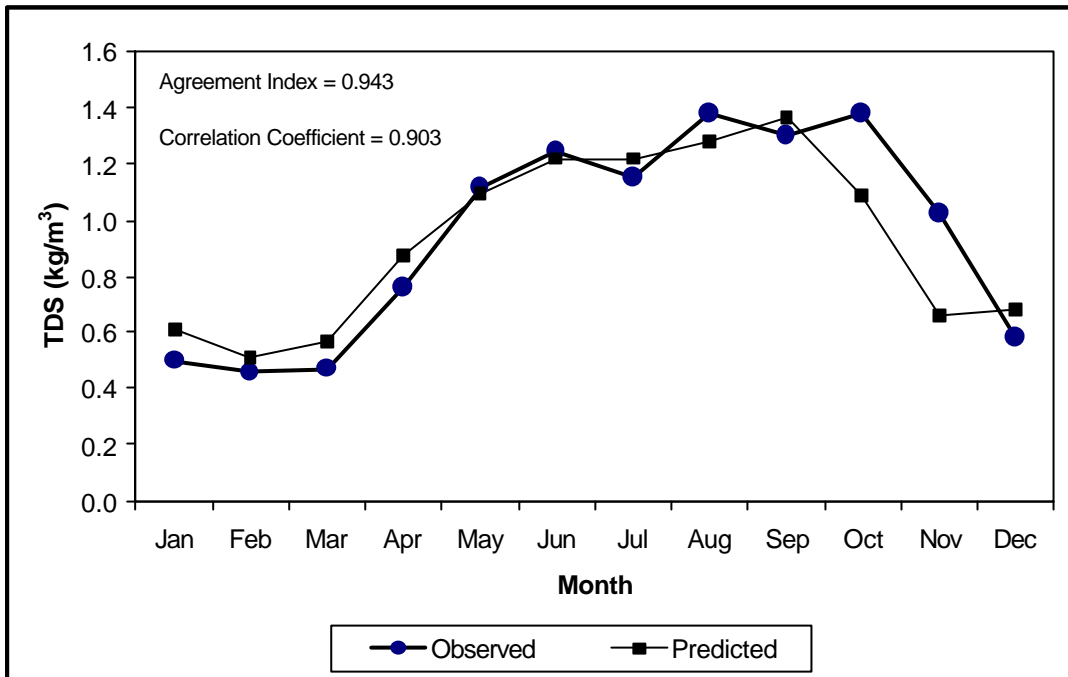
Figure 5.21: Predicted and observed monthly river total dissolved salts concentration

Table 5.15: Salt transport model parameters

Model Parameter	Symbol	Units
Urban surface wash-off parameter	0.0085	1/mm
Rural natural surface wash-off parameter	0.00085	1/mm
Rural agricultural surface wash-off parameter	0.0009	1/mm
Solubility limit	50	kg/m^3
Salt leach rate	3.5×10^{-6}	$kg/m^3/d$
First Langmuir adsorption constant	0.000024	kg/kg
Second Langmuir adsorption constant	0.418	kg/m^3
Soil void fraction	0.5	-
Soil density	1200	kg/m^3
Urban anthropogenic salt generation rate	0.7	$t/km^2/y$
Rural natural anthropogenic salt generation rate	0.03	$t/km^2/y$
Rural agricultural anthropogenic salt generation rate	0.5	$t/km^2/y$

c) Model parameter sensitivity analysis

The model parameters shown in Table 5.15 were varied by ± 50%, and the effect on the Agreement Index and correlation coefficient determined. The results of this analysis are shown in Table 5.16.

It is evident from the parameter sensitivity analysis results that, in terms of the change in Agreement Index over the range in which the parameters were adjusted, the rural natural salt generation rate is the most sensitive parameter followed by the solubility limit. These parameters are discussed in more detail in **Section 5.4**.

d) Sediment component of the hydrosalinity model

The parameters used to model sediment generation and transport are given in Table 5.17. The values of the model parameters shown in Table 5.17 (except a and b) are values recommended by Paling et al. (1989). The values of a and b were taken from Pye (1994). The parameter values were varied by ±50%, and the effect on the river concentration Agreement Index determined. No significant difference in Agreement Index was observed. This is due to the small contribution that adsorbed salt has to total salt transport. Adsorbed salt comprises 0,04% of the total salt load from surface runoff, and 0.001% of the total salt load in the river (refer to **Section 5.3.2e**). Due to the insignificant role that salt adsorbed onto sediments has on the overall salt balance, the parameters shown in Table 5.17 were accepted as being adequate without further adjustment.

e) Salt transport model results and discussion

The salt mass balance results for a one-year period is shown in Figure 5.22. Small errors are introduced in the mass balance around the rural agricultural surface and soil due to the programming methods. In order to calculate the salt load irrigated onto the surface during any day, the previous day's river salt concentration is used, which results in a 2.4% error in the mass balance over the rural agricultural surface and a 3.9% error in the salt balance around the rural agricultural soil. A 1.9% error in the salt balance over the river is as a result of the manner in which the river routing model is structured, as described in **Section 5.2.2 d** above.

Selected model outputs (for a 20-year simulation) are shown in Figures 5.23 to 5.31. Some of the figures include the detailed profiles over the last year of the simulation.

Table 5.16: Salt transport model parameter sensitivity analysis results

| Parameter	Change to Agreement Index (%)		Change to correlation coefficient (%)	
	-50%	+50%	-50%	+50%
$ISWP$	0.0067	-0.0074	0.0010	0.0003
$PSWP_n$	-0.3745	0.0883	-0.0151	0.0123
$PSWP_a$	0.0000	0.0000	0.0000	0.0000
C_{sat}	**31.1652 (1)**	**0.0000**	**2.3617**	**0.0000**
$LeachRate$	-0.0047	0.0047	0.0000	0.0000
A	0.0164	-0.0161	-0.0029	0.0032
B	0.9089	0.0061	0.000	-0.0001
F_{void}	0.9083	0.0209	0.0153	-0.0040
r_{soil}	0.0156	-0.0152	-0.0030	0.0034
G_{Us}	-0.0483	0.0487	-0.0114	0.0115
G_{Rns}	**18.8472**	**15.1962**	**0.0165**	**-0.0072**
G_{Ras}	0.7372	0.7703	0.0002	-0.0002

Note (1): The solubility limit was varied between 1 and 75 kg/m³

Table 5.17: Sediment model parameters

Model Parameter	Symbol	Units	Value
Catchment cover density	C_g	-	0.8
Sediment detachment coefficient	K_D	N/mm^2	0.0138
Erosivity factor	K_s	kg/N/m^2	0.5
Loose soil density	r_s	Kg/m^3	1500
Sediment diameter	D_s	mm	0.2
Sediment specific gravity	S_s	-	2.65
First constant in suspended sediment-river flow relationship	a	-	20
Second constant in suspended sediment-river flow relationship	b	-	0.3

For the initial conditions chosen, and the model parameters used (Tables 5.2, 5.4, 5.8, 5.9, 5.11,5.15 and 5.17), it is evident that steady state is achieved after approximately 15 years. The initial conditions used in the simulation were as follows:

- River depth = 5 m

- Soil moisture salt concentration = 0.5 kg/m^3

- Groundwater salt concentration = 0.5 kg/m^3

- Observed groundwater flow = 0.02 mm/d

- Salt storage on urban surface = 30 t/km^2

- Salt storage on rural natural surface = 1 t/km^2

- Salt storage on rural agricultural surface = 64 t/km^2

- Erodible soil depth = 0.005 m

- Loose soil depth = 0.003 m
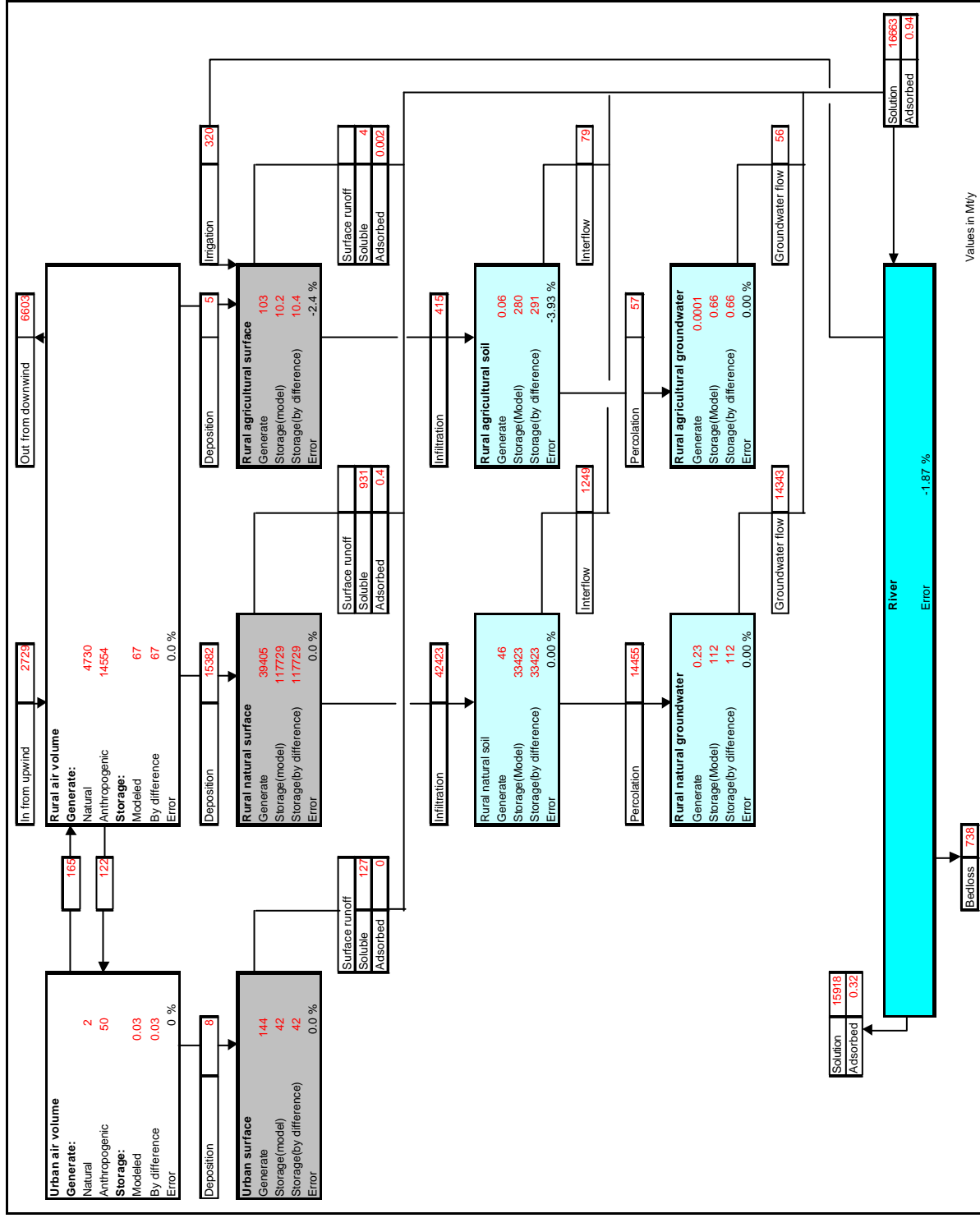
Figure 5.22: Unit catchment salt mass balance
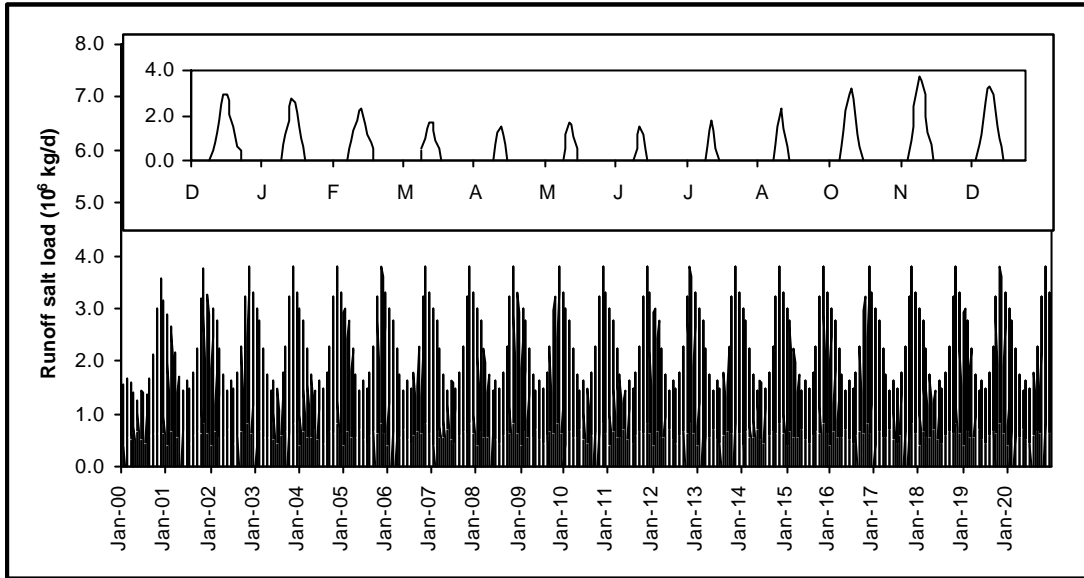
Figure 5.23: Modelled urban surface runoff salt load for a 20-year simulation
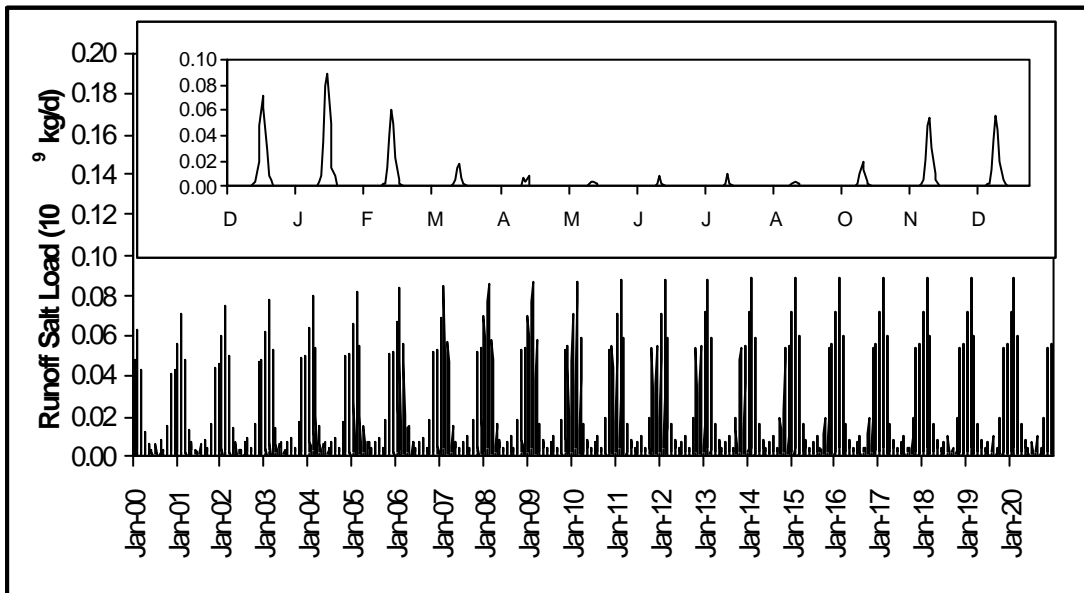
**Figure 5.24: Modelled rural natural surface runoff salt load for a 20-year simulation**
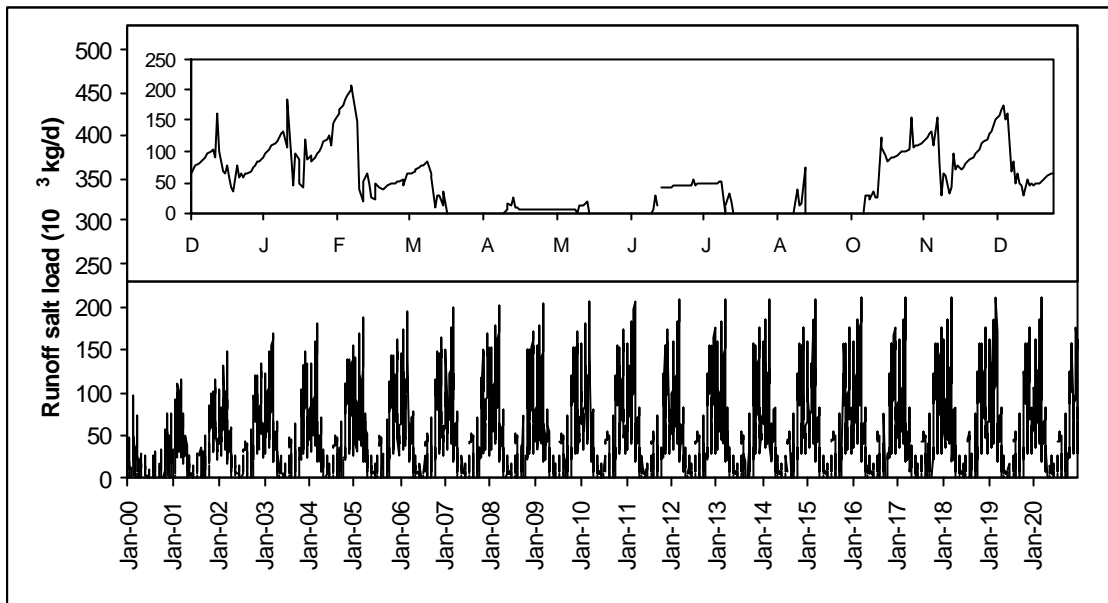
Figure 5.25: Modelled rural agricultural surface runoff salt load for a 20-year simulation
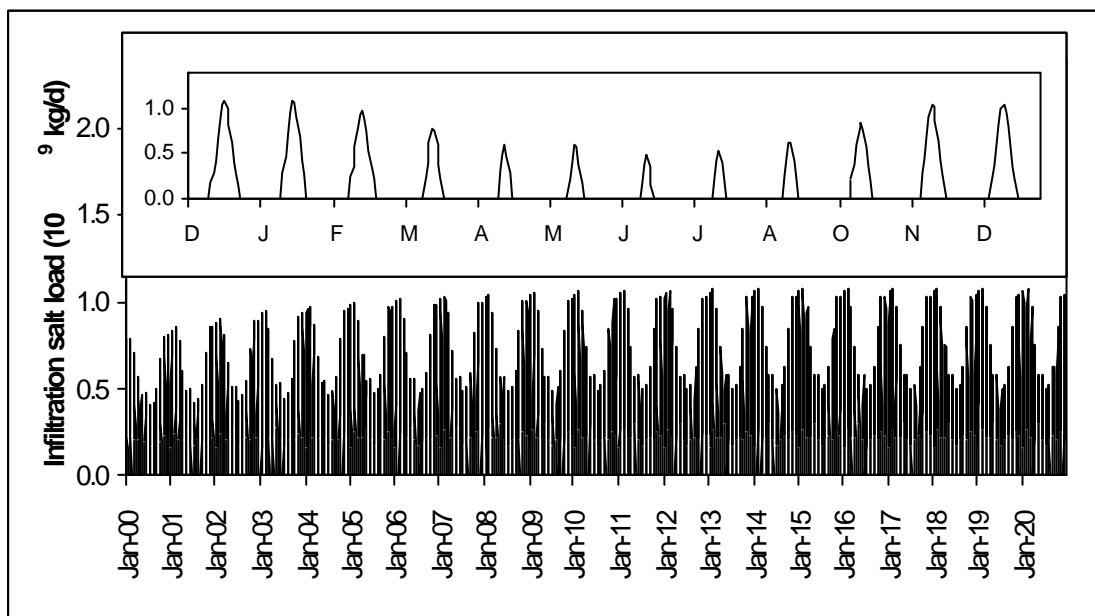

**Figure 5.26: Modelled rural natural infiltration salt load for a 20-year simulation**
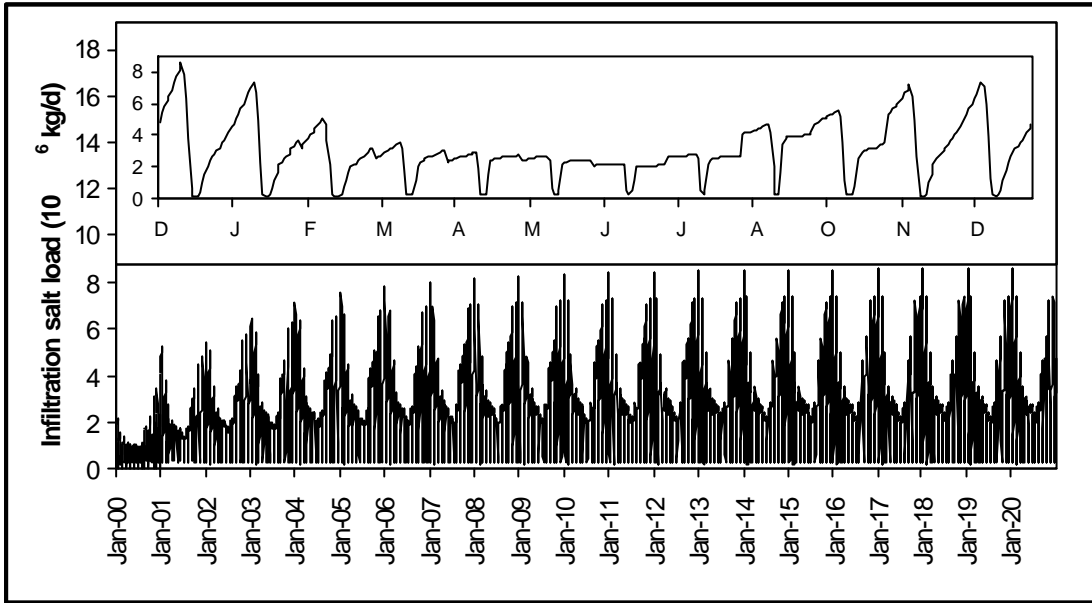
**Figure 5.27: Modelled rural agricultural infiltration salt load for a 20-year simulation**
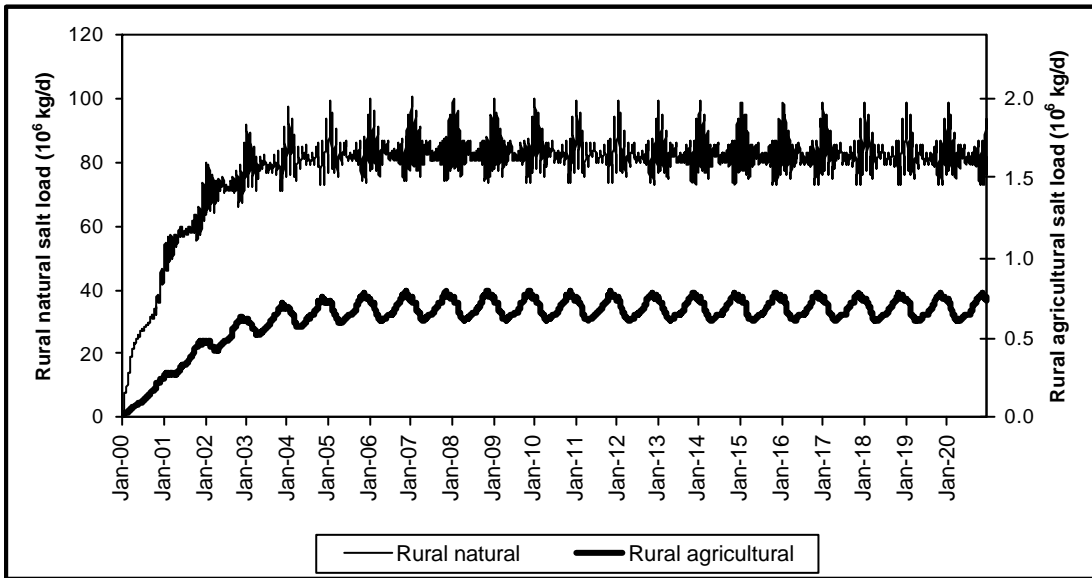
**Figure 5.28: Modelled salt load entering the river from groundwater for a 20-year simulation**
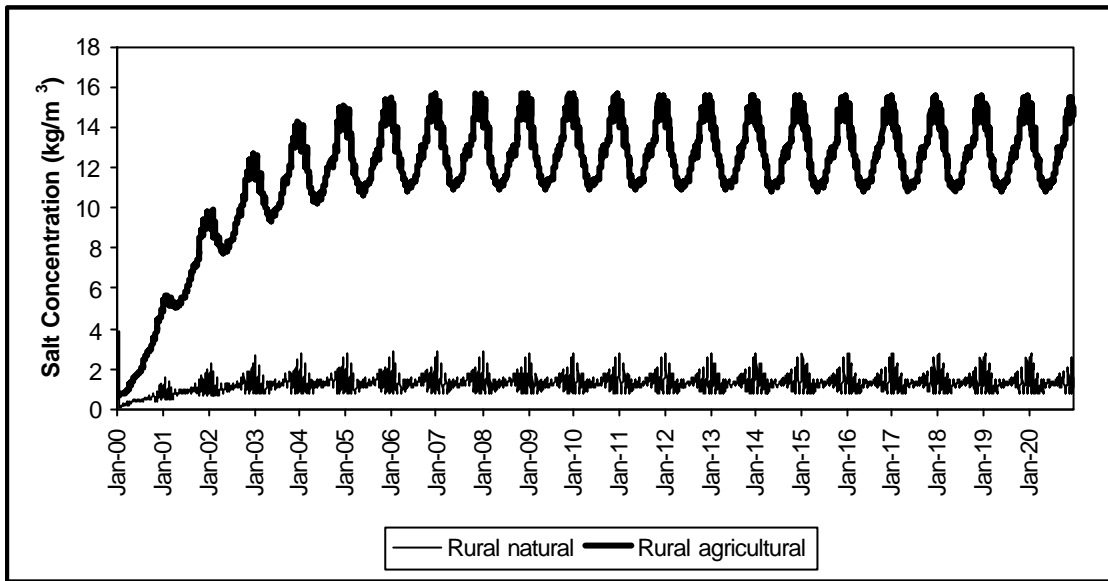
**Figure 5.29: Modelled soil moisture salt concentration for a 20-year simulation**
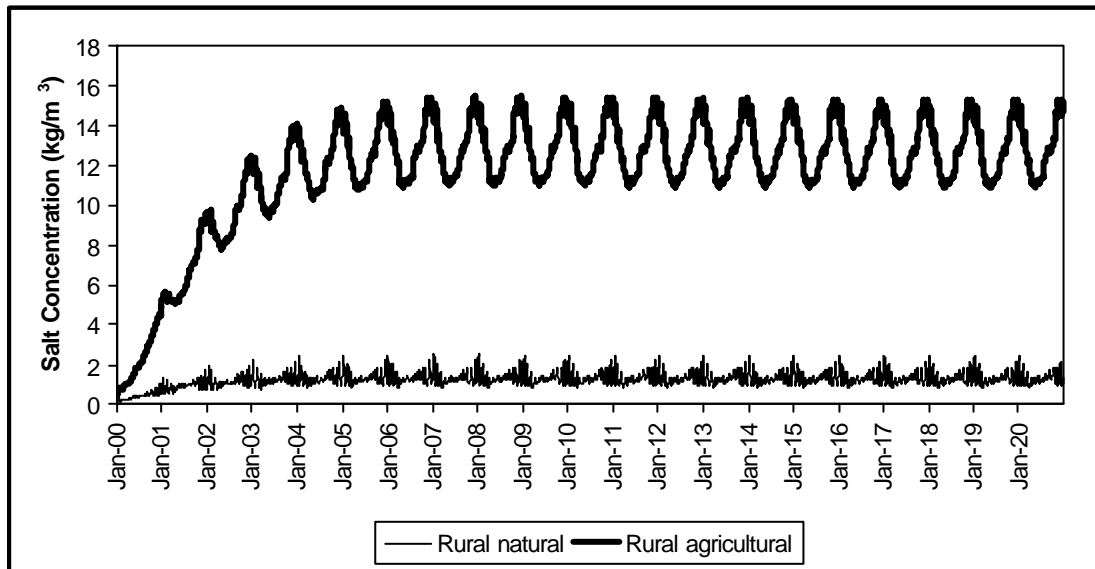
Figure 5.30: Modelled groundwater salt concentration for a 20-year simulation
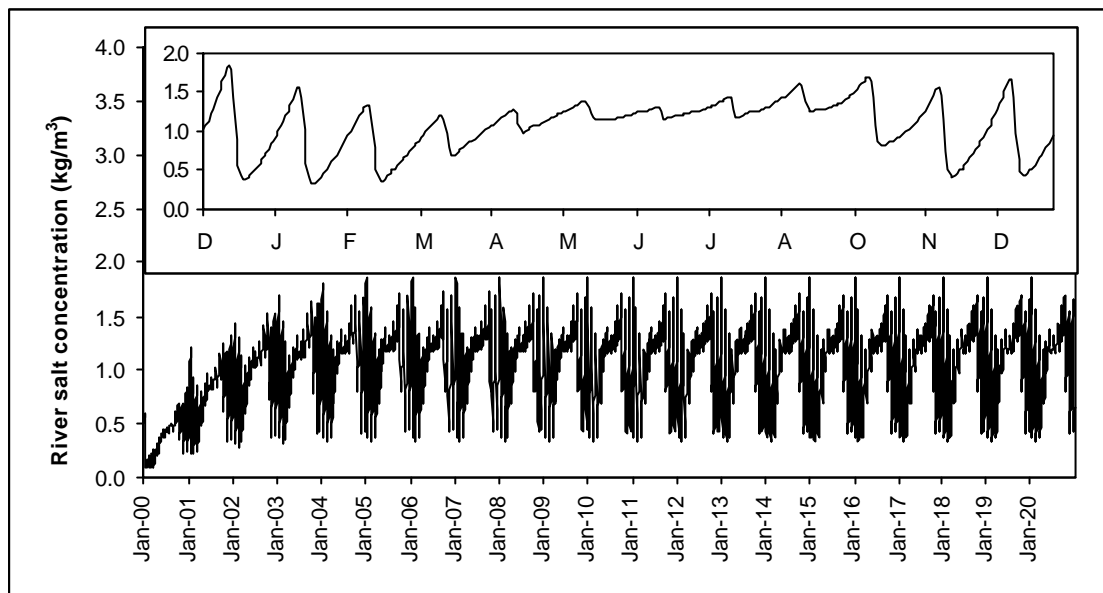
Figure 5.31: Modelled river salt concentration for a 20-year simulation

Changes made to the above initial conditions change the time it takes for the concentrations in the various compartments to reach steady state, however, the ultimate steady state concentrations do not change. The time required to reach steady state is, however, not important in calculating the salinity effects potentials because the potentials are calculated by subtracting the predicted concentrations **without** any emissions into the compartments from the predicted concentrations **with** emissions into the compartments. Only the difference between these two values is important when calculating the salinity potentials. This is discussed in more detail in **Section 5.4**.

The salt load associated with the surface runoff is shown in Figures 5.23, 5.24 and 5.25 (the inserts in these figures show typical annual profiles once steady state has been achieved) for the urban, rural natural and rural agricultural surfaces respectively. Values for the initial salt storage on the rural surfaces were chosen that resulted in steady state being reached in less than 10 years. Steady state is reached much quicker on urban surfaces, because salt is allowed to be washed off as a solid. Wash off of salt and infiltration of salt only occurs when surface runoff and infiltration occurs, which is determined by the minimum ($Z_{\min}$) and maximum ($Z_{\max}$) infiltration rates, rainfall (P_h), soil moisture (S) and soil moisture capacity (ST) according to Equations [4-21] to [4-26]. The influence that irrigation has on the runoff and infiltration salt loads is evident in Figures 5.25 and 5.27 respectively. Irrigation of water from the river, with its associated salt load, results in an increase in the salt load and duration of surface runoff and infiltration.

The same initial soil moisture and groundwater salt concentrations were used in the simulations, and the resulting soil moisture and groundwater salt concentration profiles are shown in Figures

5-52

5.29 and 5.30 respectively. It can be seen that the soil moisture salt concentration reaches steady state before the groundwater salt concentration does. Choosing a higher initial groundwater salt concentration would have resulted in steady state being reached quicker. It is also evident that the sub-surface salt concentrations on the agricultural area are, on average, approximately 10 times higher than those on the natural areas. This is due to the cycling-up effect of irrigation. Even though the subsurface concentrations on the agricultural areas are higher than the natural areas, the salt load associated with the subsurface water entering the surface water (Figure 5.28) is higher for the natural area, due to the small fraction of total surface area that is assumed to be irrigated.

The groundwater salt concentrations are not used in calculating the salinity effects potentials, however, the necessity of including the groundwater compartment in the model is evident from the above figures. Approximately 86% of the salt load in the river originates from the groundwater flow into the river, and only 6% and 8% originate from surface runoff and interflow respectively. It is also evident that salt adsorption has a negligible effect on the transport and distribution of salt in the various compartments. Adsorbed salts make-up, on average, only 0.2% of the total salt mass in the rural agricultural soil, and 0.9% of the total salt in the rural natural soil. Adsorbed salt makes up 0.04% of the total salt load entering the river, and the total adsorbed salt load in the river (as salt adsorbed onto suspended sediment and bed load) makes up only 0.002% of the total salt load in the river.

The average soil moisture and groundwater concentrations in the rural natural and rural agricultural areas at steady state are approximately 2 kg/m^3 and 20 kg/m^3 respectively. Besides the average monthly river flow and concentration data used to verify the model of the hypothetical "unit South African catchment", there are very little data available to verify the concentrations in the soil moisture and groundwater compartments. Some data are available on groundwater total dissolved salts concentrations, and these are given in **Appendix C** The groundwater data set available indicates a range of concentrations from 0.5 to 2.1 kg/m^3, with an average of 1.3 kg/m^3. Total dissolved salt concentrations in the groundwater of several areas in South Africa are in the range 5 to 10 kg/m^3. The rural natural groundwater concentrations fall within the range of reported values, however, the rural agricultural groundwater concentrations predicted by the model appear to be high. This is possibly due in part to the limited data set of measured salt concentrations in irrigated areas, and in part due to the fraction of rural area irrigated (FI) used in the model. The value of FI used in the model was estimated from the "area normally under irrigation" data published by Midgley et al. (1994), and will thus exclude areas where irrigation does take place, but not on a regular basis. The value of FI is thus probably underestimated.

Figures 5.32 to 5.40 show the effects of varying the three most sensitive **hydrological** model parameters on the salt concentrations in the soil and surface water. The figures show the profile over the last year of a 20-year simulation.

Increasing the nominal maximum infiltration rate (Z_{max}) results in a reduction in the volume of surface runoff and an increase in the volume of infiltration, particularly during high rainfall events. The associated salt load infiltrating therefore increases accordingly, resulting in an increase in soil moisture and surface water salt concentrations. The effect on the river salt concentration is a combination of the reduction in salt load entering the river from surface runoff and an increase in subsurface salt load entering the river as Z_{max} increases.

An increase in rainfall interception losses (PI) results in a decrease in the amount of rainfall available for runoff and infiltration, and consequently to a decrease in the soil moisture and surface water flow. The net input of salt from atmospheric deposition, anthropogenic generation and leaching, however, remains virtually the same. The mass of salt leached from the soil decreases because it is a function of soil moisture, but the mass of salt leached is small compared to the other sources of salt. The concentration of salt in the soil moisture and surface water therefore increases.

An increase in the percolation rate at soil moisture capacity (FT) results in a greater subsurface flow at the expense of evaporation and surface flow, particularly during dry periods. The associated salt loads therefore increase accordingly, resulting in higher soil moisture and surface water salt concentrations.
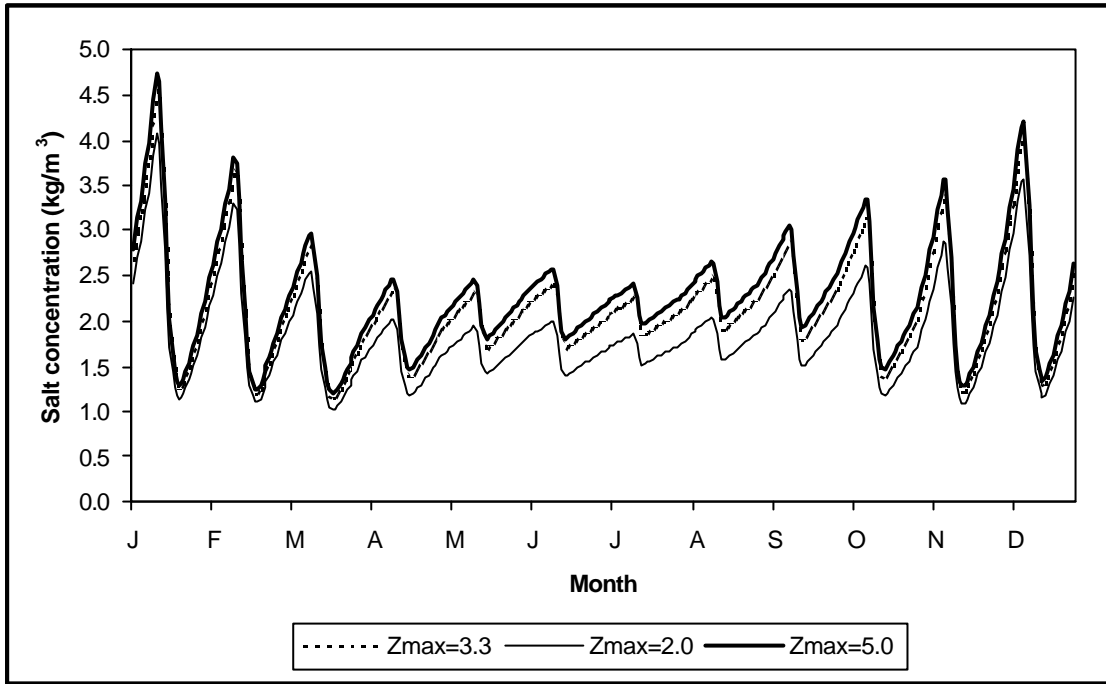
Figure 5.32: Sensitivity of modelled rural natural soil moisture salt concentration to the parameter Z_{max}
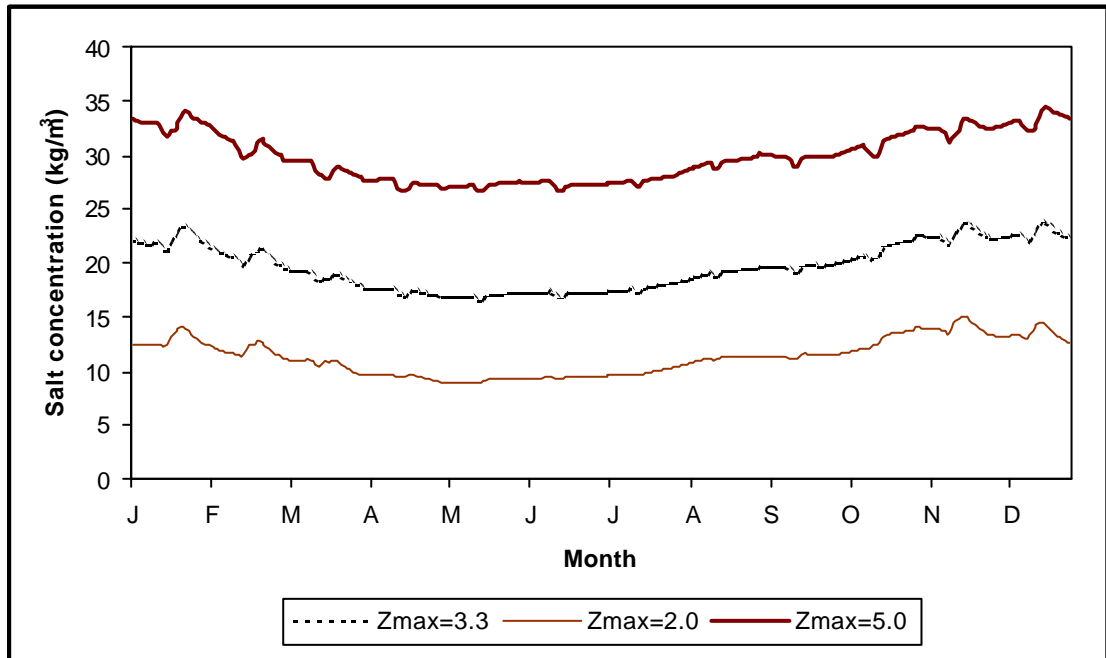

Figure 5.33: Sensitivity of modelled rural agricultural soil moisture salt concentration to the parameter Z_{max}
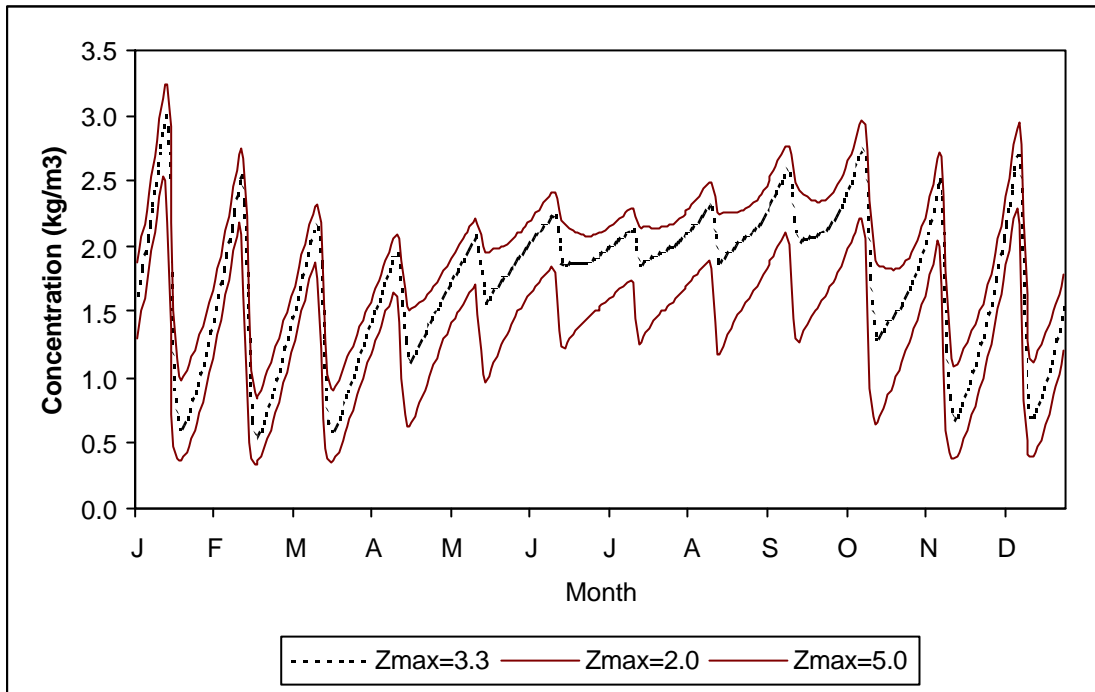
Figure 5.34: Sensitivity of modelled river salt concentration to the parameter Z_{max}
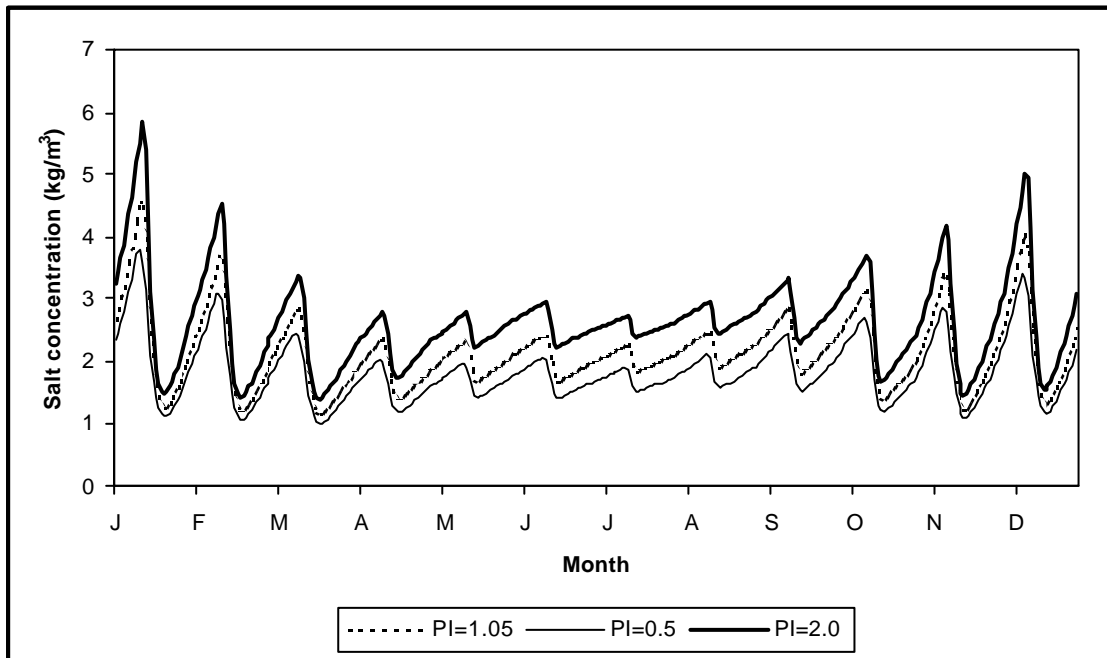

Figure 5.35: Sensitivity of modelled rural natural soil moisture salt concentration to the parameter PI
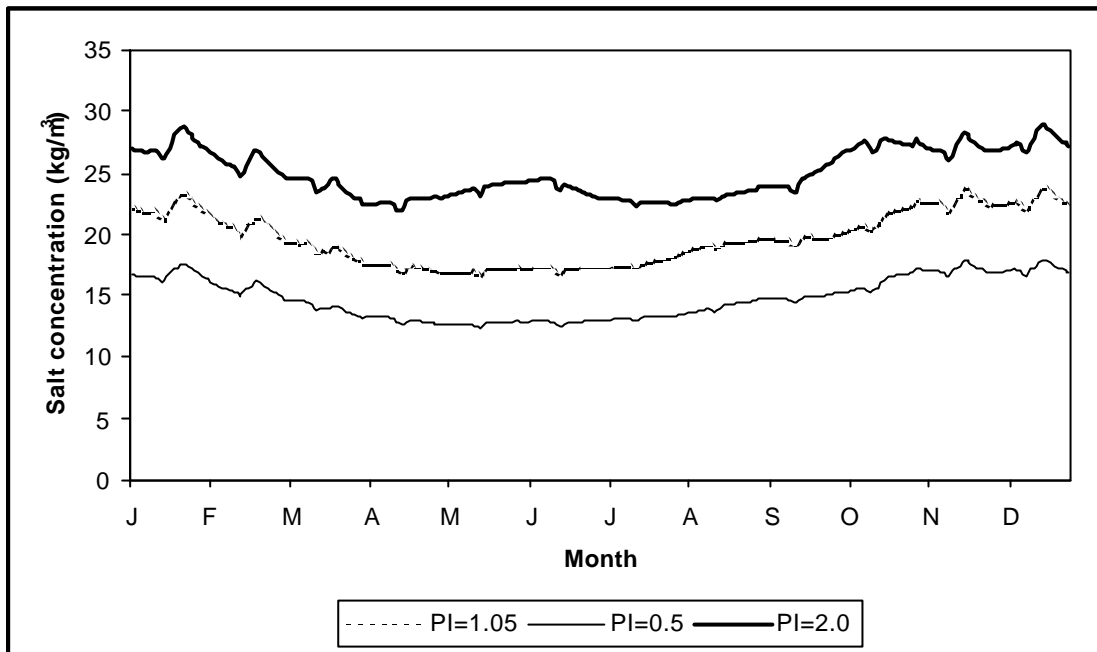
Figure 5.36: Sensitivity of modelled rural agricultural soil moisture salt concentration to the parameter PI
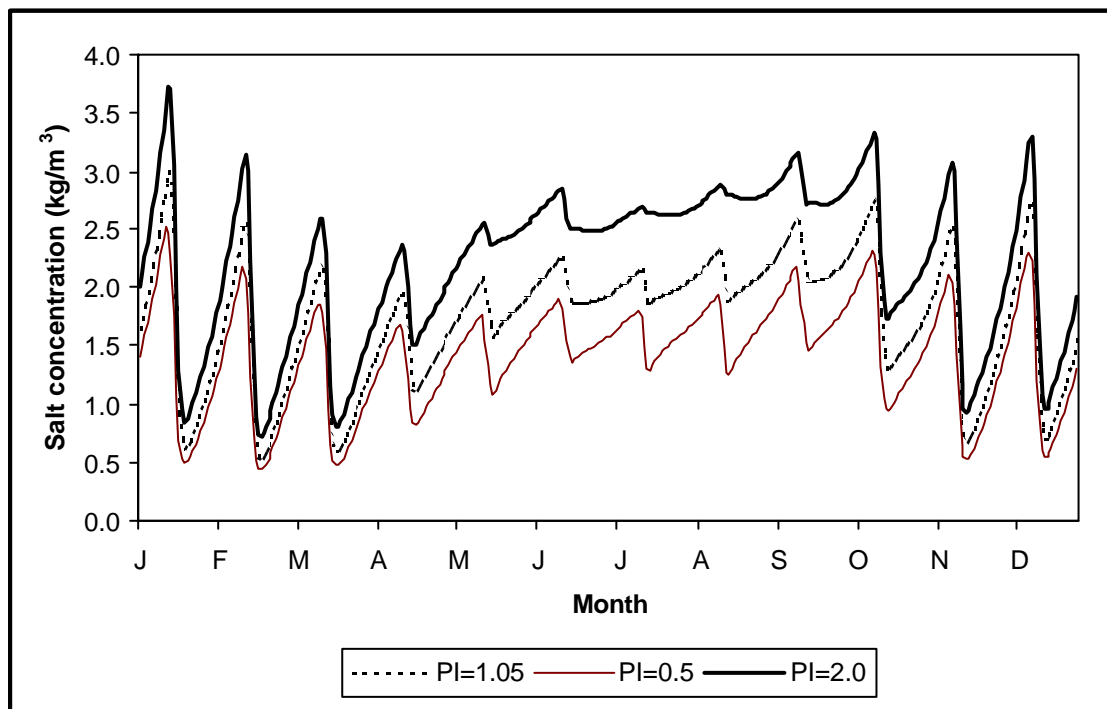
Figure 5.37: Sensitivity of modelled river salt concentration to the parameter PI
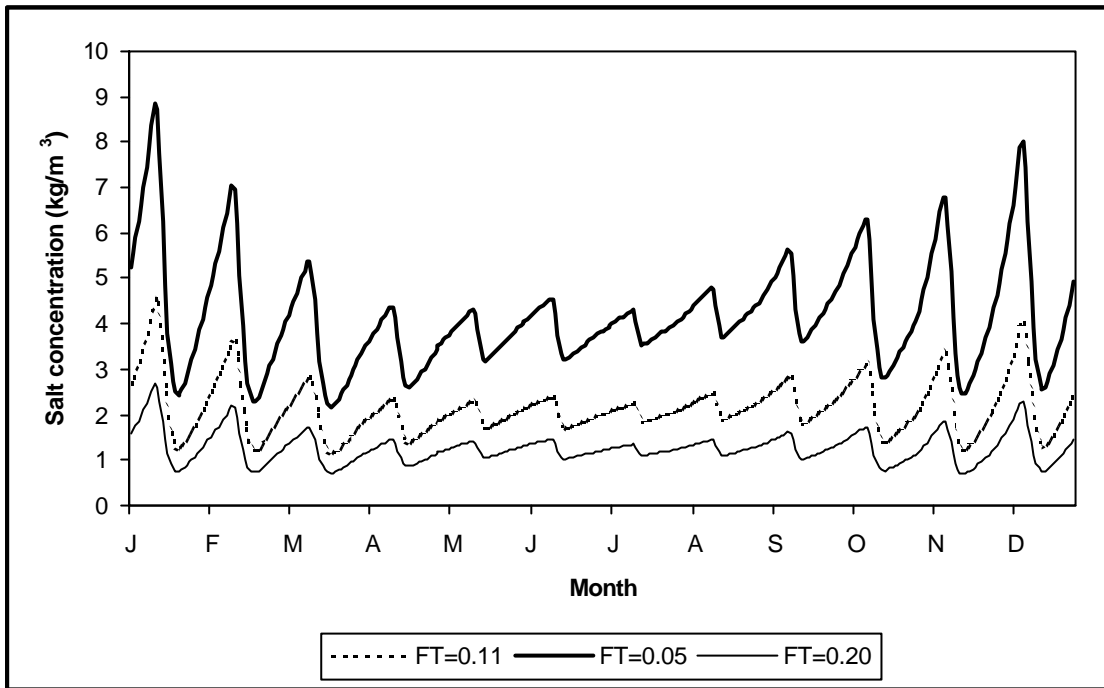
Figure 5.38: Sensitivity of modelled rural natural soil moisture salt concentration to the parameter *FT*
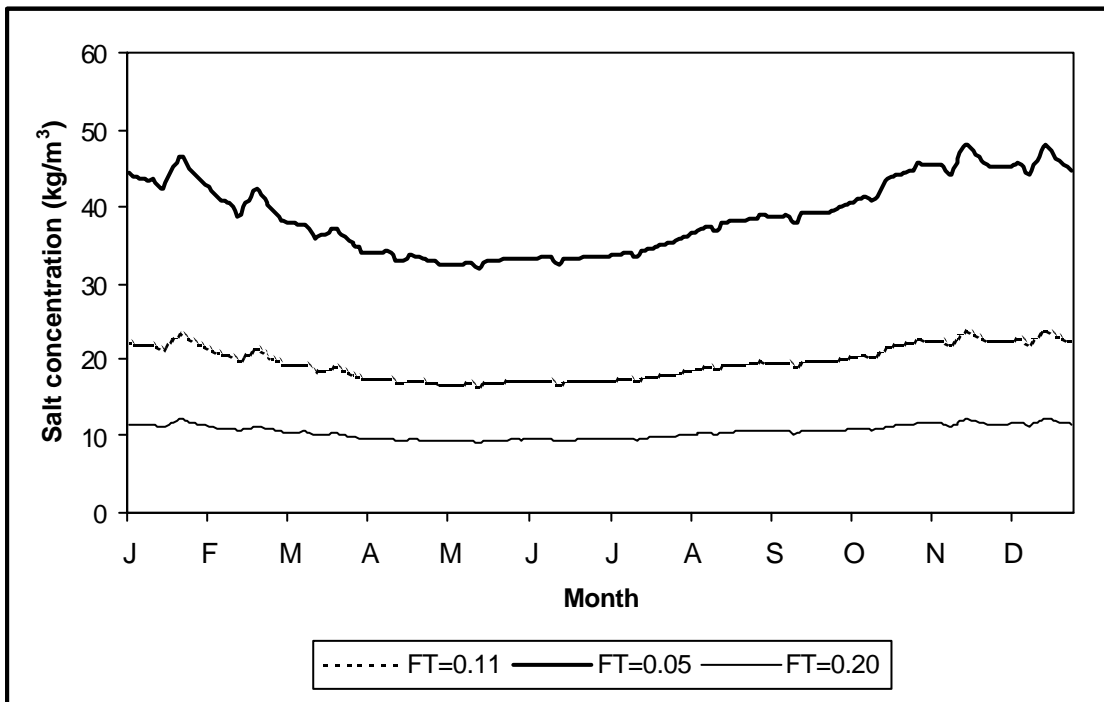

Figure 5.39: Sensitivity of modelled rural agricultural soil moisture salt concentration to the parameter *FT*
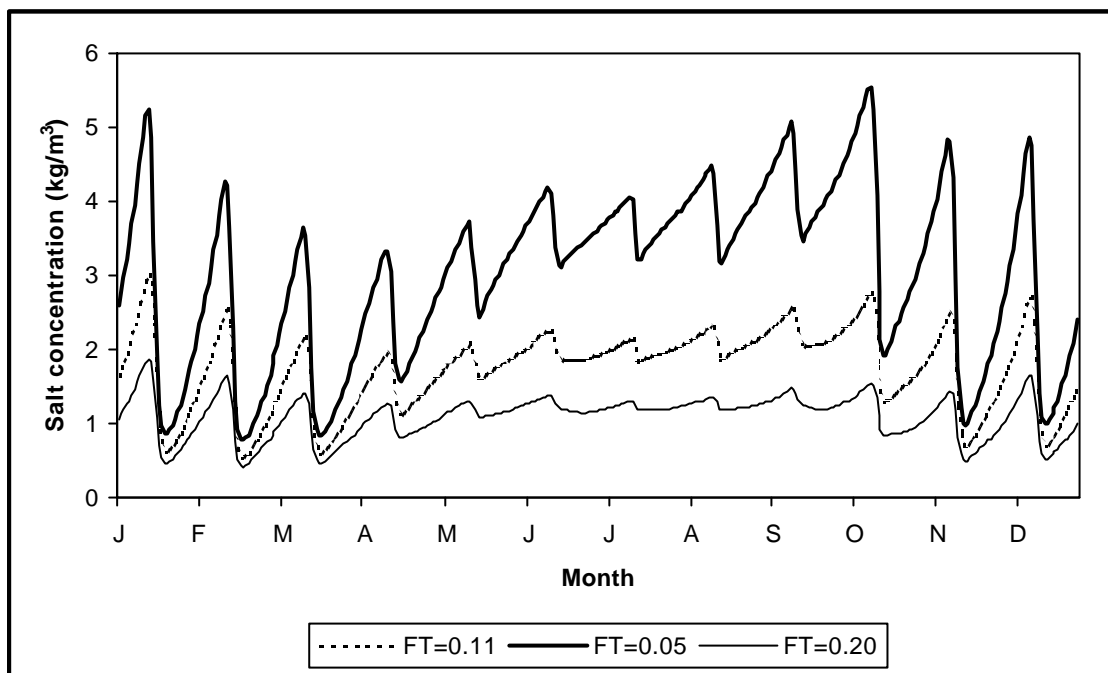
Figure 5.40: Sensitivity of modelled river salt concentration to the parameter FT

Figures 5.41 to 5.46 show the effect of varying the two most sensitive **salt transport** model parameters; the rural natural surface anthropogenic salt generation rate (G_{rns}) and the salt "solubility" (C_{sat}) on the soil moisture and surface water salt concentrations.

Increasing the anthropogenic salt generation rate increases the net salt input into the system and therefore the salt concentrations in the soil moisture and surface water increases.

If the solubility limit of salt in the soil moisture is exceeded, then the concentration of salt in the soil moisture is set equal to the solubility limit, and the appropriate mass of salt is precipitated, which, if sufficient water is available to lower the concentration to below the solubility limit, will re-dissolve. This is evident in Figures 5.44 to 5.46. The concentration of salt in the rural natural soil moisture varies between 1.2 and 4.5 kg/m^3 (all other parameters unchanged), and hence at a solubility limit of 1 kg/m^3, the limit is exceeded at all times, and the concentration in the soil moisture remains equal to the solubility limit. The salt concentration in the rural agricultural soil moisture varies between 16.5 and 23.8 kg/m^3 (all other parameters unchanged), and hence at a solubility limit of 20 kg/m^3, the profile shown in Figure 5.45 is obtained. Any precipitated salt remains in the soil, and therefore if the solubility limit is exceeded, the salt load entering the river will decrease.
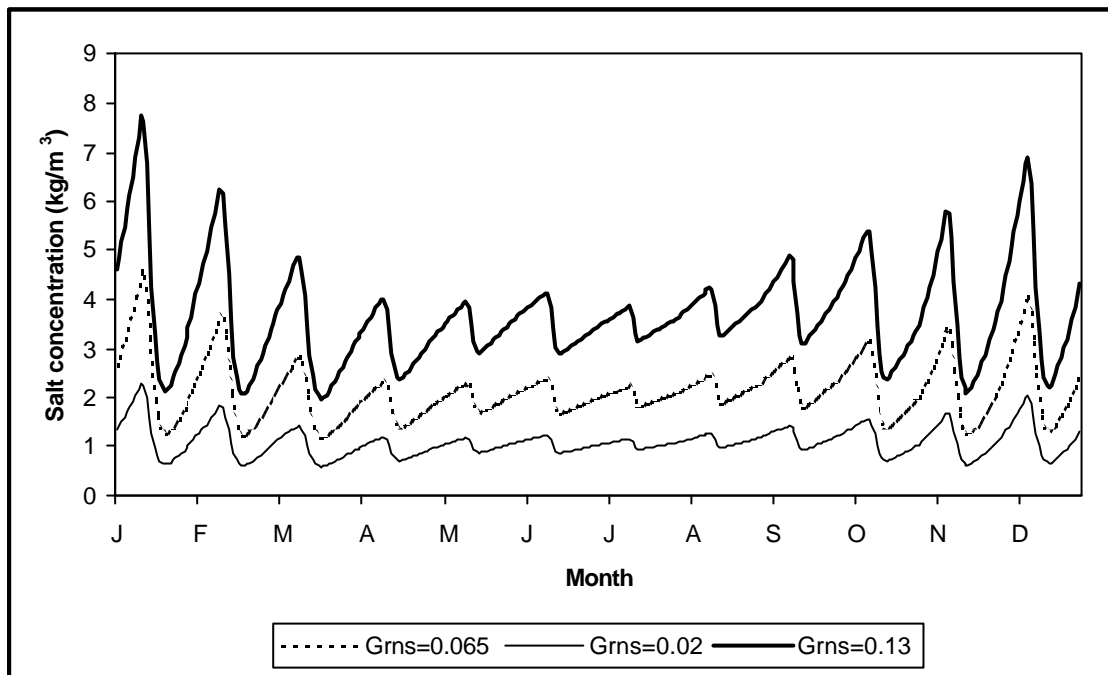
Figure 5.41: Sensitivity of modelled rural natural soil moisture salt concentration to the parameter G_{rns}
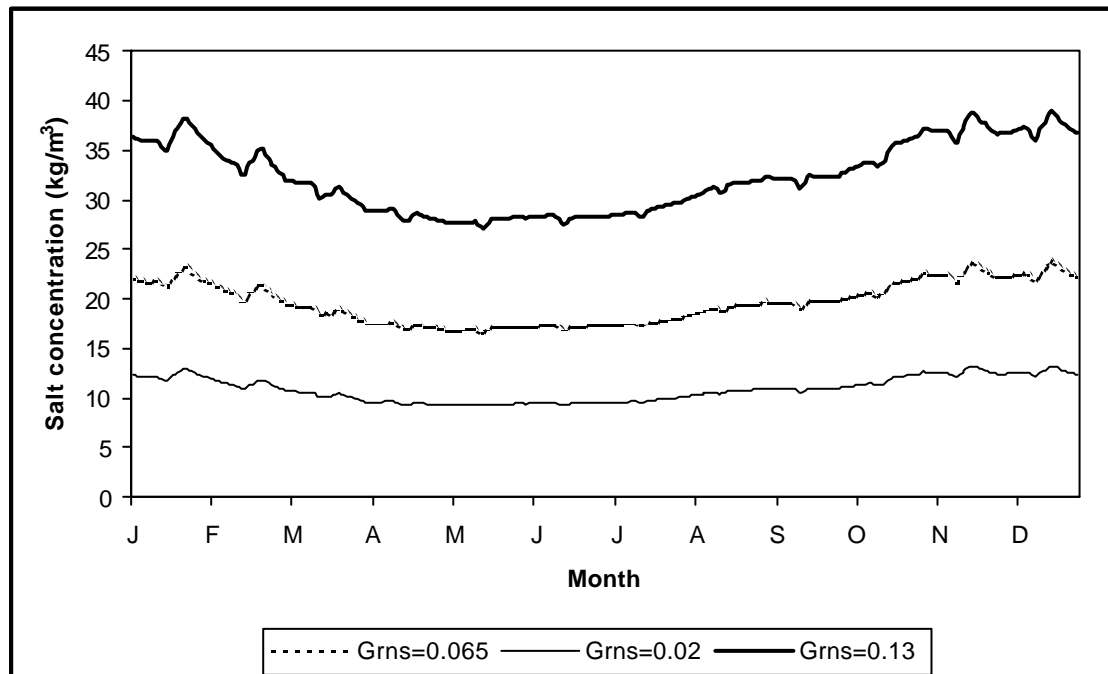
Figure 5.42: Sensitivity of modelled rural agricultural soil moisture salt concentration to the parameter G_{rns}
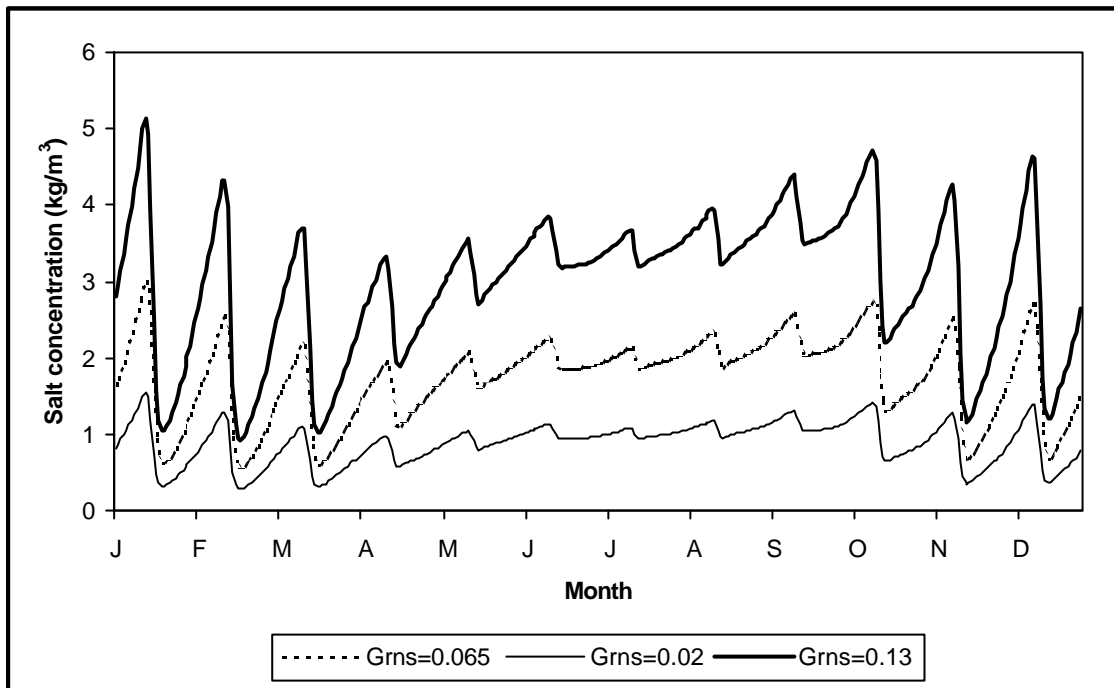
Figure 5.43: Sensitivity of modelled river salt concentration to the parameter G_{rns}
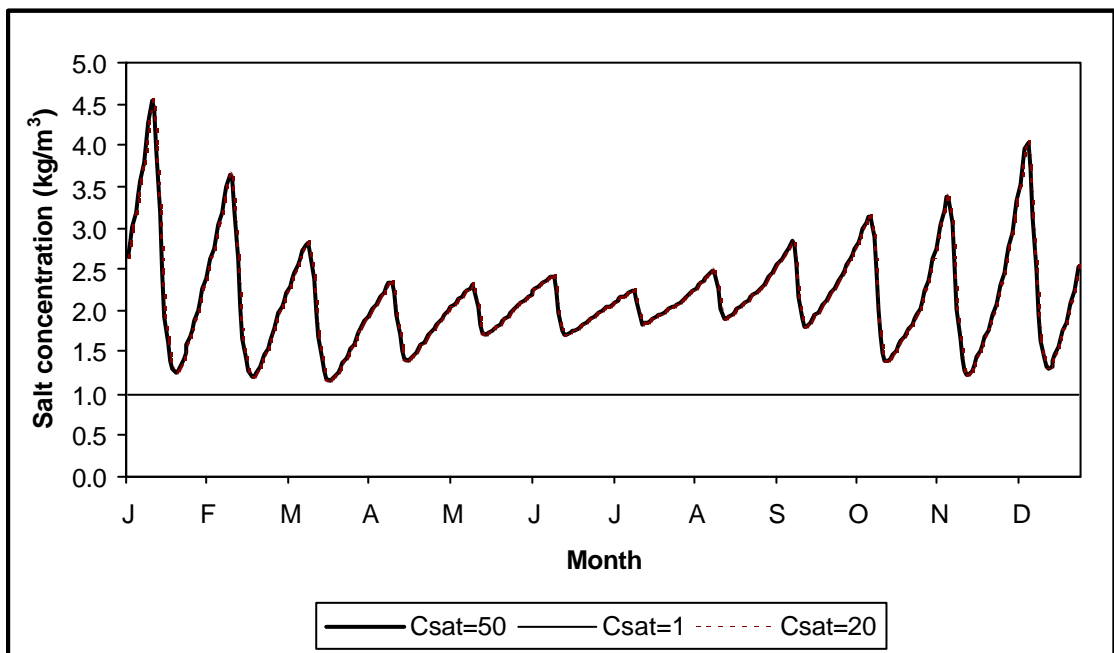

Figure 5.44: Sensitivity of modelled rural natural soil moisture salt concentration to the parameter C_{sat}
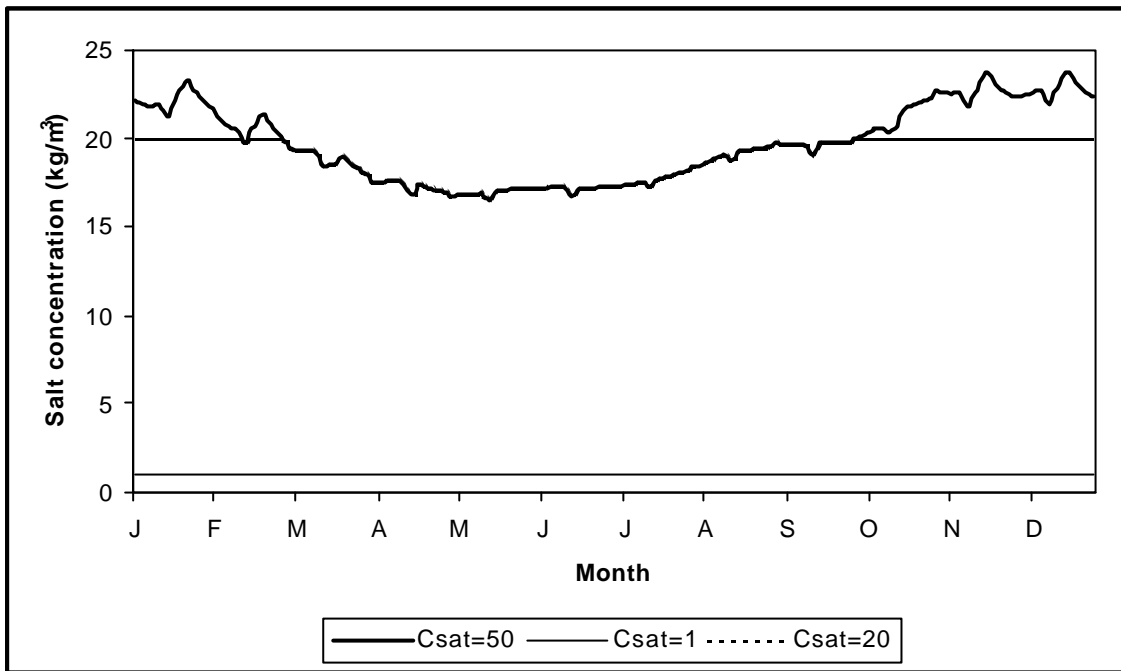
**Figure 5.45: Sensitivity of modelled rural agricultural soil moisture salt concentration to the parameter** C_{sat}
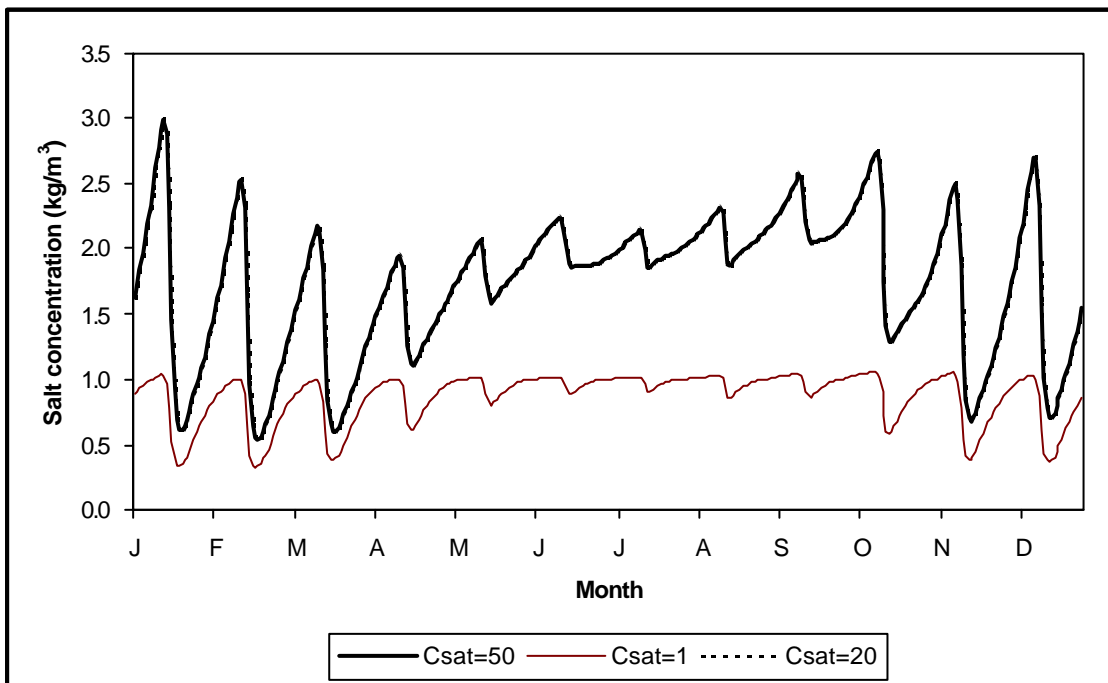
Figure 5.46: Sensitivity of modelled river salt concentration to the parameter C_{sat}

5.4 THE SENSITIVITY OF FATE FACTORS TO MODEL PARAMETERS

The method for calculating effects potentials for salinity impacts is proposed in **Section 3.3.1** (where the definition of symbols are given), and the general equation is given by:

$$Effects\,Potential = Fate\,Factor\,x\,Effect\,Factor$$

[5-2]

Where:

$$Fate\,Factor = \frac{\sum_{i=1}^{N}[PEC_i - PEC_i^0]}{M}$$

[5-3]

$$Effect\,Factor = \frac{1}{PNEC}$$

[5-4]

Fate factors are calculated for each compartment relevant to salinity effects (soil moisture and surface water compartments), for emissions into each initial release compartment (air, soil and surface water).

It has been shown above that parameter values influence the correlation between observed and predicted concentrations and that some parameters influence this correlation more than others. It will be shown below that some parameters in fact influence the values of the fate factors, and again, some parameters more than others. It is therefore important that the correct values for these parameters be chosen to calibrate the model. Understanding the influence that these parameters have on the fate factors also serves as an additional check to ensure that the model results are consistent with what would be expected to occur in reality.

The six most sensitive parameters, in terms of their influence on the correlation between observed and predicted values, were evaluated to determine the sensitivity of the fate factors to these parameters. This was done by running a number of 20-year simulations (2000 to 2020) of

the environmental fate model using different values of the selected parameters, with and without an imposed impulse emission into the various initial release compartments. An impulse magnitude of 1 x 10^8 kg of 1-year duration, starting on 1 January 2002 was used as the basis for comparison. The influence of impulse magnitude, duration and starting date is discussed in detail in **Chapter 7**. The results of the simulations are shown in Table 5.18. The fate factors listed in Table 5.18 are interpreted as follows (using the first line in the table as an example): A 20-year simulation is run with the value of the parameter F_{salt} set equal to 0.3 without an imposed emission, and the concentration profiles in the rural natural soil, rural agricultural soil and river are obtained. The simulation is then repeated with the same value of F_{salt}, but with an imposed emission into the urban air volume of 1×10^8 kg for duration of 1 year starting on 1 January 2002, and the concentration profiles are obtained. The fate factors are then calculated by subtracting the concentration profiles with the imposed impulse emission from those without the imposed impulse emission, summed over the 20-year simulation, and divided by the impulse magnitude.

It is evident that the parameter F_{salt} (the fraction soluble salt associated with aerosols) influences the fate factors significantly when salt is released into the atmosphere, but not when salt is released into the other initial release compartments. A doubling of the parameter F_{salt} results in a doubling of the fate factors when the release occurs into the atmosphere, but only results in an increase in fate factors by a small fraction of a percent when released into other compartments (refer to Table 5.18).

The parameter Z_{max} (maximum infiltration rate) has a significant impact on the fate factors. This parameter, in conjunction with Z_{min} (minimum infiltration rate) determines the frequency and volume of surface runoff events, and thus determines the split between runoff and infiltration flows, with their associated salt loads. The influence that the parameter Z_{max} has on the fate factors is demonstrated by examining its effect on the concentration differential profiles. By way of an example, Figure 5.47 shows the modelled rural agricultural soil moisture salt concentration profile for an impulse emission onto the rural agricultural surface for different values of the parameter Z_{max} (note that the fate factors are the areas beneath the curves shown in Figure 5.47).

Table 5.18: Sensitivity of fate factors to selected model parameters

Parameter	Parameter value	Initial release compartment	Fate Factor (y/m³x10⁸)		
			Rural agricultural soil	Rural natural soil	River
G_A^R (t/km²/d)	0.02	Air	4.90	0.55	0.47
	0.04	Air	4.90	0.55	0.47
	0.06	Air	4.90	0.55	0.47
	0.02	River	63.81	0.00	6.26
	0.04	River	63.81	0.00	6.26
	0.06	River	63.81	0.00	6.26
	0.02	Rural natural soil	11.64	1.41	1.14
	0.04	Rural natural soil	11.64	1.41	1.14
	0.06	Rural natural soil	11.64	1.41	1.14
	0.02	Rural agricultural soil	646.43	0.00	0.45
	0.04	Rural agricultural soil	646.43	0.00	0.45
	0.06	Rural agricultural soil	646.43	0.00	0.45
Z_{max} (mm/h)	1.8	Air	2.41	0.46	0.33
	3.3	Air	4.90	0.55	0.47
	4.95	Air	7.51	0.59	0.55
	1.8	River	38.53	0.00	5.43
	3.3	River	63.81	0.00	6.26
	4.95	River	92.86	0.00	6.81
	1.8	Rural natural soil	5.74	1.16	0.80
	3.3	Rural natural soil	11.64	1.41	1.14
	4.95	Rural natural soil	17.71	1.49	1.31
	1.8	Rural agricultural soil	437.63	0.00	0.28
	3.3	Rural agricultural soil	646.43	0.00	0.45
	4.95	Rural agricultural soil	861.76	0.00	0.69
PI (mm)	0.5255	Air	3.67	0.48	0.39
	1.051	Air	4.90	0.55	0.47
	1.5765	Air	5.61	0.62	0.54
	0.5255	River	49.20	0.00	5.30
	1.051	River	63.81	0.00	6.26
	1.5765	River	72.76	0.00	7.18
	0.5255	Rural natural soil	8.73	1.23	0.94
	1.051	Rural natural soil	11.64	1.41	1.14
	1.5765	Rural natural soil	13.33	1.58	1.32
	0.5255	Rural agricultural soil	598.87	0.00	0.36
	1.051	Rural agricultural soil	646.43	0.00	0.45
	1.5765	Rural agricultural soil	628.02	0.00	0.50

Table 5.18 (continued): Sensitivity of fate factors to selected model parameters

| Parameter	Parameter value	Initial release compartment	Fate Factor (y/m³x10⁸)		
			Rural agricultural soil	Rural natural soil	River
	0.3	Air	2.45	0.28	0.24
	0.6	Air	4.50	0.55	0.47
	0.9	Air	7.34	0.83	0.71
	0.3	River	63.81	0.00	6.26
F_{salt}	0.6	River	63.81	0.00	6.26
(-)	0.9	River	63.81	0.00	6.26
	0.3	Rural natural soil	11.64	1.41	1.14
	0.6	Rural natural soil	11.64	1.41	1.14
	0.9	Rural natural soil	11.64	1.41	1.14
	0.3	Rural agricultural soil	646.43	0.00	0.45
	0.6	Rural agricultural soil	646.43	0.00	0.45
	0.9	Rural agricultural soil	646.43	0.00	0.45
	0.015	Air	4.90	0.55	0.47
	0.03	Air	4.90	0.55	0.47
	0.045	Air	4.90	0.55	0.47
	0.015	River	63.81	0.00	6.26
	0.03	River	63.81	0.00	6.26
G_{Rns}	0.045	River	63.81	0.00	6.26
(t/km²/y)	0.015	Rural natural soil	11.64	1.41	1.14
	0.03	Rural natural soil	11.64	1.41	1.14
	0.045	Rural natural soil	11.64	1.41	1.14
	0.015	Rural agricultural soil	646.43	0.00	0.45
	0.03	Rural agricultural soil	646.43	0.00	0.45
	0.045	Rural agricultural soil	646.43	0.00	0.45
	1	Air	0.00	0.07	0.10
	5	Air	0.00	0.55	0.47
	50	Air	4.90	0.55	0.47
	1	River	0.00	0.00	6.22
	5	River	0.00	0.00	6.22
C_{sat}	50	River	63.81	0.00	6.26
(kg/m³)	1	Rural natural soil	0.00	0.18	0.18
	5	Rural natural soil	0.00	1.41	1.14
	50	Rural natural soil	11.64	1.41	1.14
	1	Rural agricultural soil	0.00	0.00	0.03
	5	Rural agricultural soil	0.00	0.00	0.02
	50	Rural agricultural soil	646.43	0.00	0.45
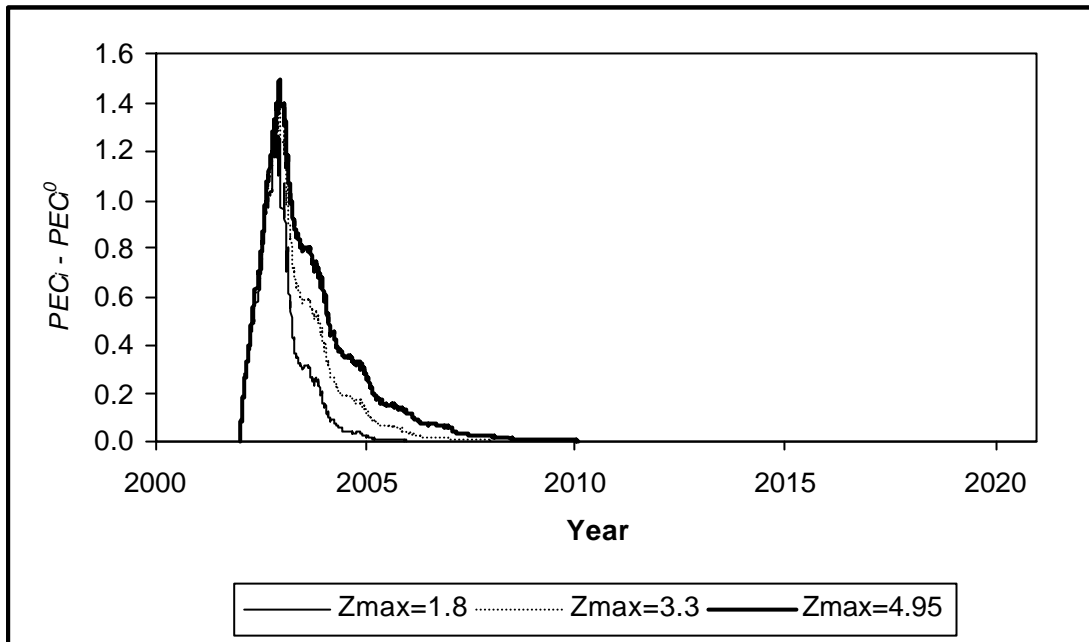
Figure 5.47: Modelled rural agricultural soil moisture salt concentration differential profiles for an impulse emission onto the rural agricultural surface for different values of the parameter $Z_{\max}$ (PEC_i is the salt concentration – in mg/L in the rural agricultural soil moisture after a release onto the rural agricultural surface and PEC_i^0 is the salt concentration – in mg/L - without a release)

It is evident that the concentration differentials are larger for larger values of $Z_{\max}$ and that concentration differentials take longer to reach zero for larger values of $Z_{\max}$, and thus the fate factors are larger for larger values of $Z_{\max}$. The magnitude and duration of the concentration differential is due to the influence that the parameter $Z_{\max}$ has on the split between surface runoff and infiltration and the frequency of runoff and infiltration events, and can be explained by means of an example. If, for example, 100 kg is deposited onto a surface and at a $Z_{\max}$ value of 1.8 mm/h and 80% of the deposited salt leaves the surface as runoff then 80 kg of salt will leave the surface as runoff and 20 kg will infiltrate into the soil moisture. If a $Z_{\max}$ value of 3.3 mm/h results in 50% split between runoff and infiltration, then 50kg will leave the surface as runoff and 50 kg will infiltrate into the soil moisture. If an emission of 50 kg is imposed onto the surface, then at a $Z_{\max}$ value of 1.8 mm/h, 120 kg will leave the surface as runoff and 30 kg will infiltrate. At a

Z_{max} value of 3.3 mm/h, 75 kg will leave the surface as runoff and 75 kg will infiltrate. The differential in mass infiltrating for a Z_{max} of 3.3 mm/h is 10 kg, and for Z_{max} the concentration differential is 25 kg. The salt concentration in the soil moisture is directly related to the mass of salt entering through infiltration, and thus the concentration differential will be larger at higher values of Z_{max}.

It is also evident that for emissions into the river, the fate factors for the rural natural soil are zero for all values of Z_{max} and that for emissions onto rural agricultural soil, the fate factors for rural natural soil are zero for all values of Z_{max}. This is due to the fact that there are no hydrological links from the river to the natural surface or from the agricultural soil to the natural soil.

The explanation for the influence of the parameter PI (rainfall interception loss) on the fate factors is the same as the explanation given above for the influence of the parameter Z_{max} on the fate factors. The split between infiltration and runoff is not only a function of Z_{min} and Z_{max}, but also of net rainfall, as determined by Equations [4-21] to [4-26].

5.5 CONCLUDING REMARKS

The following conclusions are made regarding the environmental fate model development, calibration and parameter sensitivity:

- The non steady state environmental fate model developed can predict environmental concentrations at a daily time-step in all the compartments relevant to the calculation of salinity potentials. The environmental fate model includes all the major processes governing the distribution of common ions in the various compartments. The model results (or outputs) were evaluated and are in agreement with expected behaviour.
- The simple atmospheric deposition model developed cannot be calibrated at a daily time-step due to the lack of data; however, model outputs are in the same order of magnitude as the limited published data.
- Predicted surface water flow and quality correlate well with calculated values for the "unit catchment" as defined. There is however a degree of uncertainty and variability in the calculated values for the "unit catchment", and therefore in the fate factors.
- Simple parameter sensitivity analyses were performed on the various components of the overall model, in an attempt to identify the sensitive model parameters and refine the model calibration. The parameter sensitivity analyses are by no means exhaustive, and it is possible that the same level of agreement between predicted and observed (calculated

for the "unit catchment") can be achieved with a different set of model parameters. The approach adopted in calibrating the model is, however, sound.

- Some model parameters (particularly those that influence the distribution of surface and subsurface flow) do influence the values of the fate factors (and therefore the salinity potentials). The implicit assumption is however that if there is a good correlation between the observed and predicted values, then the resulting fate factors will be correct.

- Although the hydrosalinity model developed has been applied, calibrated and validated in several catchments in South Africa, the combined multimedia fate model applied to the 'unit South African catchment' as developed has not been validated, and can only be done once further data are available.

CHAPTER 6

EFFECTS ASSESSMENT

In this chapter the methodology for determining no-effect concentrations (reciprocal of effect factors) used to determine salinity potentials is presented. In Section 6.1 the methodology generally adopted for determining effect factors is presented and the differences in methodology and approach adopted in this study are highlighted. The fate factors for the various salinity impacts defined in Chapter 3 are discussed and presented in Section 6.2. The no-effect concentrations used to calculate salinity potentials is summarised in Section 6.3.

6.1 INTRODUCTION

The effects potential was defined (by Equation [5-2]) as the product of a fate factor and an effect factor, the effect factor being the reciprocal of the predicted no-effect concentration (or PNEC). In principle, the PNEC is calculated by dividing the lowest short-term LC_{50} (concentration at which 50% of the test organisms die) or long term NOEC (no observed effect concentration) by an appropriate assessment factor. The assessment factors reflect the degree of uncertainty in extrapolating from laboratory toxicity test data for a limited number of species to the "real" environment. Assessment factors applied for long-term results are smaller as the uncertainty of extrapolation from laboratory data to the natural environment is reduced (EC, 1996).

In this study, the South African Water Quality Guidelines (DWAF, 1996) are used as a basis for determining no-effect concentrations. The guidelines specify a target water quality range, within which no measurable adverse effects are expected for long-term continuous use. The target water quality ranges quoted in the South African Water Quality Guidelines (DWAF, 1996) have been derived from quantitative and qualitative criteria, and include assessment factors. No additional assessment factors are therefore applied to the target water quality ranges.

Two different scenarios are evaluated in determining the fate factors (or no-effect concentrations). In the first scenario, the target water quality ranges quoted in the South African Water Quality Guidelines (DWAF, 1996) for the most sensitive species or water use applications are used. This

"worst case" scenario, in effect, means that the water is suitable for all water users without any risk of effects, regardless of the relative scale of a particular water user compared to the total water use. This could if fact mean that no-effect concentrations are selected that protect one particular crop, for example, that may only represent a small fraction of the total crop production in the country. In the second scenario, an "aggregated" no-effect concentration is calculated based on the relative scale of water used for a particular application, and the no-effect concentration for that particular water use. In the calculation of an aggregated no-effect concentration, an attempt is made to determine the concentration that would have no effect on 95% of the water users.

6.2 EFFECT FACTORS

The no-effect concentrations (reciprocal of effect factors) for salinity effects (listed **in Section 3.1.1**) are discussed below, and are based on the South African Water Quality Guidelines (DWAF, 1996)

6.2.1 Aquatic ecotoxicity

Plants and animals possess a wide range of physiological mechanisms and adaptations to maintain the necessary balance of water and dissolved ions in cells and tissues. This ability is extremely important in any consideration of the effects of changes in total dissolved salts on aquatic organisms. The individual ions making up the total dissolved salts also exert physiological effects on aquatic organisms. Changes in concentration of the total dissolved salts can affect aquatic organisms at three levels, namely:

- effects on, and adaptations of, individual species;
- effects on community structure; and
- effects on microbial and ecological processes such as rates of metabolism and nutrient cycling.

The rate of change of the total dissolved salts concentration, and duration of change, appears to be more important than absolute changes in the total dissolved salts concentration, particularly in systems where the organisms may not be adapted to fluctuating levels (DWAF, 1996).

The South African Department of Water Affairs and Forestry guidelines for the impact of total dissolved salts on aquatic ecosystems are as follows:

- Total dissolved solids concentrations should not be changed by more than 15% from the normal cycles of the water body under unimpacted conditions at any time of the year.
- The amplitude and frequency of natural cycles in total dissolved solids concentrations should not be changed.

In view of the above, no single value is used for the aquatic ecotoxicity no-effect concentration. The no-effect concentrations are calculated as a function of the background salt concentration. The aquatic ecotoxicity effects potential ($AEEP$) for the "worst case" scenario is therefore calculated as follows (where the subscript irc refers to the initial release compartment):

$$AEEP_{irc} = \frac{\sum_{i=1}^{N}[PEC_i^R - PEC_i^{R,0}]}{1.15\,PEC_i^{R,0}\,M^R} \qquad\qquad [6\text{-}1]$$

For the "aggregated" scenario, the no-effect concentration was calculated as follows:

$$AEEP_{irc} = \frac{\sum_{i=1}^{N}[PEC_i^R - PEC_i^{R,0}]}{1.2\,PEC_i^{R,0}\,M^R} \qquad\qquad [6\text{-}2]$$

The assumption inherent in Equation [6-2], is that 95% of aquatic organisms will not be affected by a 20% increase in the salt concentration.

6.2.2 Livestock production

Guidelines for the effects of total dissolved salts on livestock, issued by the South African Department of Water Affairs and Forestry (DWAF, 1996) are shown in Table 6.1.

For the "worst case" scenario, a no-effect concentration of 1 kg/m^3 was chosen. For the "aggregated" scenario, the lower concentrations of the ranges in the category 000+ were chosen as no-effect concentrations for each type of livestock and the concentration at which 95% of the

numbers of livestock (shown in Table 6.2) was extrapolated. A value of 1.09 kg/m^3 was used for the "aggregated" no-effect concentration.

Table 6.1: Guidelines for the effects of total dissolved salts on livestock (DWAF, 1996)

TDS (kg/m^3)	Sheep	Beef	Dairy	Pigs and poultry
0 - 1	0000	0000	0000	0000
1 – 2	0000	0000	000+	000+
2 – 3	0000	000+	000+	00++
3 – 4	000+	000+	00++	0+++
4 – 5	000+	000+	0+++	++++
5 – 6	000+	000+	0+++	++++
6 – 7	00++	00++	++++	++++
7 – 10	00++	0+++	++++	++++
10 – 13	00++	++++	++++	++++
>13	0+++	++++	++++	++++

Legend

Effects (E) are dependent on the Action (A):

0000		Target water quality guideline
	E	No significant adverse effects
	A	Immediate access allowed without any previous exposure to saline waters
000+	E	Possible initial reluctance to drink, but should be temporary. No significant adverse effects
	A	Immediate access allowed with previous exposure to saline water.
	E	Initial reluctance to drink may lead to a decline in water intake, and subsequently production. However, the stock should adapt within a relatively short period of time (within a week) and return to normal production level.
	A	Immediate access allowed without any previous exposure to saline waters.
00++	E	Care should be taken when allowing stock access to these waters, specifically for intensive systems. Initial reluctance to drink may lead to a decline in water intake and subsequently production. However, the stock should adapt to the water within a relatively short period of time (within a week) and return to normal production levels. Increased need to adapt stock to salinity levels.
	A	Immediate access allowed only with previous exposure to saline waters.
0+++	E	Production will in all likelihood decline significantly. Stock should survive (at maintenance level) and recover when offered water with TDS within the target water quality level, provided exposure is not too long. Increased need to adapt stock to salinity levels. Some species can tolerate once adapted.
	A	Immediate access allowed only with previous exposure to saline waters for a limited period of time.
++++	E	Extreme caution should be taken when allowing stock access to these ranges. Some species can tolerate once adapted.
	A	No immediate access allowed. Stock must be adapted incrementally to water.

Table 6.2: Calculation of no-effect concentrations for livestock watering

Livestock	Numbers (1)	No-effect concentration (kg/m^3)
Cattle	1.35×10^7	2
Sheep	2.54×10^7	3
Pigs	1.59×10^6	1
Goats	2.43×10^6	3
Poultry	5.18×10^7	1

(1) NDA, 2002

6.2.3 Agricultural crops

Crop yield loss is directly related to total dissolved salts concentration above a certain threshold concentration. Threshold and yield loss relationships for many species of plans are published in the literature. The major crops grown in South Africa are listed in Table 6.3, which also contains the threshold concentrations for these crops. In the literature reviewed, the crops most sensitive to salinity are beans and carrots, with threshold concentrations of 0.455 kg/m^3, and this value was used for the "worst case" scenario.

For the "aggregated" scenario, the concentration at which 95 % of the crops are unaffected was extrapolated from the total annual production and no-effect concentrations shown in Table 6.3. A value of 1.01 kg/m^3 was used for the "aggregated" scenario.

6.2.4 Damage to man-made environment

The norms used by the South African Department of Water Affairs and Forestry to measure the suitability of water supply, in terms of the presence of dissolved salts are (DWAF, 1996):

- the extent of damage caused to equipment and structures as a result of dissolved salts;
- the extent to which the dissolved solids in the water supply interfere with industrial processes;
- the extent of impairment of product quality caused by the presence of dissolved salts; and

- the degree of complexity involved in the treatment and/or disposal of wastes generated as a result of the presence of dissolved salts.

The Department of Water Affairs and Forestry have defined 4 categories of processes according to the degree to which they are affected by the presence of dissolved salts. Category 1 processes require high quality water, while category 4 processes require low quality water. The target water quality ranges for category 1 to category 4 processes are shown in Table 6.4.

Within the target water quality ranges, no effects on equipment and structures, interference with processes, product quality and complexity of waste treatment are expected. For the "worst case" scenario, a no-effect concentration of 0.1 kg/m^3 was used.

Table 6.3: Calculation of no-effect concentration for agricultural crops

Crop	Production (tons)(1)	No-effect concentration (kg/m^3)	Reference	Comments
Maize	8 040 000	1.105	Barnard et al., 1998	-
Wheat	2 316 000	5.590	Barnard et al., 1998	Grain
Sugar cane	21 659 000	1.105	Maas., 1990	-
Grain sorghum	211 000	4.420	Barnard et al., 1998	
Ground nuts	74 000	2.080	Maas, 1990	Peanuts
Sunflower	677 000	1.495	Kotby-Amacher et al., 1997	-
Deciduous and other soft fruit	1 484 000	0.930	Kotby-Amacher et al., 1997	Average of 15 fruits
Citrus fruit	1 529 000	1.105	Maas, 1990	Oranges
Subtropical fruit	58 8000	1.110	Maas, 1990	-
Vegetables	2 093 000	2.037	Kotby-Amacher et al., 1997	Average of 23 vegetables
Potatoes	1 655 000	1.105	Barnard et al., 1998	
Soya beans	2 247 000	3.250	Barnard et a.l, 1998	Grain
Oats	22 000	3.380	Kotby-Amacher et al., 1997	-
Barley	161 000	5.200	Barnard et al., 1998	Grain
Rye	2 000	7.410	Barnard et al., 1998	Grain
Dry beans	111 000	0.650	Barnard et al., 1998	Seeds/pods
Cowpea	5 600	1.040	Barnard et al., 1998	Shoots
Cotton	32 182	5.005	Maas, 1990	-
Tobacco	34 000	1.105	Kotby-Amacher et al., 1997	-

(1) NDA, 2002, values are in tons produced in 2002

An industry may consist of any or all of the categories of processes, and in order to calculate the concentration at which 95% of the water users categories would not experience any adverse effects, one would need to know the water usage for each category for each industry in South Africa. This information is not available and it was assumed that at a concentration of 0.2 kg/m^3, 95% of the water use categories would not experience any adverse effect.

Table 6.4: No effect concentrations for various categories of industrial processes (DWAF, 1996)

Category	Target Water Quality Range (kg TDS/m^3)
Category 1	0 – 0.10
Category 2	0 – 0.20
Category 3	0 – 0.45
Category 4	0 – 1.60

6.2.5 Natural vegetation

No data are available on the effect of dissolved salts on natural vegetation in South Africa. Most riparian plants in Australia can tolerate salinities greater than 5 kg/m^3, and sensitive species will only be adversely affected by salinities above 2 kg/m^3. In the United States it has been proposed that, for the protection of wildlife habitats, salinity should not vary by more than 1 kg/m^3 in water where the natural salinity is below 3.5 kg/m^3 (WRC, 2000b). Threshold salinity limits for 27 different grasses and forage crops are reported by Maas (1990). Values vary from 0.98 kg/m^3 to 4.49 kg/m^3, with an average of 2.15 kg/m^3. For the "worst case" scenario a no-effect concentration of 0.98 was used to calculate effects potentials. For the "aggregated" scenario, a no-effect concentration of 2 kg/m^3 was assumed.

6.2.6 Wildlife

High (> 3 kg/m^3) salinities may have an effect on the productivity and reproductive capacity of wildlife. This may be the case for the more sensitive animals, but at salinities below 1.2 kg/m^3 there will be no real effect on animals and birds (WRC, 2000b). Drinking water criteria for livestock and poultry are acceptable as criteria for wildlife (WRC, 2000b). A value of 1.2 kg/m^3 was assumed for the "worst case" scenario, and a value of 3 kg/m^3 was assumed for the aggregated scenario.

6.2.7 Aesthetic effects

The South African Water Quality Guidelines for the effects of salinity on human health, household distribution systems and water heating appliances are given in Table 6.5.

Aesthetic effects generally encompass taste, odour and colour. Dissolved salts do not impart colour or odour to water, and therefore the no-effect concentration for aesthetic effects is for taste only. A value of 0.45 kg/m^3 was used to for the "worst case" scenario, and a value of 2 kg/m^3 was used for the "aggregated" scenario.

Table 6.5: Effects of dissolved salts on human health, aesthetics, household distribution systems and water appliances (DWAF, 1996).

TDS range (kg/m^3)	Aesthetic/Economic effects	Health effects
0 – 0.45	The taste threshold for dissolved salts in water is in the region of 0.3 kg/m^3, hence a slightly salty taste may be detected above this concentration. The threshold varies according to salt composition. No effect on plumbing or appliances.	No health effects.
0.45 – 1.00	Water has a noticeably salty taste, but is well tolerated. No effects on plumbing or appliances.	No health effects are likely.
1.00 – 2.00	Water has a marked salty taste and would probably not be used on aesthetic grounds if alternative supplies are available. Some effects on plumbing and appliances, such as increased corrosion or scaling may be detected.	Consumption of water does not appear to produce adverse health effects in the short term.
2.00 – 3.00	Water tastes extremely salty. Corrosion and/or scaling of pipes and appliances will increase.	Short-term consumption may be tolerated, but with probable disturbance of the body's salt balance.
> 3.00	Water tastes extremely salty and bitter. Effects such as scaling and/or corrosion increase.	Short-term consumption leads to disturbance of the body's salt balance. At high concentrations, noticeable short-term health effects can be expected.

6.3 SUMMARY

Table 6.6 summarises the no effect concentrations used to calculate salinity potentials, and ultimately the total salinity potential (in **Chapter 7**) for the "worst case" scenario and the "aggregated" scenario.

Table 6.6: Summary of no-effect concentrations

Potential salinity impact	No-effect concentration (kg/m^3)	
	Worst case	Aggregated
Effects of aquatic environment	<15 % increase	<20 % increase
Effects on livestock production	1.00	1.09
Effects on agricultural production	0.46	1.01
Damage to man-made environment	0.10	0.20
Effects on natural vegetation	0.98	2.00
Effects on wildlife	1.20	3.00
Aesthetic effects	0.45	2.00

CHAPTER 7

SALINITY POTENTIALS

In this chapter the calculated salinity potentials are presented and discussed. In environmental life cycle assessment, the magnitude of the emission impulse is determined during the life cycle inventory step. The temporal distribution of the impulse emission is, however, not known. In Section 7.1 the effects that impulse characteristics have on the values of the salinity potentials is evaluated in order to confirm that salinity potentials are linearly related to impulse magnitude, and that salinity potentials are not a function of the temporal distribution of the impulse emission. In Section 7.2, the calculated salinity potentials are presented and discussed. The effect that the inclusion of a salinity impact category has on the types of decisions that life cycle assessment support are evaluated by reworking the example presented in Chapter 2. The methodology and results of the method developed to include salinity in environmental life cycle assessment is evaluated in terms of the requirements for defining new impact categories, which were presented in Section 2.3. Finally, in Section 7.3, a discussion of the uncertainty associated with the results is presented and forms the basis for determining recommendations for further work.

7.1 THE EFFECTS OF IMPULSE CHARACTERISTICS ON SALINITY POTENTIALS

The life-cycle inventory stage of a life-cycle assessment results in a list of substances released into the environment and the total mass of these substances released, or in other words, an impulse emission. The temporal and spatial distribution of the impulse emission is generally unknown. Spatial distribution is taken into account in the model developed, by defining a "unit linity potentials are therefore only relevant to the catchment, as defined. Regarding temporal distribution, the date on which the impulse emission

starts, and the duration of the impulse is generally not known. The analysis presented below will demonstrate that this information is not required for the calculation of salinity potentials.

7.1.1 Impulse magnitude

Firstly, the linearity of the salinity potentials needs to be confirmed. In other words, the value of the salinity potential due to a release of y kg of salt into the environment should be half the value if $2y$ kg is released into the environment.

A number of 20-year (7 300 d) simulations were done with varying impulse magnitudes into the initial release compartments. The impulse duration was arbitrarily set at 1 year. The results are shown in Table 7.1

Table 7.1: Effect of impulse magnitude on effects potentials

Impulse magnitude (kg)	Impulse starting date	Impulse duration (y)	$\sum_{i=1}^{7300}[PEC_i - PEC_i^0]$		
			Rural agricultural soil moisture	Rural natural soil moisture	River
1×10^4	1 January 2001	1	0.0727	0.00020	0.0008
1×10^5	1 January 2001	1	0.7268	0.00198	0.0083
1×10^6	1 January 2001	1	7.2678	0.01987	0.0833
1×10^8	1 January 2001	1	726.7805	1.9687	8.3276
1×10^{10}	1 January 2001	1	41612.57	196.86	812.16
1×10^{12}	1 January 2001	1	259328.48	19676.64	78532.96

It is evident from Table 7.1 that the sum of the difference in predicted environmental concentrations over the simulation period (and hence the effects potentials) are a linear function of impulse magnitude up to an impulse magnitude of 1×10^8, but at higher impulse magnitudes this is not the case. At higher impulse magnitudes, the solubility limit in the rural agricultural soil moisture was exceeded, as shown in Figure 7.1.
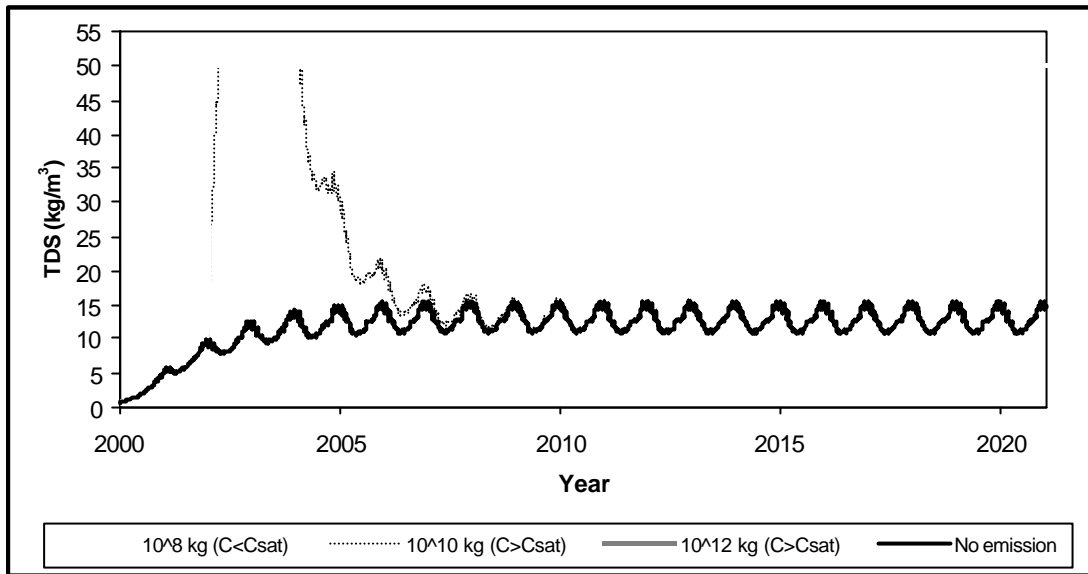
Figure 7.1: Modelled rural agricultural soil moisture salt concentration for different impulse magnitudes.

Once the solubility limit has been exceeded (in this case, 50 kg/m^3), the salt concentration in the soil moisture remains constant (at the value of the solubility limit) until the sufficient water has passed through the soil to re-dissolve the precipitated salt. For an impulse magnitude of 1×10^{10} kg the solubility limit was reached approximately 3 months after the impulse started, and dissolution started at approximately 2 years after the start of the impulse. For the impulse magnitude of 1×10^{12} kg, the solubility limit was reached approximately 2 weeks after the start of the impulse, and remained above the solubility limit throughout the duration of the simulation. The sum of the difference in concentrations is therefore greater than expected when the solubility limit is exceeded, and is thus no longer a linear function of impulse magnitude. In practice, it is unlikely that emissions would be released that would result in the solubility limit being exceeded, or at the very least, this would be prevented by the environmental authorities. The remainder of the analysis was therefore done with an impulse magnitude of 1×10^8 kg.

7.1.2 Impulse duration

The effect of impulse duration was determined by keeping the impulse magnitude and impulse starting date constant, at 1×10^8 kg and 1 January 2002 respectively. The impulse duration was varied and the effect on the effects potentials determined, as shown in Table 7.2.

Table 7.2: Effect of impulse duration on effects potentials

Impulse magnitude (kg)	Impulse starting date	Impulse duration (y)	$\sum_{i=1}^{7300}[PEC_i - PEC_i^0]$		
			Rural agricultural soil moisture	Rural natural soil moisture	River
1×10^8	1 January 2002	0.2	761.78	2.02	7.40
1×10^8	1 January 2002	0.4	755.28	1.96	8.10
1×10^8	1 January 2002	0.6	741.10	1.96	8.53
1×10^8	1 January 2002	0.8	726.78	1.97	8.33
1×10^8	1 January 2002	1.0	726.46	1.96	8.31
1×10^8	1 January 2002	3.0	726.46	1.96	8.31

It is evident from Table 7.2 that for impulse durations of less than one year, effects potentials vary with impulse duration, but for impulse durations of greater than one year, there is very little variation in effects potentials. This is due to the fact that for impulse durations of less than one year, seasonal variations in hydrological parameters, such as rainfall and evaporation, will influence the distribution of salts, whereas over one hydrological cycle (one year), this is not the case. It is unlikely that an environmental life cycle assessment of an activity occurring over a time period of less than one year would be conducted. The salinity potentials are therefore independent of the duration of the impulse emission.

7.1.3 Impulse start date

The effect of impulse start date was evaluated by keeping the impulse magnitude and impulse duration constant, at 1×10^8 kg and 1 year respectively, and varying the starting date of the impulse. The results are shown in Table 7.3.

It is evident from Table 7.3 that salinity potentials are independent of impulse starting.

Table 7.3: Effect of impulse starting date on effects potentials

Impulse magnitude (kg)	Impulse starting date	Impulse end date	Impulse duration (y)	$\sum_{i=1}^{7300}[PEC_i - PEC_i^0]$		
				Rural agricultural soil moisture	Rural natural soil moisture	River
1×10^8	1 January 2002	1 January 2003	1	726.78	1.97	8.33
1×10^8	1 January 2003	1 January 2004	1	726.72	1.96	8.32
1×10^8	1 January 2004	1 January 2005	1	726.63	1.95	8.32

7.1.4 Simulation length

The next important factor to be considered when calculating the effects potentials is the simulation length. The duration of the simulation must be sufficient to allow the difference in predicted environmental concentrations (with and without an emission impulse) to approach zero. Figures 7.2 to 7.5 show the difference in predicted environmental concentrations (indicated as Delta PEC on the figures) as a function of time over a 20-year simulation. The figures are for a 1- year impulse of 1×10^8 kg starting on 1 January 2001.

It is evident from the Figures 7.2 to 7.5 that the difference in predicted environmental concentrations (with and without an imposed emission impulse) is approximately zero after 20 years. The salinity effects potentials can therefore be regarded as infinite time horizon potentials.
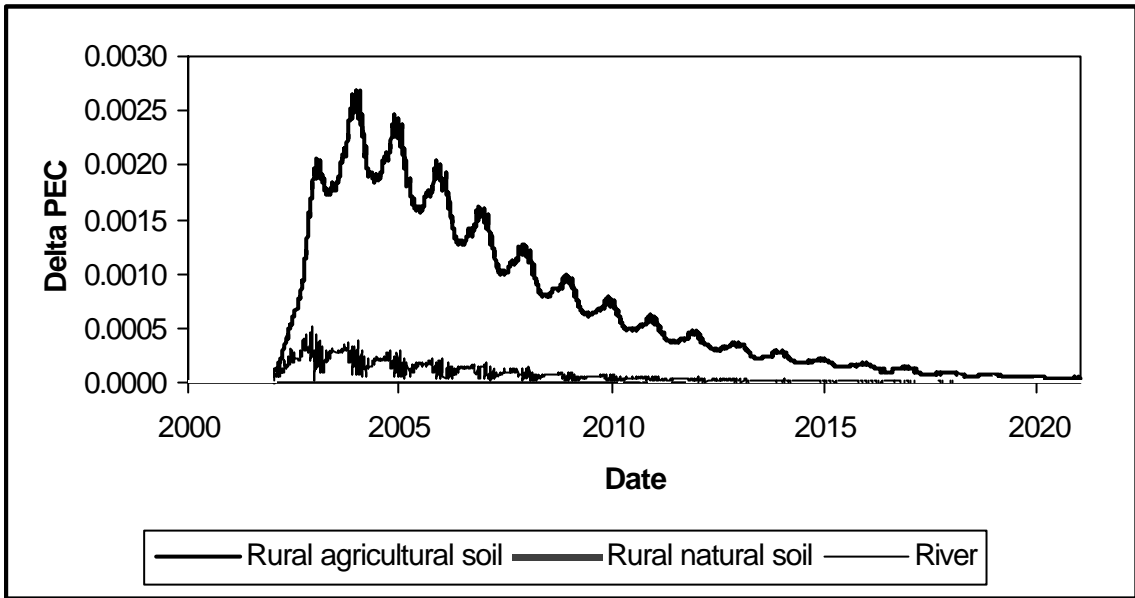
Figure 7.2: Delta PEC (in mg/L) for an emission impulse into the atmosphere
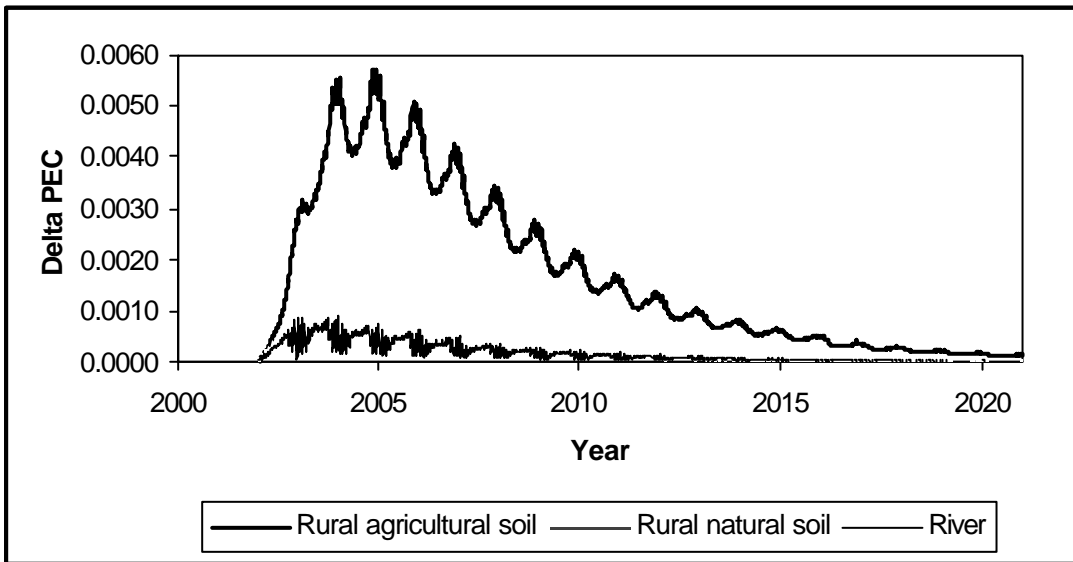
Figure 7.3: Delta PEC (in mg/L) for an emission impulse onto the rural natural surface
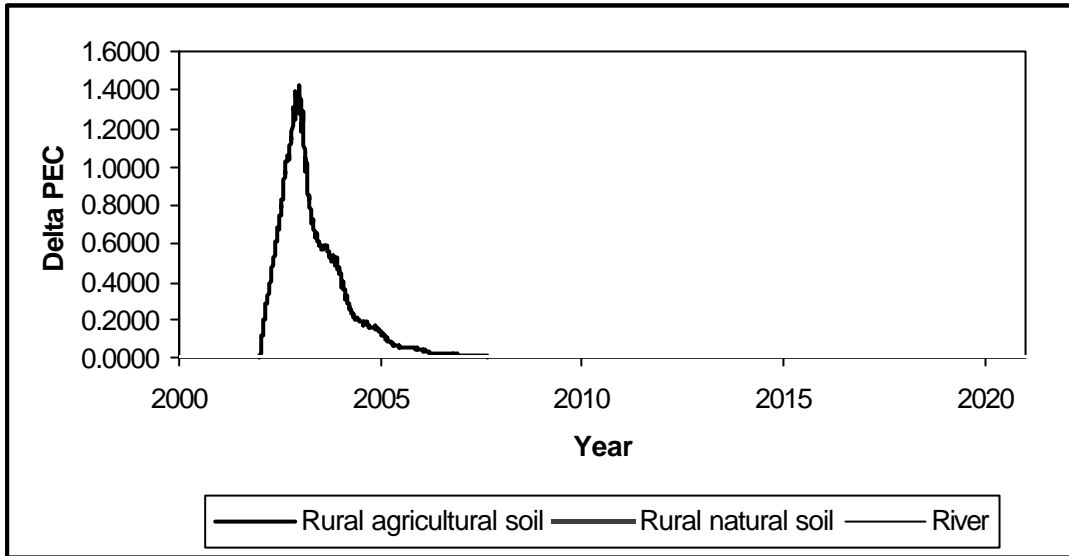
Figure 7.4: Delta PEC (in mg/L) for an emission impulse onto the rural agricultural surface
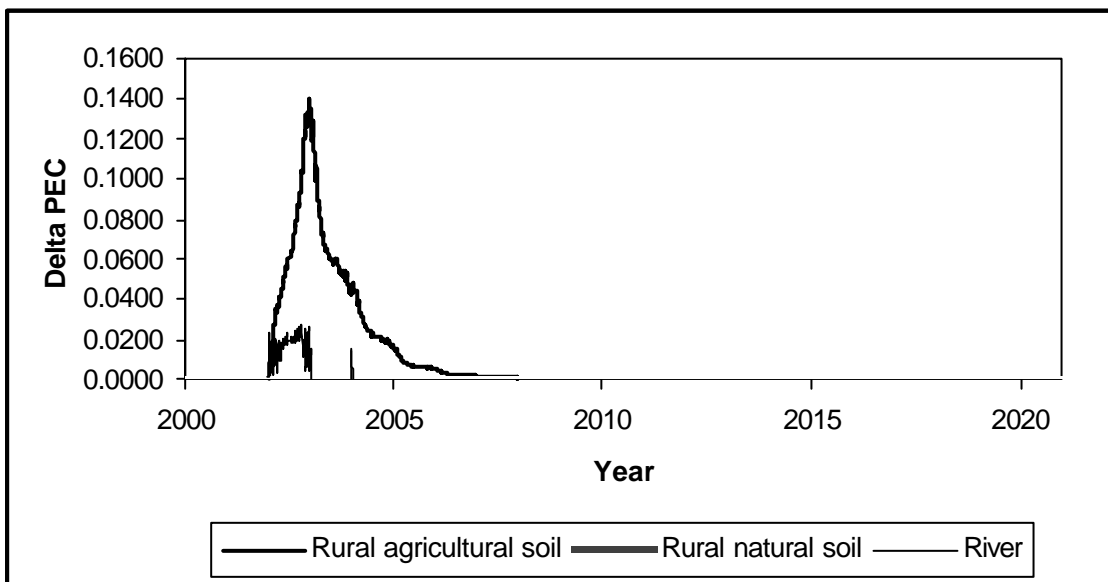
Figure 7.5: Delta PEC (in mg/L) for an emission impulse into the river

7.2 SALINITY EFFECTS POTENTIALS AND TOTAL SALINITY POTENTIALS

Effects potentials were therefore calculated from a 20-year simulation, with an impulse magnitude of 1 x 10^8 kg, of 1-year duration, starting on 1 January 2001. The effects potentials are shown in Tables 7.4 and 7.5. The effects potentials shown in Table 7.4 are calculated using the "aggregated" no-effect concentrations shown (and discussed in **Chapter 6**). The effects potentials shown in Table 7.5 are calculated using the minimum, or "worst case" no-effects concentrations shown (and discussed in **Chapter 6**). The effects potentials have been normalised so that the total salinity potential for emission onto agricultural soil is equal to unity. The effects potentials and total salinity potential are therefore expressed as kg TDS equivalents per kg, and are for an infinite time horizon.

The total salinity potentials for using the aggregated no-effect concentrations differ from the total salinity potentials using the minimum (or worst-case) no-effect concentrations by only 4%. In keeping with the European Commission guidelines for risk assessment (EC, 1996), it is recommended that the salinity potentials using the minimum no-effect concentrations be used.

The totals of the vertical columns of Tables 7.4 and 7.5 represent the effects potentials if emissions occur into each initial release compartment simultaneously. It is evident that, for all weighting factors set equal to unity, potential effects on agricultural production far outweigh any of the other potential salinity effects, followed by material damage effects.

The contribution to the total salinity potential for emissions into each initial release compartment (for minimum no-effect concentrations) is shown graphically in Figure 7.6. Figure 7.7 shows the relative contributions to total salinity potentials for different effects potentials and initial release compartments.

Table 7.4: Effects potentials calculated from aggregated no-effect concentrations

PNEC (kg/m³)	1.20PEC	1.01	2.00	1.09	3.00	0.20	2.00	
Weighting factor	1	1	1	1	1	1	1	
			Effects potentials (kg TDS equivalent/kg)					
Initial release compartment	*AEEP* (aquatic ecotoxicity)	*ACEP* (agricultural crops)	*NVEP* (natural vegetation)	*LEP* (livestock)	*NWEP* (natural wildlife)	*MDP* (material damage)	*AeEP* (aesthetic)	*TSP* (total salinity potential)	Contribution (%)
Atmosphere	0.00052	0.00753	0.00043	0.00068	0.00025	0.00368	0.00037	**0.01346**	**1.11**
River	0.00725	0.09820	0.00000	0.00892	0.00324	0.04863	0.00486	**0.17111**	**14.06**
Rural natural surface	0.00122	0.01791	0.00110	0.00163	0.00059	0.00889	0.00089	**0.03224**	**2.65**
Rural agricultural surface	0.00050	0.99477	0.00000	0.00064	0.00023	0.00351	0.00035	**1.00000**	**82.18**
Total	**0.00949**	**1.11841**	**0.00153**	**0.01187**	**0.00431**	**0.006472**	**0.00647**	**1.21680**	
Contribution (%)	**0.78**	**91.91**	**0.13**	**0.98**	**0.35**	**5.32**	**0.53**		

Table 7.5: Effects potentials calculated from minimum no-effect concentrations

	AEEP	ACEP	NVEP	LEP	NWEP	MDP	AeEP	TSP	
PNEC (kg/m^3)	1.15PEC	0.46	0.98	1.00	1.20	0.10	0.45		
Weighting factor	1	1	1	1	1	1	1		
				Effects potentials (kg TDS equivalent/kg)					
Initial release compartment	AEEP (aquatic ecotoxicity)	ACEP (agricultural crops)	NVEP (natural vegetation)	LEP (livestock)	NWEP (natural wildlife)	MDP (material damage)	AeEP (aesthetic)	TSP (total salinity potential)	Contribution (%)
Atmosphere	0.00028	0.00754	0.00040	0.00034	0.00028	0.00336	0.00075	0.01294	1.07
River	0.00397	0.09824	0.00000	0.00443	0.00369	0.04432	0.00985	0.16450	13.61
Rural natural surface	0.00067	0.01792	0.00102	0.00081	0.00068	0.00810	0.00180	0.03100	2.57
Rural agricultural surface	0.00027	0.99523	0.00000	0.00032	0.00027	0.00320	0.00071	1.00000	82.75
Total	**0.00519**	**1.11894**	**0.00142**	**0.00590**	**0.00491**	**0.05898**	**0.01311**	**1.20844**	
Contribution (%)	**0.43**	**92.59**	**0.12**	**0.49**	**0.41**	**4.88**	**1.08**		
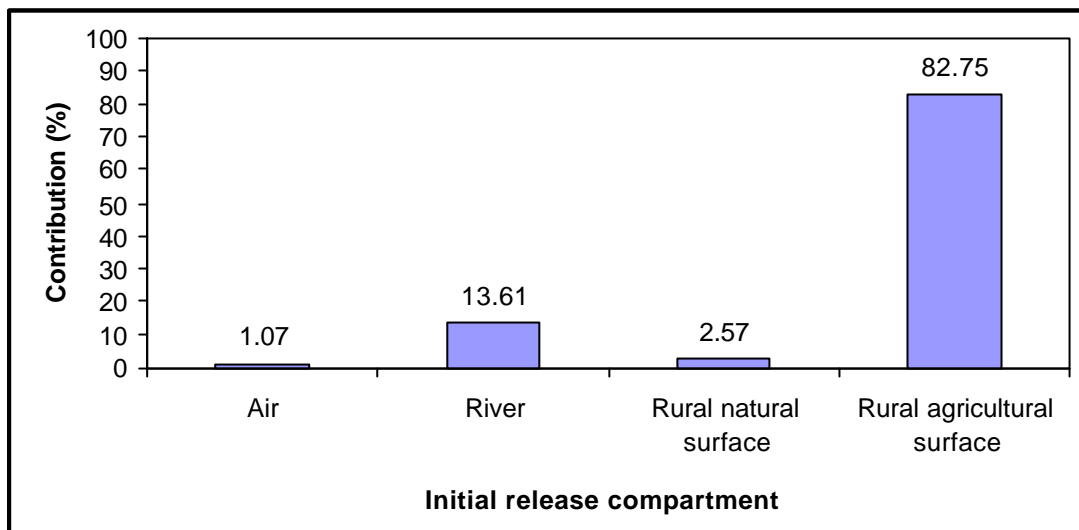
Figure 7.6: Contribution to total salinity potential for individual emissions into each initial release compartment (for minimum no-effect concentrations)

It is evident from the Tables 7.4 and 7.5, and Figures 7.6 and 7.7 that the total salinity potential for emissions onto the rural agricultural surface by far outweighs (82.8%) the salinity potentials for releases into other compartments, followed by the salinity potential for emissions into the river (13.6%), onto rural natural surfaces (2.6%) and into the atmosphere (1.1%). Salination is recognised as one of the major threats to the water resources of South Africa, along with eutrophication, microbial contamination, erosion and acidification. The major contributors to salination in South Africa are attributed to municipal and industrial wastes, urban storm water runoff, irrigation return water, seepage from mining activities and solid waste disposal sites. Rapid population growth has led to urbanisation, intensification of agricultural production, and industrialisation. Furthermore, government policies that have encouraged monoculture and intensive use of agrochemicals have resulted in over-use of the land, and degradation of vegetation and soils. Approximately 54 000 ha of agricultural land has been severely affected by salination, and approximately 128 000 ha moderately affected. Approximately 10% of the irrigated land in South Africa is severely affected by salination. The conversion of natural ecosystems for intensive agricultural or forestry production, or for grazing purposes, have been identified as major pressures on plant diversity in the country (DEAT, 1999). The Department of Water Affairs and Forestry have implemented a policy that prohibits the irrigation of water containing wastes, which is enshrined in the National Water Act (DWAF, 1998), which classifies the irrigation of

water containing wastes as a scheduled process, to which certain conditions apply. The salinity potentials support this policy.
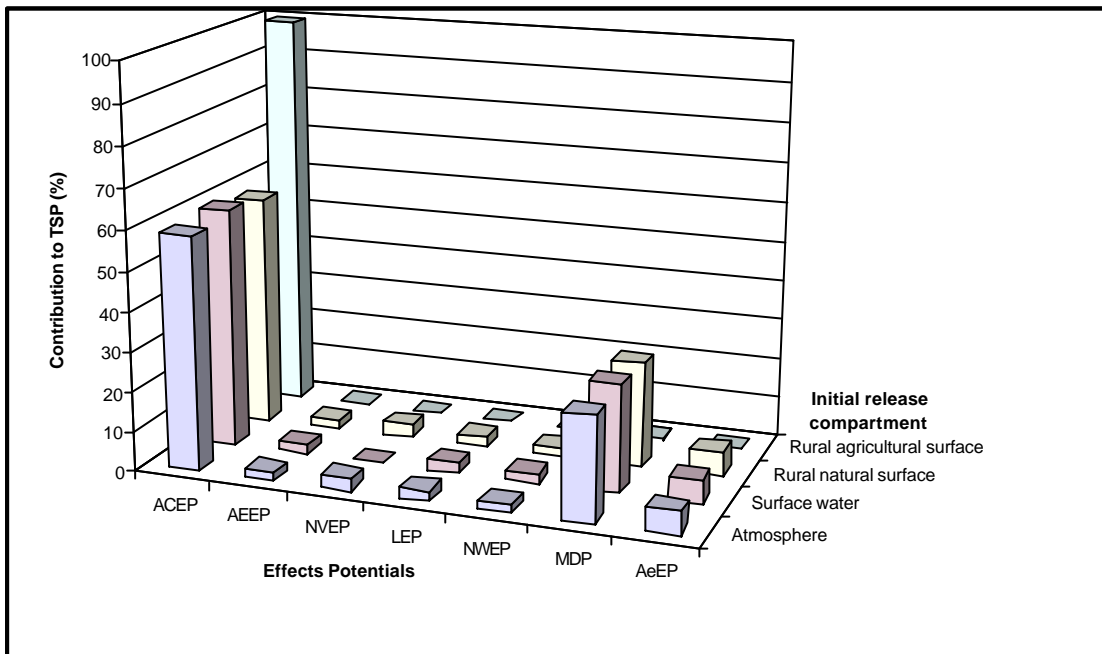
Figure 7.7: Relative contributions to total salinity potentials for different effects potentials and initial release compartments (for minimum no-effect concentrations)

For almost 40 years, South Africa has subscribed to the policy of managing water quality through returning water to its source, and setting effluent standards. Even though these standards were largely adhered to, the quality of receiving water bodies deteriorated, and the policy has now changed to one of management according to receiving water quality objectives, aimed at maintaining the ecological functions of the aquatic ecosystems (DEAT, 1999). The salinity potential for emissions into the river is the second highest which appears to support the move towards managing water resources through the setting of receiving water quality objectives. If one looks at the effects potentials, however, the potential salinity effects are greatest to agricultural crop production, followed by material damage effects. Aquatic ecotoxicity effects rank second last, and are lower than potential aesthetic effects. In reality, aquatic ecotoxicity effects could indeed be low compared to other effects. In a study conducted by the Water Research Commission on the economic cost effects of salinity (WRC, 2000a) in the middle Vaal River area, the highest direct cost of salinity was to the household sector (due to material damage effects), followed by the manufacturing sector. Direct costs of salinity to the agricultural sector ranked the lowest (in part, due to the salt tolerant crops grown in middle Vaal catchment). Unfortunately the

study concluded that the cost effects on the natural environment could not be determined, and were not included. The results of the study do, however, indicate that material damage has significant cost implications, which is supported by the material damage effects potentials, which rank second in their contribution to total effects potentials. It should be borne in mind that dose-response data for salinity on aquatic organisms are very limited. It is therefore not known if the guidelines recommended by the Department of Water Affairs and Forestry (< 15% increase in total dissolved salts concentration) are over- or under-protective.

By examining the salinity potentials, one could deduce that the most environmentally benign way of disposing of salts would be to release them into the atmosphere, particularly if emissions are above stable inversion layers. A large portion of the salt released in this way will be transported off-shore (refer to **Section 4.1.1**), and deposition will take place over a larger area. It should, however, be borne in mind that the atmospheric model developed is very simplistic, and assumes complete mixing in the urban and rural air volumes. In reality, localised areas of high concentration will occur in the vicinity of the emission, which will result in far greater localised deposition rates, which in turn may result in greater surface and sub-surface water salt concentrations. In addition, human health effects are not taken into account in the calculation of salinity potentials. Large emissions into the atmosphere may result in localised aerosol concentrations that exceed safe levels. The second lowest contributor to total salinity potential results from emissions to rural natural land. This is obviously not a practical method for the disposal of salts, since even distribution of the salts over the entire rural natural area would be required.

The results and discussion presented above are for effects potentials having equal weights. Weighting factors can be used to determine the relative importance (or value) of the salinity sub-impacts considered (effects potentials). One could, for example, weight potential aesthetic effects as being half as important as material damage effects, and so on. These choices are, for the time being, subjective, and will remain so until a scientifically valid method for expressing potential effects in a common currency have been developed. It is therefore recommended that, until such a method is developed, equal weightings be assigned to the effects potentials. The work done by the Water Research Commission on the economic cost effects of salinity (WRC, 2000a) are a step in the direction of being able to determine the relative weighting, based on economic considerations. Ideally, weightings should be based on social, economic, and ecological considerations.

In **Chapter 2** a simple worked example was used to demonstrate the methodology for carrying out life cycle assessments, and the types of decisions that the results of an LCA might support.

The worked example is repeated below, with the inclusion of salinity. Table 7.6 shows the equivalency factors, and Table 7.7 shows the impact profile, which is represented graphically in Figure 7.8. Although the impact categories cannot be compared with each other (without first normalizing), the relative changes in the impact scores remain the same as before, but the salinity potential decreases by 80%. Based on this information, the decision may be made that the decrease in salinity potential is sufficiently large to implement the effluent treatment plant.
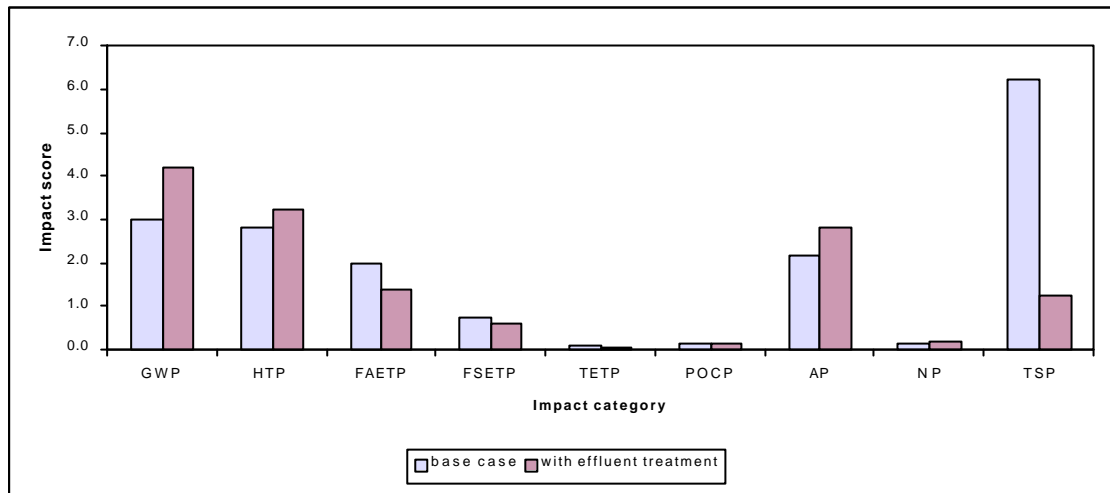
Figure 7.8: Impact profile for the LCA worked example, including salinity

Table 7.7: Impact profile for the worked example LCA, including salinity

Impact category	Impact score	
	Base case	With effluent treatment
Global warming [GWP](kg CO_2 equ.)	3.000	3.600
Human toxicity [HTP](kg 1,4-DCB equ.)	2.811	3.240
Fresh water exocoxicity [FAETP](kg 1,4-DCB equ.)	2.021	1.400
Fresh water sediment ecotoxicity [FSETP](kg 1,4-DCB equ.)	0.764	0.604
Terrestrial ecotoxicity [TETP](kg 1,4-DCB equ.)	0.102	0.077
Photochemical oxidant formation [POCP](kg ethylene eq.)	0.120	0.131
Acidification [AP](kg SO_2 eq.)	2.170	2.821
Nutrification [NP](kg PO_4 eq.)	0.157	0202
Salinity[TSP](kg TDS eq.)	6.21	1.228

Table 7.6: Equivalency factors for worked example, including salinity

	TSP	GWP	HTP	FAETP	FSETP	TETP	POCP	AP	NP
Emissions to air									
Carbon dioxide		1							
Carbon monoxide			**0.012**				0.027		
Oxides of nitrogen (NOx)	0.01294		**0.78**				0.028	0.5	0.13
Sulphur dioxide	0.01294		0.096				0.048	1.2	
Particulate matter (PM10)	0.01035 *		0.82						
Hydrogen sulphide	0.01294		0.22						
Ammonia	0.01294		0.1					1.6	0.35
Carbon disulphide	0.01294		1.6	0.33	0.0027	0.0051			
Emissions to fresh water									
Ammonia									0.33
Phosphate			0.00052						1.0
Chemical oxygen demand									**0.022**
Lead			12	9.6	250	4.8×10^{-22}			
Total dissolved salts	0.16450								
Emissions to agricultural soil									
Chemical oxygen demand									
Carbon disulphide			3.6	0.34	0.28	1.6			
Hydrogen sulphide									
Lead			3300	6.5	170	330			
Cadmium			20000	7800	2000	1700			
Copper			94	5900	1500	140			
Dichloromethane			2.4	0.00016	0.00011	0.00025			
Total dissolved salts		1							

GWP = global warming potential (kg CO_2 eq./kg)

HTP = human toxicity potential (kg 1,4-DCB eq./kg)

FAETP = fresh water ecotoxicity potential (kg 1,4-DCB eq./kg)

FSETP = fresh water sediment ecotoxicity potential (kg 1,4-DCB eq./kg)

TETP = terrestrial ecotoxicity potential (kg 1,4-DCB eq./kg)

POCP = photochemical oxidant formation (kg ethylene eq/kg)

AP = acidification potential (kg SO_2 eq./kg)

NP = nutrification potential (kg PO_4 eq./kg)

TSP = total salinity potential (kg TDS eq./kg)

Values in **bold** are taken from UNEP (1996), all other values are taken from Guinee et al. (2000)

* Particulate matter is assumed to comprise 80% potentially soluble salts

The requirements for defining new impact categories are presented in **Section 2.3**, and summarised in Table 2.5. The extent to which these requirements have been met by the proposed method developed is evaluated below.

General starting point

"A framework shall be developed which is open to further scientific progress and further detailing of new information"

> The proposed method developed certainly meets this requirement, and recommendations regarding further development of the method and information gaps are discussed in **Chapter 8**.

Starting points for total categories

"The categories shall together enable encompassing assessment of relevant impacts, which are known today"

> The obligatory and non-obligatory impact categories defined by the ISO 14042 standard are listed in **Section 1.1**. The nature of salinity impacts are such that some of the salinity impacts (such as aesthetic impacts, and damage to man-made environment) do not fall within the impact categories defined, and the inclusion of these impacts into methodology therefore encompasses a wider range of impacts than currently covered by defined impact categories.

"The categories should have the least overlap possible"

> Some of the salinity impacts as defined in the method developed (such as aquatic ecotoxicity) do overlap with existing impact categories. The question therefore arises as to whether to exclude some of the salinity sub-impacts that are already defined in the existing impact categories or to include them. Salination of water resources is a local or regional problem and characterisation of salinity impacts therefore requires models with a higher degree of spatial differentiation than for environmental problems that are global in nature (such as global warming). Furthermore, the characterisation models should be relevant to the area in which the problem occurs. It was shown in **Chapter 2** that existing characterisation models are not suited for the characterisation of salinity impacts under local conditions. It is therefore recommended that salinity impacts that overlap with

existing impact categories be included in the salinity impact category developed. This will require that LCA practitioners ensure that impacts are not double accounted for. This can be done relatively easily by using existing impact categories to account for toxic ions, such as manganese, mercury, and so on, and to use the salinity impact category to account for impacts resulting from common ions.

"The total of the impact category should amount to not too high a number"

The approach adopted in the development of an impact category, and the characterisation of salinity impacts is the same as for existing categories and characterisation models. The salinity potentials have therefore been normalised to give a total salinity potential equal to unity for emissions of salts onto agricultural soil. All other total salinity potentials are less than unity.

Starting points for separate impact categories

"The category indicator can be chosen anywhere in the environmental mechanism of an impact category, from environmental interventions to category end-points."

The availability and selection of no-effect concentrations (**Chapter 6**) is such that category indicators have been chosen at midpoints (refer to Figure 2.4).

"The category indicator should be modelled in a scientifically and technically valid way in relation to the environmental interventions"

Scientific and technically valid techniques were used to model the fate of salts in the various environmental compartments. No-effect concentrations were based on the South African Water Quality Guidelines (DWAF, 1996) in which quantitative (including assessment factors) and qualitative techniques were used to determine no-effect concentrations for life-long exposure.

"The category indicator shall have sufficiently clear links to the category end-

The links between category indicator and category end-points were established and discussed in **Chapter 2**.

"It must be possible that characterisation factors are multiplied by mass or other units indicating the magnitude of the environmental interventions"

Characterisation factors (salinity potentials) have been developed that meet this requirement.

In summary it can be stated that the proposed method for incorporating salinity into life cycle assessment meets the requirements for defining new impact categories.

7.3 UNCERTAINTY AND VARIABILITY

Examples of the types of uncertainty and variability related to the various phases of conducting an environmental life cycle assessment are shown in Table 7.8. The work presented in this document has, in the context of conducting environmental life cycle assessments, a very narrow focus. A method is developed for the characterisation of salinity impacts, and therefore the discussion of uncertainty and variability is limited to the characterisation step in Table 7.8, and more specifically the uncertainty and variability as it affects the results of the proposed characterisation model, and consequently the results of the LCA. There are two major sources of uncertainly and variability, namely environmental fate modelling, and environmental effects assessment.

Environmental fate modelling

Salinity is, as stated, a local or regional problem, and therefore a higher degree of spatial differentiation is required than, for example, global warming. The ultimate aim for characterising salinity would be to differentiate at a catchment scale. This would, however, require that the spatial distribution of life cycle activities be known. In the absence of this information, characterisation models generally integrate over time and space, over the entire globe. In this study, a compromise was made by defining the "unit South African catchment". This required the regionalisation of model parameters in instances where these parameters were available on a smaller scale, and in other instances very little data were available. The methodology used to regionalize the published model parameters, and the limited data for other parameters are sources of uncertainty. Published model parameter values were regionalised by calculating area-weighted averages. For some parameters (for example, the soil moisture capacity) this method would be valid, but for other parameters (for example, the power of the soil moisture-percolation relationship) this method of regionalisation is questionable.

Various simplifying assumptions were made in the environmental fate model, particularly the atmospheric deposition model component. These assumptions would introduce further uncertainty regarding the relative distribution of salts in the various compartments, and therefore in the salinity potentials. Additional uncertainty is introduced due to the modelling of dissolved salts as a lumped parameter, which in practice does not have one solubility limit, or one set of Langmuir adsorption constants.

It was shown in **Section 5.4** that some of the fate factors (and therefore salinity potentials) were sensitive to some of the model parameters. The implicit assumption was that if there was good correlation between the predicted environmental concentrations and the observed (or regionalised) values, then the parameter values were correct, or most appropriate. A large degree of uncertainty and variability is, however, associated with the observed values, particularly regarding the dissolved salt concentrations in the "unit river". The methodology for determining the observed values is presented in **Appendix B**, where it was highlighted that in some catchments the water quality database was very limited.

Effects assessment

Although there are clear causal relationships between interventions and salinity effects, there is unquestionably a lack of dose-response data. This is particularly true for aquatic ecotoxicity effects. No-effect concentrations were chosen based on the target water quality given in the South African Water Quality Guidelines (DWAF, 1996), for which assessment (or safety) factors were used to reflect the degree of uncertainty in extrapolating from the (limited) laboratory toxicity test on a limited number of species to the real word situation. Uncertainty in this regard can be reduced by extensive toxicity testing.

Table 7.8: Examples of types of uncertainty and variability related to the phase of LCA (Huijbregts, 2001)

Source	LCA Phase					
	Goal and scope	Inventory	Choice of impact categories	Classification	Characterisation	Weighting
Parameter uncertainty		Inaccurate emission measurements	Impact categories not known		Uncertainty in life times of substances	Inaccurate normalisation data
Model uncertainty		Linear instead of non-linear modelling	Leaving out known impact categories	Contribution to impact category is not known	Characterisation factors not known	Weighting criteria are not operational
Uncertainty due to choices	Functional unit	Use of several allocation methods			Using several characterisation methods within one category	Using several weighting methods
Temporal variability		Differences in yearly emission inventories			Change in temperature over time	Change of social preferences over time
Spatial variability		Regional differences in emission inventories			Regional differences in environmental sensitivity	Regional differences in distance to (political) targets
Variability between objects/sources		Differences in emissions between factories which produce the same product			Differences in human characteristics	Differences in individual preferences, when using the panel method

CHAPTER 8

CONCLUSIONS AND RECOMMENDATIONS

This work presented in this thesis stemmed out of the apparent lack of a method for incorporating salinity effects into environmental life cycle assessments. Salination of the water resources is a well-known problem in South Africa, and is of strategic concern. Any environmental decision support tool that does not allow the evaluation of salinity effects therefore has limited applicability in the South African context. The starting-point for the work presented in this thesis was to evaluate existing impact categories, and the characterisation models used to calculate equivalency factors for these impact categories, in an attempt to incorporate salinity effects into existing categories and/or characterisation models. The types of effects that elevated (above normal background levels) dissolved salt concentrations have on the natural and man-made environment were evaluated, and it was concluded that, although there was some overlap with existing impact categories, some of the salinity effects could not be described by existing impact categories. It was also concluded that there are clear and quantifiable causal relationships between interventions and salinity effects. A separate salinity impact category was therefore recommended that includes all salinity effects, including; aquatic ecotoxicity effects, damage to man-made environment, loss of agricultural production (livestock and crops), aesthetic effects and effects to natural fauna and flora. Once a conceptual model for a separate salinity impact category had been formulated, existing characterisation models were evaluated to determine their applicability for modelling salinity effects. Salination is a local or regional problem, and in order to characterise salinity effects, an environmental fate model would be required in order to estimate salt concentrations in the various compartments, particularly surface and subsurface water. The USES-LCA model (which is based on the USES 2.0 model) was evaluated because it is a well developed and accepted environmental fate model that has been adapted to calculate toxicity potentials for LCA, and intuitively would seem to be suited to be used for calculating salinity effects, some of which are toxicological in nature. It was however concluded that the USES-LCA model is not suitable for the calculation of salinity potentials. The major reasons for this were:

- In the USES-LCA model the globe is modelled as a closed system using a series of nestled multi-media fate models on different geographical scales, with Western Europe being defined as the smallest regional (or "starting") scale. Substance independent model parameters used may result in equivalency factors that are therefore not

necessarily valid to South African conditions. Furthermore, salination is a local or regional problem, and that a higher degree of spatial differentiation is required.

- Although the USES-LCA model accounts for some of the salinity impacts, it does not account for all.

- Sub-surface water and solute transport modelling in the USES-LCA model is inadequate for the degree of accuracy and relevance needed to account for salinity effects.

- Perhaps the biggest obstacle in using the USES-LCA model as is, or in some modified form to account for salinity effects is that it has been developed to handle organic compounds, and is not suited for estimating the fate of ionic compounds.

It was therefore decided to develop an environmental fate model that would overcome the limitations of The USES-LCA model, in terms of modelling the movement of salts in the environment. In terms of spatial differentiation, the same approach that was adopted in the USES-LCA model was adopted in developing an environmental fate model for South African conditions. This was done by defining a "unit South African catchment" (including the air volume above the catchment), which consists of an urban surface, rural agricultural soil (an associated soil moisture), rural natural soil (and associated moisture), groundwater (natural and agricultural) and one river with a flow equal to the sum of the flows of all rivers in South Africa, and a concentration equal to the average concentration of each river in the country. A non steady state environmental fate model (or, hydrosalinity model) was developed that can predict environmental concentrations at a daily time-step in all the compartments relevant to the calculation of salinity potentials. The environmental fate model includes all the major processes governing the distribution of common ions in the various compartments. In terms of the environmental fate model the following conclusions and recommendations are made:

- The non steady-state hydrosalinity model developed was based on existing models that are well accepted and are in general use in South Africa. Many of the model parameters are available for all catchments in the country at quaternary catchment level, which made the definition of the "unit catchment" and the calibration of the model relatively simple. A simple non steady-state atmospheric deposition "box-model" was therefore developed to predict aerosol (and associated salt) deposition at a daily time-scale, in accordance with the daily time-step hydrosalinity model. Some simplifying assumptions were made in the development of the atmospheric deposition model that are clearly a great simplification of what actually occurs in nature. The atmospheric deposition model cannot be calibrated at a daily time-step due to the lack of data; however, model outputs are in the same order of magnitude as the (limited) published data. In addition, most of the model parameters used do not affect the value of the fate factors, and those parameters that do, do not

have a major effect on the value of the fate factors. It is not recommended that complex atmospheric dispersion models be developed. These models require a large number of parameters, and it is doubtful that such models could be developed for a "unit South African environment". It is, however, recommended that more data be collected to refine the model parameters used (particularly the fraction of salt associated with aerosols), and that more data be collected that will enable better calibration of the model.

- Predicted surface water flow and quality correlate well with calculated values for the "unit catchment" as defined. There is however a degree of uncertainty and variability in the calculated values for the "unit catchment", and therefore in the fate factors, and ultimately the salinity potentials. It is recommended that the method used to calculate the average monthly surface water quality be refined, and that uncertainty and variability in the data be quantified, with the aim of quantifying the variability and uncertainty associated with the calculated salinity potentials.

- Simple parameter sensitivity analyses were performed on the various components of the overall model, in an attempt to identify the sensitive model parameters and refine the model calibration. The sensitivity of model outputs to the model parameters varied is understood, and agrees with expected behaviour. The parameter sensitivity analyses are, however, by no means exhaustive, and it is possible that the same level of agreement between predicted and observed (calculated for the "unit catchment") can be achieved with a different set of model parameters. The approach adopted in calibrating the model is sound, however, it is recommended that more detailed sensitivity analyses be conducted using multi-variate statistical techniques to refine the model calibration.

- Some model parameters (particularly those that influence the distribution of surface and subsurface flow) do influence the values of the fate factors (and therefore the salinity potentials). It is recommended that more data be collected to refine these parameters.

- For a number of reasons, salts were modelled as a lumped parameter (total dissolved salt) and therefore certain model parameters (such as solubility limit, and adsorption constants) are also lumped parameters. It is recommended that the common ions be modelled separately and that separate salinity potentials be calculated for each ion. This would however require some level of speciation to be built into the model, and at this stage, some data are not available, most notably the adsorption constants for individual ions. This data would therefore need to be collected.

- The assumption made in the characterization model is that all water for livestock watering and domestic use is taken from surface water. In reality, a (small) portion of water for these users is taken from groundwater. In future it is recommended that this be included in the model.

- Although the hydrosalinity model developed has been applied, calibrated and validated in several catchments in South Africa, the combined multimedia fate model applied to the 'unit South African catchment' as developed has not been validated, and can only be done once further data are available.

The effect factors used in the characterisation model were based on the target water quality ranges given by the South African Water Quality Guidelines (DWAF, 1996). It is well known that there is a severe lack of dose-response data for South African species, particularly for aquatic organisms. As these data become available, the model developed could be refined. It was, however, shown that salinity potentials using no-effect concentrations for the aggregated scenario (protection of approximately 95% of the water users) did not substantially differ from salinity potentials using the minimum (protection of all water users) no-effect concentrations.

Regarding the use of the salinity potentials in conducting environmental life cycle assessment, the following should be borne in mind:

- The salinity potentials are only relevant to South African conditions, and their use in LCA in other countries may not be applicable. This, in effect, means that the life cycle activities that generate salts should be within the borders of South Africa. It has been recognised that the LCA methodology requires greater spatial differentiation. Salination is a local or regional problem, and it is foreseen that local or regional salinity potentials would need to be calculated for different areas of the earth where salinity is a problem. The LCA practitioner would then need to know something about the spatial distribution of LCA activities in order to apply the relevant salinity potentials.
- The LCA practitioner should take care when applying the salinity potentials to prevent double accounting for certain impacts. Currently, this is simple because no equivalency factors exist for common ions, or for total dissolved salts as a lumped parameter.
- The LCA practitioner is also required to have some knowledge about the nature of salts emitted into the atmosphere when generating the life cycle inventory and applying the salinity potentials. Not all matter emitted to the atmosphere will be deposited as salt.
- The various salinity potentials that make up the total salinity potential have, in the absence of better information, all been given equal weight. Weighting of the salinity potentials will be based on subjective value judgments and should include input from policy makers in the country. It is recommended that a method be developed to weight the salinity potentials.

The distribution of salinity potentials, which make up the total salinity potential, appears to be supported by the environmental policies and legislation of South Africa.

The work presented in this thesis focuses on a method for incorporating salinity impacts into environmental life cycle assessment, and presents salinity potentials to do this. There is currently no way of normalising or weighting the LCA results for South Africa. Methods to do this still need to be developed.

Emissions in most LCAs are not continuous fluxes, but discrete pulses, since they are linked to single amount of product functions, rather than to (production) processes as such. These discrete emission pulses cause discrete "concentration pulses". While continuous concentrations are characterised by concentration (mass per unit volume) and spatial (volume or area), concentration pulses are additionally characterised by their temporal value. To handle large numbers of such concentration pulses, it is convenient to integrate them over both space and time. Integration over space (volume) delivers amounts. The double integration therefore delivers time-integrated amounts. The advantage of space- and time integration of emission pulses is that each pulse is characterised by one single value. This makes it possible to compare and assess pulses with different spatial and temporal characteristics.

Most toxicity characterisation models are steady-state models. Predicted environmental concentrations are calculated based on continuous emission fluxes imposed on the various initial release compartments. Various methods have been proposed (Guinee., et al 1996) to overcome the difference between the emission flux necessary to implement in a steady state multi media fate model and the artificial emission pulse resulting from a life cyde inventory. The most common method is to use a reference substance. Heijungs (1995) published a paper on the harmonization of methods for impact assessment. In this paper the following important conclusions were made:

- Provided there is a linear relationship between continuous fluxes and steady-state concentrations, the total time integrated exposure due to an emission pulse can be found by simply multiplying the amount of pulse emission by the coefficients that link fluxes to concentrations. A consequence of this is that pulse-oriented techniques, like LCA, need not (under certain conditions) employ complicated time-dependent unsteady-state models for impact prediction, but can use the much simpler steady-state models that have been developed for flux-oriented techniques, like risk assessment.
- The existence of equivalency factors had previously been proven assuming that the impacts of the products are marginal compared with the total impacts. Heijungs (1995)

proves that, in fact, almost every linear exposure and/or impact prediction model gives rise to equivalency factors, which can be used in every LCA, regardless of the marginality of the product's impacts.

- The impact scores calculated in LCA bear no relation to factually occurring impacts, as discussed in **Section 2.4.2**
- A reference substance is not required when calculating equivalency factors.

In the development of the characterisation model presented in this work, it was decided to develop a non steady state model for the following reasons:

- At the outset, it was uncertain as to whether there would be a linear relationship between continuous fluxes and steady-state concentrations.
- Existing non steady-state models were available, familiar and accepted for general use in South Africa. Many of the model parameters for these models were available for each catchment, at quaternary level.
- The steady state coefficients that link fluxes to concentrations were not known for the defined "unit catchment". In this regard, it may be possible to use the results of the non steady state model to determine these coefficients, thereby simplifying the model.

The values of the published equivalency factors are dependent on the mathematical definition of the local or regional environment, and these values have been calculated for Western European conditions. Equivalency factors may vary by several orders of magnitude, depending on how the local or regional conditions have been defined. It is therefore recommended that the model developed in this work be included into a global nested model, in the same way the USES-LCA model is, in order to calculate equivalency factors for other compounds, including heavy metals and organic compounds. This would result in equivalency factors for all compounds that are relevant to South Africa.

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APPENDIX A

WIND VELOCITY DATA

The South African Weather Service (http:///www.weathersa.co.za) provided monthly wind velocity data 20 sites throughout South Africa for the period 1992 to 2002. Average monthly wind velocities for the sites are summarised in Table A.1.

Table A1. Summary of wind velocities at 20 sites throughout South Africa

Location	Latitude	Longitude	Heigth(m)	Average Wind Speed (m/sec)											
				Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
George	-34.02	22.38	191	6.6	6.5	5.6	4.8	4.1	4.4	4.5	4.7	5.2	5.6	6.1	6.4
Capetown	-33.97	18.6	46	6.6	6.5	5.6	4.8	4.1	4.4	4.5	4.7	5.2	5.6	6.1	6.4
Port Elisabeth	-33.98	25.62	59	5.7	5.6	5.3	5.0	4.8	4.7	4.6	5.2	5.7	6.2	6.2	5.9
East London	-33.03	27.83	116	4.8	4.7	4.2	4.1	4.3	4.2	4.4	4.6	4.8	5.1	5.0	4.9
Langebaan	-32.97	18.17	31	4.6	4.3	3.9	3.3	2.8	3.0	3.0	3.0	3.3	4.0	4.4	4.4
Umtata	-31.53	28.67	743	3.3	3.0	2.6	2.5	2.3	1.9	2.2	2.5	3.0	3.3	3.5	3.4
Calvinia	-31.48	19.77	975	4.4	4.2	3.8	4.0	3.8	4.3	4.5	4.3	4.2	4.4	4.4	4.4
De Aar	-30.67	24.00	1287	5.5	5.1	4.5	4.1	3.8	3.9	4.2	4.4	4.9	5.3	5.6	5.6
Springbok	-29.67	17.90	1006	4.4	4.2	4.0	4.2	4.4	4.9	5.2	4.6	4.4	4.5	4.4	4.4
Durban	-29.97	30.95	8	4.6	4.5	4.2	3.9	3.3	3.2	3.6	4.1	4.7	5.0	4.8	4.6
Bloemfontein	-29.10	26.30	1354	3.2	2.9	2.5	2.3	2.0	2.0	2.2	2.5	3.0	3.4	3.5	3.6
Kimberly	-28.80	24.77	1197	4.3	4.0	3.6	3.3	3.1	3.2	3.6	3.7	4.1	4.5	4.5	4.6
Upington	-28.42	21.27	841	4.1	3.8	3.5	3.5	3.2	3.4	3.7	3.7	3.6	4.0	4.1	4.2
Bethlehem	-28.25	28.33	1686	3.1	3.0	2.7	2.2	2.1	2.0	2.2	2.4	3.1	3.5	3.4	3.2
Johannesburg	-26.15	28.23	1695	3.4	3.2	3.0	3.0	3.0	3.1	3.3	3.6	4.0	4.2	3.9	3.7
Ermelo	-26.50	29.98	1766	4.2	4.1	3.9	3.9	3.9	4.2	4.4	4.7	5.3	5.1	4.9	4.4
Mafikeng	-25.78	25.53	1282	3.7	3.6	3.2	3.3	3.0	3.0	3.6	3.7	4.5	4.8	4.6	4.2
Pretoria	-25.73	28.18	1310	1.4	1.3	1.1	0.9	0.7	0.7	0.9	1.3	1.6	1.7	1.7	1.6
Irene	-25.92	28.22	1524	3.3	3.1	2.9	2.8	2.8	2.8	3.0	3.1	3.5	3.7	3.6	3.4
Pietersburg	-23.87	29.45	1237	2.6	2.6	2.3	2.2	2.5	2.7	2.6	2.6	2.8	2.9	2.5	2.5
Minumum				**1.4**	**1.3**	**1.1**	**0.9**	**0.7**	**0.7**	**0.9**	**1.3**	**1.6**	**1.7**	**1.7**	**1.6**
Average				**4.2**	**4.0**	**3.6**	**3.4**	**3.2**	**3.3**	**3.5**	**3.7**	**4.0**	**4.3**	**4.4**	**4.3**
Maximum				**6.6**	**6.5**	**5.6**	**5.0**	**4.8**	**4.9**	**5.2**	**5.2**	**5.7**	**6.2**	**6.2**	**6.4**

APPENDIX B

CHARACTERISATION OF THE "UNIT SOUTH AFRICAN

B.1 SURFACE WATER RESOURCES

B1.1 Drainage regions

Data presented by Midgley et al. (1994) were used to characterise the surface water resources of the "unit South African catchment". South Africa is divided into 22 drainage regions, as depicted in Figure B1.
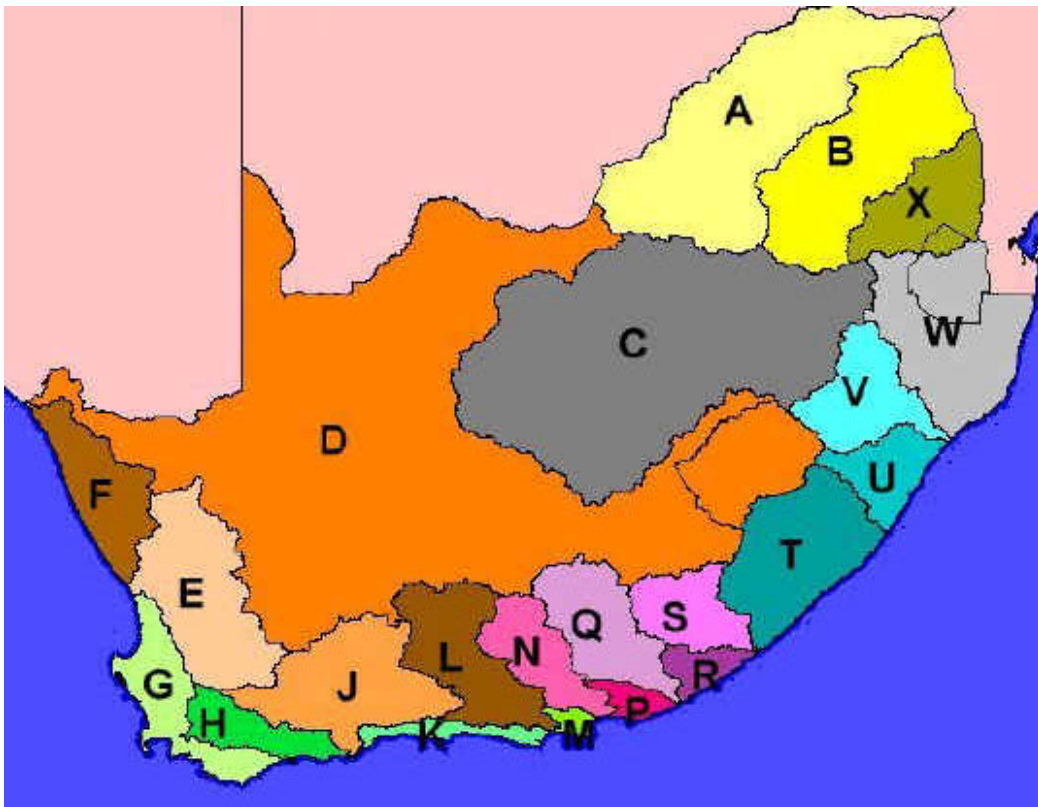
Figure B1: Drainage regions of South Africa.

Each drainage region is sub-divided into primary drainage regions, which in turn are sub-divided into secondary, tertiary and quaternary sub-catchments. Average monthly rainfall and evaporation data are presented for each drainage region at quaternary sub-catchment level. Simulated monthly surface water flows are calculated at secondary catchment level using a modified version of the model originally developed by Pitman (1973).

B1.2 Surface area

The total surface area of each drainage region, the area assumed to be impervious and the areas normally irrigated are shown in Table B1.The data presented in Table B1 were used to calculate fraction impervious (urban) area (0.00034) and the fraction of the total rural area under irrigation (0.00034).

B1.3 Rainfall

In the work presented by Midgley et al. (1994), South Africa has been divided into different rainfall zones. Rainfall data (expressed as a percentage of mean annual precipitation) are given for each rainfall zone as well as mean annual precipitation for each catchment at quaternary level. The rainfall zone applicable to each catchment at quaternary level is presented, and from this information, the average monthly rainfall for each catchment is calculated as an area weighted average. The mean monthly rainfall for each drainage region, and for the country as a whole, is presented in Table B2.

B1.4 Evaporation

Mean monthly evaporation is calculated in a similar manner to mean monthly precipitation. Evaporation data (expressed as a percentage of mean annual precipitation) are given for each evaporation zone as well as mean annual evaporation for each catchment at quaternary level. The evaporation zone applicable to each catchment at quaternary level is presented, and from this information, the average monthly evaporation for each catchment is calculated as an area weighted average. The mean monthly evaporation for each drainage region, and for the country as a whole, is presented in Table B3.

B1.5 Model parameters

The model parameters used by Midgley et al (1994) to calibrate surface water flow at quaternary catchment level were used to calculate area weighted average parameter values for each drainage region, and for the country as a whole. The regionalised parameter values are given in Table B 4.

B1.6 Surface water flow

Simulated natural monthly river flow data are presented by Midgley et al. (1994) at secondary catchment level. The natural monthly river flow was decreased to account for stream flow reduction due to forestry; using the fraction that runoff is decreased due to forestry (taken from DWAF, 1986). The total river flow was then calculated by summing the flows from each secondary catchment. The monthly average river flow values are shown in Table B 5.

B1.7 River losses

Channel bed losses and losses due to wetlands are reported by Midgely et al (1994) at quaternary catchment level. The total loss for all rivers amounts to 1 349 million m^3/y. For a river 1 000 km long and 1 km wide, this amounts to a bedloss of 3.7 mm/d.

B1.8 Irrigation factors

The irrigation flow requirements are calculated from the crop water demand, as shown in Equations [4-39] and [4-40]. Rainfall, evaporation and irrigation data from Schulze et al (1997) were used to back-calculate the irrigation demand factor. The results are shown in Table B 6.

Table B1: Drainage regions surface area, impervious area and area normally irrigated.

Drainage Region	Area (km^2)	Impervious area (km^2)	Area normally irrigated (km^2)
A	109604	83.189	523.57
B	5310	0	2.233
C	191328	260.995	342.05
D	877721	2.054	729.165
E	49066	0	348.471
F	28623	0	0
G	24978	54.538	491.522
H	15532	5.34	427.128
J	45702	4.518	621.66
K	7223	9.64	136.734
L	34852	0	145.08
M	2630	22.082	16.3
N	21248	0	61.93
P	5322	0	16.8
Q	30243	0.963	320.46
R	7936	10.102	64.53
S	20485	2.56	149.32
T	46684	3.878	257.5
U	18312	68.45	219.25
V	28864	19.59	251.35
W	59200	18.095	798
X	31157	2.37	596.835
Total	**1662020**	**568.363**	**6519.888**

Table B2: Mean monthly rainfall for each drainage region

Drainage Region	Mean monthly Rainfall (mm/m)											
	OCT	NOV	DEC	JAN	FEB	MAR	APR	MAY	JUN	JULY	AUG	SEP
A	40.7	74.5	88.8	99.0	82.6	67.9	35.5	12.5	5.9	4.1	4.3	13.6
B	53.7	94.2	105.5	114.9	97.3	77.2	40.8	14.5	7.2	7.3	6.2	19.8
C	48.3	70.3	75.8	89.9	79.7	77.4	44.6	18.1	7.7	6.8	9.3	19.0
D	10.3	14.4	15.9	19.3	21.0	22.6	13.5	6.7	3.4	3.0	3.8	5.1
E	11.5	11.0	7.7	5.3	8.2	11.5	19.5	26.3	36.9	27.8	28.7	15.3
F	8.7	5.8	5.1	2.0	4.5	6.9	11.3	17.2	24.8	19.0	21.0	10.2
G	32.7	22.9	14.9	13.9	16.5	21.6	40.9	64.0	78.4	69.8	68.3	43.4
H	62.9	57.9	33.4	36.2	44.2	53.7	71.2	77.9	85.1	79.7	91.1	62.5
J	19.8	24.7	19.4	17.8	23.2	30.3	27.0	22.7	19.6	18.9	20.9	17.6
K	88.7	85.1	72.0	72.0	70.0	83.6	71.8	76.6	62.7	68.0	83.3	85.2
L	25.0	32.3	29.0	27.4	38.8	48.2	30.9	24.2	14.2	17.1	19.0	19.3
M	57.0	58.1	41.3	38.8	43.2	60.2	47.6	42.7	34.6	38.7	41.8	50.9
N	29.4	34.7	30.8	28.7	39.2	48.7	29.6	22.1	11.9	16.3	17.7	20.0
P	59.2	59.4	43.8	40.9	49.8	64.7	42.6	42.8	33.9	35.1	37.2	51.2
Q	37.5	47.3	44.9	43.6	56.1	66.0	36.3	24.9	13.7	16.0	18.4	23.9
R	46.3	54.1	41.8	43.1	48.4	58.5	33.7	24.3	15.5	18.7	23.2	34.0
S	49.6	67.2	68.6	71.4	76.7	81.1	41.5	25.1	13.2	16.1	20.0	32.9
T	87.3	117.7	125.6	134.2	128.0	126.5	58.4	33.9	20.1	22.5	28.4	56.2
U	89.1	116.4	127.2	134.8	125.6	122.9	58.8	35.9	21.5	19.3	31.8	57.2
V	78.9	111.5	127.1	140.9	121.3	101.3	45.1	20.8	11.7	12.4	20.7	42.5
W	81.6	111.1	118.0	125.6	112.0	96.0	51.3	27.5	18.1	17.2	20.4	45.9
X	66.5	113.5	124.6	136.9	122.8	97.2	48.9	18.7	10.5	11.1	10.4	31.9
Total	1084.8	1384.1	1361.2	1436.7	1409.1	1424.2	900.8	679.5	550.8	545.2	625.7	757.6
Average	36.0	51.5	54.9	60.7	56.9	54.3	31.8	18.2	12.8	11.9	13.8	19.8

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Table B3: Mean monthly evaporation

Drainage region	Evaporation (mm)											
	OCT	NOV	DEC	JAN	FEB	MAR	APR	MAY	JUN	JULY	AUG	SEP
A	203.3	195.6	203.6	198.9	163.2	157.0	123.3	106.2	87.0	97.3	129.9	169.9
B	169.9	161.5	173.7	170.5	143.1	141.3	111.1	96.7	78.6	86.8	113.3	144.0
C	203.2	216.9	235.4	227.3	177.9	159.5	116.7	90.7	71.1	81.0	116.1	161.2
D	111.0	129.1	147.0	145.4	112.7	99.0	68.8	50.6	38.9	43.5	59.8	83.3
E	207.3	265.0	314.5	321.5	265.5	243.4	159.2	100.5	71.4	71.9	100.4	146.7
F	196.2	233.4	252.3	258.8	209.5	196.0	141.7	110.8	97.5	92.6	113.2	145.8
G	131.9	177.5	214.6	218.7	181.3	162.8	100.4	57.5	45.0	43.4	54.2	82.9
H	149.5	189.2	230.9	234.8	190.4	163.1	105.2	66.3	47.3	49.4	65.6	97.7
J	185.5	230.9	277.8	283.2	230.5	200.5	133.4	88.6	65.0	69.0	92.2	128.3
K	155.1	185.0	226.7	224.5	176.8	153.5	113.0	87.9	77.5	78.7	93.6	113.5
L	192.7	226.2	272.5	273.7	214.9	184.3	130.2	96.3	76.0	82.7	109.2	142.3
M	147.8	174.6	209.1	214.4	171.9	148.3	107.6	75.9	55.0	59.5	81.3	109.1
N	175.2	205.5	246.8	248.6	195.8	167.9	119.2	87.6	67.9	74.3	99.2	129.5
P	145.7	172.1	206.1	211.3	169.5	146.2	106.0	74.8	54.3	58.7	80.2	107.6
Q	170.2	194.0	226.7	224.7	178.1	154.9	110.3	84.1	67.3	74.7	103.7	133.9
R	135.6	144.1	164.5	164.1	134.6	121.6	89.1	70.3	101.1	83.6	81.8	103.4
S	149.6	163.1	186.4	186.2	149.7	136.5	105.8	87.9	75.9	85.2	103.4	124.6
T	233.6	251.5	279.7	275.4	227.1	207.5	154.4	118.9	97.9	110.7	159.4	197.8
U	114.6	120.5	136.5	134.7	118.4	117.9	90.6	75.3	64.4	70.3	86.8	100.9
V	141.1	145.1	156.5	153.8	132.2	127.2	101.6	85.9	72.0	79.5	104.5	122.6
W	134.6	137.8	150.7	152.9	130.2	126.1	95.4	80.0	66.7	73.5	96.2	118.9
X	142.6	142.3	161.7	169.4	145.2	142.5	108.1	94.3	77.5	83.6	105.9	128.4
Average	**159.0**	**175.5**	**197.2**	**195.6**	**157.1**	**142.7**	**103.1**	**79.2**	**63.1**	**69.3**	**93.7**	**124.9**

Table B4: WR90 model parameters

Drainage Region		POW (-)	SL (mm)	ST (mm)	FT (mm/m)	GW (1/d)	ZMIN (mm/m)	ZMAX (mm/m)	PI (mm)	TL (d)	GL (d)	R (-)
A	Area weighted average	1.28	0.00	198.98	3.46	0.08	141.55	958.46	1.48	0.25	0.75	0.49
	Minimum	0.00	0.00	55.00	0.00	0.00	25.00	727.11	1.09	0.18	0.00	0.36
	Average	1.71	0.00	208.68	5.69	0.13	181.47	973.01	1.50	0.26	1.18	0.50
	Maximum	3.00	0.00	500.00	50.00	1.00	999.00	1000.00	1.50	0.50	10.00	0.50
B	Area weighted average	0.00	0.00	250.00	0.00	0.00	100.00	800.00	1.50	0.25	0.00	0.50
	Minimum	0.00	0.00	105.54	0.00	0.00	0.00	520.64	0.93	0.15	0.00	0.31
	Average	1.39	0.00	227.66	7.29	0.03	380.78	884.91	1.51	0.28	0.34	0.50
	Maximum	3.00	0.00	600.00	50.00	0.20	999.00	1000.00	1.50	0.50	2.50	0.50
C	Area weighted average	1.17	0.00	134.48	1.58	0.01	250.25	790.82	1.47	0.26	0.04	0.20
	Minimum	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	Average	1.91	0.00	117.47	2.93	0.01	436.65	791.62	1.48	0.25	0.05	0.32
	Maximum	3.00	0.00	300.00	8.00	0.40	999.00	1100.00	1.50	0.50	2.00	0.50
D	Area weighted average	0.15	0.01	61.61	0.75	0.01	50.04	286.93	0.66	0.12	0.01	0.03
	Minimum	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	Average	0.93	0.00	94.88	4.84	0.00	260.07	644.78	1.46	0.24	0.00	0.15
	Maximum	3.00	0.10	300.00	25.00	0.10	999.00	999.00	1.50	0.28	0.10	0.50
E	Area weighted average	0.25	0.00	107.33	7.27	0.00	10.52	355.96	1.40	0.24	0.00	0.00
	Minimum	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	Average	0.54	0.00	127.30	16.22	0.00	8.92	401.96	1.46	0.26	0.00	0.00
	Maximum	2.00	0.00	250.00	75.00	0.00	15.00	600.00	1.50	1.50	0.25	0.00
F	Area weighted average	0.00	0.00	110.38	0.00	0.00	16.56	529.82	1.66	0.28	0.00	0.00
	Minimum	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	Average	0.00	0.00	100.00	0.00	0.00	15.00	480.00	1.50	0.25	0.00	0.00
	Maximum	0.00	0.00	238.20	0.00	0.00	35.73	1143.36	3.57	0.60	0.00	0.00
G	Area weighted average	0.00	0.00	195.00	0.00	0.00	0.00	350.00	1.39	0.23	0.00	0.00
	Minimum	1.65	0.00	253.16	20.56	0.00	18.86	441.23	1.53	0.25	0.00	0.00
	Average	2.00	0.00	270.00	100.00	0.00	30.00	500.00	1.50	0.25	0.00	0.00
	Maximum	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H	Area weighted average	1.37	0.00	227.87	18.17	0.00	16.37	321.00	1.50	0.25	0.00	0.00

Model Parameters

Table B4: continued

J	Minimum	0.00	0.00	150.00	0.00	0.00	0.00	180.00	1.50	0.25	0.00
	Average	1.39	0.00	231.16	23.20	0.00	15.51	338.70	1.50	0.25	0.00
	Maximum	2.00	0.00	450.00	75.00	0.00	50.00	900.00	1.50	0.25	0.00
	Area weighted average	0.49	0.00	152.84	1.87	0.00	9.79	356.25	1.50	0.25	0.00
K	Minimum	2.00	0.00	151.27	29.22	0.00	7.83	326.64	2.24	0.25	0.00
	Average	2.00	0.00	100.00	8.00	0.00	0.00	150.00	1.50	0.25	0.00
	Maximum	2.00	0.00	145.00	30.80	0.00	7.38	312.50	2.25	0.25	0.00
	Area weighted average	2.00	0.00	250.00	50.00	0.00	30.00	600.00	4.00	0.25	0.00
L	Minimum	0.33	0.00	133.28	1.64	0.00	10.01	406.96	1.34	0.22	0.00
	Average	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	Maximum	0.61	0.00	165.18	3.04	0.00	12.50	458.04	1.47	0.25	0.00
	Area weighted average	1.59	0.00	250.00	10.00	0.00	20.00	550.00	1.50	0.25	0.27
M	Minimum	0.00	0.00	123.46	2.65	0.00	31.73	388.15	1.50	0.25	0.00
	Average	0.00	0.00	100.00	0.00	0.00	20.00	360.00	1.50	0.25	0.00
	Maximum	1.50	0.00	143.75	2.50	0.00	38.13	442.50	1.69	0.28	0.25
	Area weighted average	3.00	0.00	150.00	5.00	0.00	45.00	420.00	1.50	0.25	0.50
N	Minimum	0.18	0.00	113.29	0.12	0.00	7.85	423.34	1.50	0.25	0.03
	Average	0.00	0.00	100.00	0.00	0.00	0.00	380.00	1.50	0.25	0.00
	Maximum	0.18	0.00	117.65	0.12	0.00	6.47	443.53	1.59	0.26	0.03
	Area weighted average	3.00	0.00	200.00	2.00	0.00	45.00	600.00	1.50	0.25	0.50
P	Minimum	1.11	0.00	168.48	0.74	0.00	35.76	486.53	1.50	0.25	0.18
	Average	0.00	0.00	150.00	0.00	0.00	20.00	420.00	1.50	0.25	0.00
	Maximum	1.13	0.00	168.75	0.75	0.00	35.63	487.50	1.50	0.25	0.19
	Area weighted average	3.00	0.00	200.00	2.00	0.00	45.00	600.00	1.50	0.25	0.50
Q	Minimum	0.43	0.00	111.72	0.75	0.00	10.66	466.01	1.48	0.25	0.07
	Average	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	Maximum	0.61	0.00	115.22	1.20	0.00	11.74	476.38	1.52	0.25	0.10
	Area weighted average	3.00	0.00	150.00	12.00	0.00	45.00	480.00	1.50	0.25	0.50
R	Area weighted average	3.00	0.00	162.76	5.33	0.00	45.00	458.31	1.50	0.25	0.50

Table B4: continued

	Minimum	3.00	0.00	150.00	4.00	0.00	45.00	420.00	1.50	0.25	0.00	0.50
	Average	3.00	0.00	161.67	6.40	0.00	45.00	462.67	1.50	0.25	0.00	0.50
	Maximum	3.00	0.00	200.00	12.00	0.00	45.00	600.00	1.50	0.25	0.00	0.50
S	Area weighted average	3.00	0.00	118.41	8.24	0.02	301.22	646.18	1.50	0.25	0.20	0.50
	Minimum	3.00	0.00	45.00	3.00	0.00	30.00	500.00	1.50	0.25	0.00	0.50
	Average	3.00	0.00	116.29	8.55	0.02	287.67	638.36	1.50	0.25	0.26	0.50
	Maximum	3.00	0.00	200.00	40.00	0.20	999.00	999.00	1.50	0.25	2.50	0.50
T	Area weighted average	3.00	0.00	120.26	17.08	0.00	999.00	999.00	1.50	0.25	0.00	0.48
	Minimum	3.00	0.00	45.00	10.00	0.00	999.00	999.00	1.50	0.25	0.00	0.50
	Average	3.05	0.00	123.60	16.82	0.00	1014.14	1014.14	1.52	0.25	0.00	0.51
	Maximum	3.00	0.00	200.00	30.00	0.00	999.00	999.00	1.50	0.25	0.00	0.50
U	Area weighted average	3.00	0.00	193.16	21.10	0.01	999.49	999.49	1.50	0.25	0.16	0.50
	Minimum	3.00	0.00	100.00	15.00	0.00	999.00	999.00	1.50	0.25	0.00	0.50
	Average	3.00	0.00	232.26	20.32	0.01	999.00	999.00	1.50	0.25	0.16	0.50
	Maximum	3.01	0.00	300.00	50.00	0.10	1001.05	1001.05	1.50	0.25	2.50	0.50
V	Area weighted average	3.02	0.00	118.77	20.17	0.00	1005.30	1005.30	1.51	0.25	0.11	0.50
	Minimum	3.00	0.00	100.00	15.00	0.00	999.00	999.00	1.50	0.25	0.00	0.50
	Average	3.00	0.00	121.63	22.27	0.01	999.00	999.00	1.50	0.25	0.15	0.50
	Maximum	3.20	0.00	200.00	50.00	0.10	1066.69	1066.69	1.60	0.27	2.50	0.53
W	Area weighted average	2.73	0.00	239.64	15.24	0.01	465.04	922.61	1.49	0.28	0.15	0.53
	Minimum	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	Average	2.67	0.00	214.97	17.81	0.02	448.53	928.80	1.51	0.30	0.14	0.50
	Maximum	3.00	0.00	600.00	60.00	0.30	999.00	999.00	1.50	0.50	2.50	1.26
X	Area weighted average	1.33	0.00	275.50	11.39	0.17	329.37	882.53	1.50	0.36	1.11	0.50
	Minimum	0.00	0.00	140.00	0.00	0.00	0.00	800.00	1.50	0.25	0.00	0.50
	Average	1.63	0.00	298.85	16.01	0.20	309.34	890.11	1.50	0.39	1.23	0.50
	Maximum	3.00	0.00	600.00	60.00	0.60	999.00	999.00	1.50	0.50	2.50	0.50
	Area weighted average	**0.706**	**0.004**	**107.446**	**3.369**	**0.014**	**149.809**	**488.128**	**1.051**	**0.183**	**0.090**	**0.140**
	Minimum	**0.00**	**0.00**	**0.00**	**0.00**	**0.00**	**0.00**	**0.00**	**0.00**	**0.00**	**0.00**	**0.00**
	Average	**1.63**	**0.00**	**166.42**	**14.06**	**0.02**	**252.43**	**633.54**	**1.54**	**0.26**	**0.16**	**0.25**
	Maximum	**3.20**	**0.10**	**600.00**	**100.00**	**1.00**	**999.00**	**999.00**	**4.00**	**1.50**	**10.00**	**1.26**

Table B5: Simulated natural river flow

Drainage Region	F *	Simulated natural river flow (million m3)											
		OCT	NOV	DEC	JAN	FEB	MAR	APR	MAY	JUN	JULY	AUG	SEP
A	0.01	52.83	123.60	219.68	424.07	480.40	357.22	189.35	95.88	68.17	56.01	46.85	40.39
B	0.11	63.99	188.49	256.13	439.50	510.05	392.48	195.44	99.10	69.34	55.44	46.63	42.38
C	0.00	271.33	537.41	506.17	769.97	764.17	628.98	314.10	123.76	50.54	40.05	40.64	119.42
D	0.00	454.00	569.77	566.70	901.50	1141.65	1376.06	804.81	368.23	183.90	152.35	177.14	272.40
E	0.00	73.04	35.42	14.73	7.54	6.61	7.37	32.60	78.03	202.06	202.09	208.22	140.43
F	0.00	0.38	0.49	0.41	0.09	0.20	0.20	0.86	1.97	9.48	4.49	3.96	1.48
G	0.01	169.13	92.56	36.28	15.93	16.11	15.29	55.54	164.09	318.56	374.50	424.04	283.79
H	0.01	136.60	101.52	45.07	37.88	44.75	62.30	158.44	266.14	322.75	333.97	324.42	137.55
J	0.02	41.94	56.25	54.46	45.21	60.93	80.12	72.23	54.53	42.24	38.32	56.76	45.71
K	0.31	101.16	88.53	63.60	52.27	49.73	66.40	62.96	77.34	63.07	69.33	100.55	107.09
L	0.02	32.13	38.34	35.42	33.71	51.54	71.84	39.16	43.22	27.95	28.67	46.53	36.73
M	0.00	16.40	14.37	8.81	4.94	4.28	12.62	10.65	13.95	10.35	15.87	17.98	20.66
N	0.00	18.62	24.04	25.78	20.81	30.72	61.23	29.20	19.02	6.50	8.94	19.35	15.83

8.9430.728.28170.82547 88.765 505. Tj 21.7275.25 315.75 45.75 0.75 75 0.75 75 0.75 75 0.75 75 45097 328.53.75 5 re f 275.25 315.75 45.75 0. 50.97 328.53.75 328.53.75 328.53.75

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Table B 6: Calculation of irrigation factor

	Rainfall (mm/m)											
Province	JAN	FEB	MAR	APR	MAY	JUN	JUL	AUG	SEP	OCT	NOV	DEC

JULJUL

B.2 SURFACE WATER QUALITY

Water quality data was obtained from the *Water Quality on Disc* database, provided by the Directorate of Hydrology and the Institute for Water Quality Studies. The database contains data for an intensive network of water quality monitoring points up to the end of September 1999.

The approach adopted and the methodology for calculating the average monthly total dissolved salt concentration in the "unit South African river" is described below.

Step 1: The river gauging station closest to the primary catchment outlet was identified and the water quality data for this station was extracted from the database. Where no gauging stations were available at the primary catchment outlet, the gauging station at the outlet of the secondary catchment was identified and the water quality data extracted from the database. Where no gauging stations were available at the seconday catchment outlet, the gauging station at the outlet of the tertiary catchment was identified and the water quality data extracted from the database. Where no gauging stations were available at the tertiary catchment outlet, the gauging station at the outlet of the quaternary catchment was identified and the water quality data extracted from the database. In some instances, no water quality data were available, particularly at quaternary level. In these instances, the data from the closest gauging station were used.

Step 2: The water quality data extracted was then examined to determine the year in which the data set for that year was the most complete (i.e. had the most data points). The year in which the data set was most complete was recorded as the "reference year".

Step 3: The average monthly salt concentrations were then calculated for the reference year. In some instances, only one data point was available for a particular month, and this value was then used as the average value for the month. In some instances, no data were available for a particular month of the reference year. In these instances, the median between the preceding month and following month was taken as the average value for that month. In a very few instances, no data was available for two successive months. In these instances, the average was calculated from the preceding year's data.

Step 4: All water quality data were then adjusted to a common year (2000) as follows; The total dissolved salt concentrations for all catchments (primary, secondary, tertiary or quaternary, depending on the catchment level for which data was available) were plotted against time, and a linear regression curve was fitted to the data, in order to identify any upward or downward trends in water quality. A growth factor (slope of the linear regression curve) was calculated for each catchment. The plotted water quality data, and the number of data points available were examined, and a decision was made to either use the calculated growth factor or not. The selected growth factor was then use to adjust the salt concentrations at the reference year to the common year (2000). It should be mentioned that in only a very few instances were the calculated growth factors used. In most cases a growth factor of zero was selected, either because of the small number of data points available, or because no obvious trend was observed. The projected salt concentration at the year 2000 was then calculated by multiplying the salt concentration at the reference year with the chosen growth factor.

Step 5: The total monthly salt load at each catchment level identified in Step 1, for the year 2000, was calculated by multiplying the river flow for that catchment by the projected salt concentration for the year 2000.

Step 6: The total monthly salt loads for the "unit South African river" were then calculated by adding the salt loads from each drainage region, and dividing by the total monthly flow for the drainage region.

The results of the water quality analysis for each drainage region are presented in Tables B7 to B28. The tables indicate the catchment (either at primary, secondary or tertiary scale), the gauging station used, the reference year selected, the number of data points available for regression analysis, the calculated growth factor and the chosen growth factor. The river flows at the catchment level chosen, and the calculated monthly salt concentrations are indicated.

Table B 29 contains a summary of the TDS data for each drainage region, and the calculated monthly "unit South African river" salt concentrations. The average monthly salt concentrations are shown graphically in Figure B3.
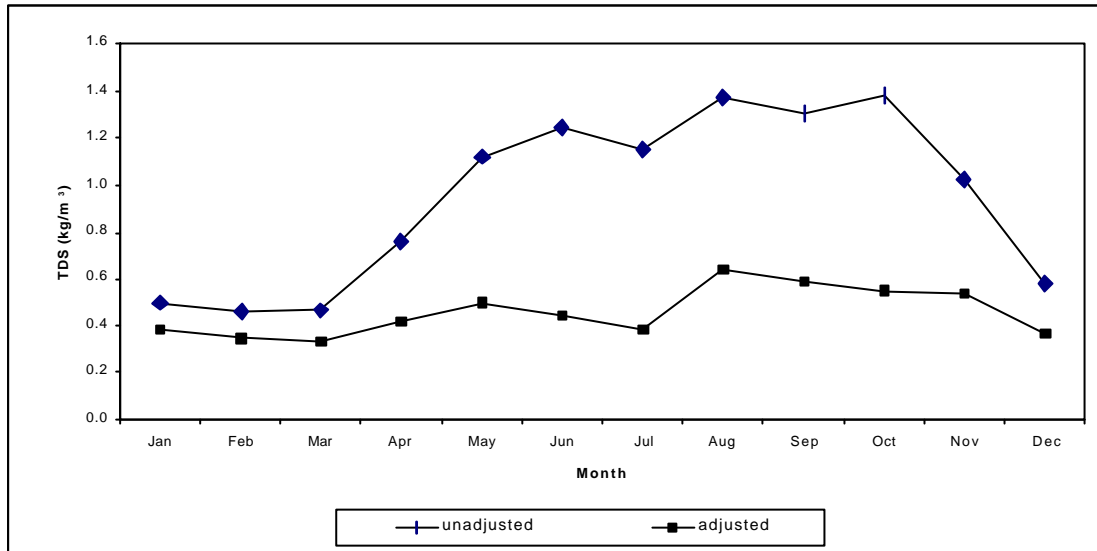
Figure B3: Average monthly total dissolved salt concentration and flow for the "unit South

From Table B9 it can be seen that The salt loads from drainage regions G and K together constitute 49% of the total annual load in the "unit river", due to the high natural salinity in these drainage regions. Their combined flow, however, only constitute 6.5% of the total annual flow in the "unit river". Figure B3 shows the unadjusted monthly average salt concentrations, and adjusted values. The adjusted values were calculated by assuming that the average monthly concentrations in drainage region G were equal to those of drainage region E, and that the average monthly concentrations in drainage region K were equal to those of drainage region J. The adjusted concentration values are most likely more representative of an "average South African river" since the rivers in drainage region G and K are generally short, and only make up a small fraction of the total flow. It was decided, however, to calibrate the model using the unadjusted values. Calibration of the model using adjusted values could be achieved by adjusting the surface salt generation rate, however, it was shown in **Section 5.4**, that adjustment of these model parameters do not influence the values of the fate factors.

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Table B7: Water quality data for drainage region A

Catchment	Guage	River		Year	n	Calculated growth factor	Growth factor used	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
A10	A1H001-A1H005		Ave TDS (ref year)	1998	423	1.227	1.227	389.20	420.00	398.40	421.33	368.00	395.25	387.50	389.40	316.00	380.00	417.33	403.00
			Ave TDS (2000)	2000				391.65	422.45	400.85	423.79	370.45	397.70	389.95	391.85	318.45	382.45	419.79	405.45
			Stream flow					2.93	2.93	3.11	2.60	0.61	0.04	0.02	0.00	0.01	0.14	0.48	1.43
A31-A32	A3H007		Ave TDS (ref year)	1982	172	-26.233	0.000	345.00	254.76	181.23	232.59	281.55	337.78	467.85	597.92	583.60	397.44	108.23	152.43
			Ave TDS (2000)	2000				345.00	254.76	181.23	232.59	281.55	337.78	467.85	597.92	583.60	397.44	108.23	152.43
			Stream flow					23.41	26.23	22.64	16.92	6.41	2.92	2.36	1.86	1.61	2.33	5.73	11.87
A21	A2H019		Ave TDS (ref year)	1999	547	-0.556	0.000	421.50	414.00	434.67	460.50	460.00	470.00	475.00	461.00	471.64	498.00	492.00	390.00
			Ave TDS (2000)	2000				421.50	414.00	434.67	460.50	460.00	470.00	475.00	461.00	471.64	498.00	492.00	390.00
			Stream flow					33.58	35.91	27.87	18.14	12.36	10.13	9.05	7.97	7.27	8.59	16.29	20.29
A22	A2H110		Ave TDS (ref year)	1986	55	19.031	0.000	614.84	603.90	634.05	671.73	671.00	507.47	504.96	541.00	630.00	726.43	717.68	568.89
			Ave TDS (2000)	2000				614.84	603.90	634.05	671.73	671.00	507.47	504.96	541.00	630.00	726.43	717.68	568.89
			Stream flow					21.51	26.59	22.68	11.28	4.27	2.52	1.89	1.42	1.33	1.78	4.99	10.89
A23	A2H021		Ave TDS (ref year)	1999	812	2.074	2.074	372.00	386.00	376.33	464.50	502.50	427.50	444.50	447.00	452.00	514.00	480.00	403.00
			Ave TDS (2000)	2000				374.07	388.07	378.41	466.57	504.57	429.57	446.57	449.07	454.07	516.07	482.07	405.07
			Stream flow					26.95	23.13	16.82	11.34	7.81	6.06	5.14	4.35	3.55	5.19	13.60	16.39
A24	A2H037	Crocodile	Ave TDS (ref year)	1990	119	52.520	5.000	480.07	456.86	496.73	533.37	496.17	536.58	571.50	576.92	567.99	559.06	586.10	543.15
			Ave TDS (2000)	2000				530.07	506.86	546.73	583.37	546.17	586.58	621.50	626.92	617.99	609.06	636.10	593.15
			Stream flow					28.49	29.44	18.90	8.90	3.18	1.64	1.28	1.02	0.80	2.01	7.12	14.07
A41	A4H004	Matlabas	Ave TDS (ref year)	1998	216	1.545	1.545	26.00	19.00	37.00	34.00	39.00	38.00	45.00	76.00	106.50	131.00	99.50	68.00
			Ave TDS (2000)	2000				29.09	22.09	40.09	37.09	42.09	41.09	48.09	79.09	109.59	134.09	102.59	71.09
			Stream flow					10.49	15.51	7.84	2.12	0.56	0.24	0.17	0.13	0.11	0.67	3.28	7.13
A42	A4H013		Ave TDS (ref year)	1998	98	-1.469	0.000	71.50	66.00	63.00	66.00	74.00	53.50	69.50	54.00	68.50	62.00	77.50	62.00
			Ave TDS (2000)	2000				71.50	66.00	63.00	66.00	74.00	53.50	69.50	54.00	68.50	62.00	77.50	62.00
			Stream flow					57.14	76.09	50.22	22.21	12.76	9.66	8.45	7.18	6.17	8.78	17.76	32.80
A50	A5H008	Palala	Ave TDS (ref year)	1997	44	7.844	0.000	65.00	9.83	52.00	78.00	81.50	77.00	108.00	103.00	142.00	100.00	80.00	59.80
			Ave TDS (2000)	2000				65.00	9.83	52.00	78.00	81.50	77.00	108.00	103.00	142.00	100.00	80.00	59.80
			Stream flow					30.76	34.08	22.10	9.20	4.54	3.08	2.34	2.07	1.61	2.88	9.27	18.43
A61-A63	A6H009		Ave TDS (ref year)	1996	328	-11.328	0.000	181.00	123.75	144.00	200.25	277.75	287.67	333.83	380.00	359.00	327.25	295.50	174.00
			Ave TDS (2000)	2000				181.00	123.75	144.00	200.25	277.75	287.67	333.83	380.00	359.00	327.25	295.50	174.00
			Stream flow					55.16	58.10	33.40	17.33	10.65	7.59	5.97	4.81	3.96	5.10	17.88	32.43
A71-A72	A7H005	Sand	Ave TDS (ref year)	1981	89	-10.450	0.000	207.80	314.22	444.63	501.00	457.56	465.50	491.44	559.00	488.76	418.52	348.28	278.04
			Ave TDS (2000)	2000				207.80	314.22	444.63	501.00	457.56	465.50	491.44	559.00	488.76	418.52	348.28	278.04
			Stream flow					23.77	14.91	8.04	2.55	0.29	0.04	0.01	0.02	0.11	0.90	4.73	8.28
A80	A8H007		Ave TDS (ref year)	1981	78	-6.305	0.000	181.00	118.67	116.75	125.00	131.40	130.33	147.00	132.67	133.25	154.80	163.50	162.00
			Ave TDS (2000)	2000				181.00	118.67	116.75	125.00	131.40	130.33	147.00	132.67	133.25	154.80	163.50	162.00
			Stream flow					26.58	30.00	22.15	8.91	3.97	2.77	2.08	1.62	1.34	1.64	3.39	7.64
A91	A9H007		Ave TDS (ref year)	1991	206	-1.827	0.000	73.00	86.00	71.00	75.67	0.00	90.00	98.33	100.67	103.50	107.00	96.00	84.00
			Ave TDS (2000)	2000				73.00	86.00	71.00	75.67	0.00	90.00	98.33	100.67	103.50	107.00	96.00	84.00
			Stream flow					56.47	73.96	70.93	41.08	20.43	15.64	12.73	10.72	9.35	9.37	13.32	25.27
A92	A9H010		Ave TDS (ref year)	1991	218	-5.105	0.000	73.00	87.00	63.00	61.00	76.33	85.75	88.60	94.80	112.00	150.00	124.00	99.00
			Ave TDS (2000)	2000				73.00	87.00	63.00	61.00	76.33	85.75	88.60	94.80	112.00	150.00	124.00	99.00
			Stream flow					26.81	33.52	30.52	16.78	8.04	5.83	4.53	3.68	3.18	3.45	5.78	12.76

n = number of water quality data points available to calculate growth factor
TDS expressed as mg/l

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Table B8: Water quality data for drainage region B

Catchment	Guage	River		Year	n	Calculated growth factor	Growth factor Used	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
B11-B12,B20,B31-B32 B41-B42,B51-B52,B60 B71-B73	B7H017	Olifants	Ave TDS (ref year)	1999	336	24.770	1.000	236.33	354.00	345.50	228.25	307.75	379.00	454.00	457.50	584.00	860.50	1137.00	252.00
			Ave TDS (2000)	2000				237.33	355.00	346.50	229.25	308.75	380.00	455.00	458.50	585.00	861.50	1138.00	253.00
			Stream flow					316.33	357.08	265.54	143.99	80.00	54.93	43.65	36.61	33.56	54.98	172.18	212.22
B81-B83			Ave TDS (ref year)	1984	27	2.542	0.000	131.33	261.50	341.50	175.00	215.50	286.50	308.00	249.50	191.00	284.00	203.00	136.00
			Ave TDS (2000)	2000				131.33	261.50	341.50	175.00	215.50	286.50	308.00	249.50	191.00	284.00	203.00	136.00
			Stream flow					95.55	130.31	112.40	47.91	19.01	14.41	11.79	10.01	8.78	8.95	14.95	36.89
B90	B9H003	Shingwidzi	Ave TDS (ref year)	1998	192	24.740	2	522.00	520.00	670.50	330.00	369.00	396.00	398.00	411.25	401.00	427.25	488.00	505.00
			Ave TDS (2000)	2000				526.00	524.00	674.50	334.00	373.00	400.00	402.00	415.25	405.00	431.25	492.00	509.00
			Stream flow					27.62	22.66	14.54	3.53	0.09	0.00	0.00	0.00	0.04	0.06	1.36	7.02

n = number of water quality data points available to calculate growth factor
TDS expressed as mg/l

Table B9: Water quality data for drainage region C

Catchment	Guage	River		Year	n	Calculated growth factor	Growth factor used	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
All	C9H011	Vaal	Ave TDS (ref year)	1981	71	-0.076	0.000	1030.50	890.67	488.00	926.50	754.33	745.00	853.67	767.21	941.02	977.30	871.37	744.04
			Ave TDS (2000)	2000				1030.50	890.67	488.00	926.50	754.33	745.00	853.67	767.21	941.02	977.30	871.37	744.04
			Stream flow					769.97	764.17	628.98	314.10	123.76	50.54	40.05	40.64	119.42	271.33	537.41	506.17

n = number of water quality data points available to calculate growth factor
TDS expressed as mg/l

Table B10: Water quality data for drainage region D

Catchment	Guage	River		Year	n	Calculated growth factor	Growth factor used	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
All except D41-D42	D8H008	Orange	Ave TDS (ref year)	1999	214	-26.035	0.000	333.67	419.50	403.60	355.00	314.00	281.50	330.67	388.00	201.25	248.50	307.50	304.40
			Ave TDS (2000)	2000				333.67	419.50	403.60	355.00	314.00	281.50	330.67	388.00	201.25	248.50	307.50	304.40
			Stream flow					883.91	1128.93	1366.52	800.92	367.72	183.88	152.34	177.13	272.38	453.70	568.22	563.61
D41-D42	D4H003	Molopo	Ave TDS (ref year)	1998	72	25.712	25.712	481.00	354.00	335.50	346.00	363.00	367.67	376.75	377.00	390.00	398.00	355.00	367.00
			Ave TDS (2000)	2000				532.42	405.42	386.92	397.42	414.42	419.09	428.17	428.42	441.42	449.42	406.42	418.42
			Stream flow					17.59	12.72	9.54	3.89	0.51	0.02	0.01	0.01	0.02	0.30	1.55	3.09

n = number of water quality data points available to calculate growth factor
TDS expressed as mg/l

Table B11: Water quality data for drainage region E

Catchment	Guage	River		Year	n	Calculated growth factor	Growth factor used	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
E33F- E33G	E3H001	Olifants	Ave TDS (ref year)	1997	546	-2.448	0.000	265.00	272.50	345.25	321.00	241.75	226.00	98.00	69.67	166.20	229.25	284.50	184.67
			Ave TDS (2000)	2000				265.00	272.50	345.25	321.00	241.75	226.00	98.00	69.67	166.20	229.25	284.50	184.67
			Stream flow					0.01	0.01	0.01	0.15	0.31	0.87	0.39	0.22	0.10	0.02	0.04	0.04
E21- E24, E40	E2H003		Ave TDS (ref year)	1997	546	-2.448	0.000	265.00	272.50	345.25	321.00	241.75	226.00	98.00	69.67	166.20	229.25	284.50	184.67
			Ave TDS (2000)	2000				265.00	272.50	345.25	321.00	241.75	226.00	98.00	69.67	166.20	229.25	284.50	184.67
			Stream flow					5.95	5.13	4.99	22.08	41.25	105.53	93.40	96.81	65.60	36.49	20.30	9.64
E10	E1H007		Ave TDS (ref year)	1988	77	0.248	0.000	61.00	52.00	49.00	62.00	15.00	49.00	48.00	48.00	54.00	52.00	50.00	48.00
			Ave TDS (2000)	2000				61.00	52.00	49.00	62.00	15.00	49.00	48.00	48.00	54.00	52.00	50.00	48.00
			Stream flow					1.39	1.22	1.93	8.60	32.57	86.07	104.00	107.97	73.33	36.28	14.42	4.42
E31-E33 A-E	F6H001*		Ave TDS (ref year)	1999	40	-72.605	0.000	3204.00	3012.00	3515.00	3388.50	3262.00	3198.00	3300.00	3861.00	3050.00	4132.00	4229.00	4015.00
			Ave TDS (2000)	2000				3204.00	3012.00	3515.00	3388.50	3262.00	3198.00	3300.00	3861.00	3050.00	4132.00	4229.00	4015.00
			Stream flow					0.19	0.25	0.44	1.71	3.76	9.21	4.13	3.13	1.36	0.24	0.64	0.62

n = number of water quality data points available to calculate growth factor

TDS expressed as mg/l

* No guaging station in catchment. Closest guaging satation used

Table B12: Water quality data for drainage region F

Catchment	Guage	River		Year	n	Calculated growth factor	Growth factor used	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
F30,F40,F50	F5H001*	Groen	Ave TDS (ref year)	1995	2	-72.605	0.000	3204.00	3012.00	3515.00	3388.50	3262.00	3198.00	3300.00	3861.00	3050.00	4132.00	4229.00	3545.00
			Ave TDS (2000)	2000				3204.00	3012.00	3515.00	3388.50	3262.00	3198.00	3300.00	3861.00	3050.00	4132.00	4229.00	3545.00
			Stream flow					0.06	0.20	0.20	0.75	1.73	8.86	4.12	3.72	1.42	0.36	0.45	0.30
F60	F6H001	Sout	Ave TDS (ref year)	1995	40	-72.605	0.000	3204.00	3012.00	3515.00	3388.50	3262.00	3198.00	3300.00	3861.00	3050.00	4132.00	4229.00	3545.00
			Ave TDS (2000)	2000				3204.00	3012.00	3515.00	3388.50	3262.00	3198.00	3300.00	3861.00	3050.00	4132.00	4229.00	3545.00
			Stream flow					0.00	0.00	0.00	0.06	0.07	0.31	0.13	0.09	0.03	0.01	0.01	0.01
F10, F20	D8H012*		Ave TDS (ref year)	1999	216	-24.381	0.000	306.33	419.50	403.60	355.00	314.00	281.50	281.00	318.80	201.25	248.50	315.00	304.40
			Ave TDS (2000)	2000				306.33	306.33	306.33	306.33	306.33	306.33	306.33	306.33	306.33	306.33	306.33	306.33
			Stream flow					0.03	0.00	0.00	0.05	0.17	0.31	0.24	0.15	0.03	0.01	0.03	0.10

n = number of water quality data points available to calculate growth factor

TDS expressed as mg/l

* No guaging station in this catchment. Closest gauging station used

Table B13: Water quality data for drainage region G

Catchment	Guage	River		Year	n	Calculated growth factor	Growth factor used	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
G30 A-H	G3H004	Verlore Vlei	Ave TDS (ref year)	1999	510	-2.555	0.000	420.50	420.00	394.25	309.00	166.00	192.56	261.15	147.00	206.67	270.67	235.25	356.00
			Ave TDS (2000)	2000				420.50	420.00	394.25	309.00	166.00	192.56	261.15	147.00	206.67	270.67	235.25	356.00
			Stream flow					0.19	0.11	0.12	1.17	4.76	13.28	9.96	11.45	6.98	3.53	1.88	0.70
G10	G1H024	Berg	Ave TDS (ref year)	1998	151	-580.127	0.000	26718.00	23716.00	28185.00	29174.00	6187.00	2581.00	451.00	813.00	573.00	11471.00	21949.00	13708.00
			Ave TDS (2000)	2000				26718.00	23716.00	28185.00	29174.00	6187.00	2581.00	451.00	813.00	573.00	11471.00	21949.00	13708.00
			Stream flow					5.37	4.16	4.83	20.84	76.56	154.63	183.13	198.83	131.03	72.36	37.70	14.72
G21A-B	G2H018 *	Diep	Ave TDS (ref year)	1990	302	3.039	3.039	492.00	491.00	501.50	512.00	544.00	510.00	536.00	495.00	498.00	510.00	520.00	473.00
			Ave TDS (2000)	2000				522.39	521.39	531.89	542.39	574.39	540.39	566.39	525.39	528.39	540.39	550.39	503.39
			Stream flow					0.17	0.09	0.07	0.53	2.55	5.66	7.32	8.95	5.19	5.89	1.39	0.52
G21 C-F	G2H014		Ave TDS (ref year)	1982	265	31.772	10.000	4449.18	1249.00	2289.00	1526.00	1307.00	1701.96	1454.89	1384.00	1978.03	1931.34	2950.22	3993.31
			Ave TDS (2000)	2000				4629.18	1429.00	2469.00	1706.00	1487.00	1881.96	1634.89	1564.00	2158.03	2111.34	3130.22	4173.31
			Stream flow					0.31	0.16	0.13	0.96	4.63	10.27	13.28	16.25	9.42	4.81	2.52	0.95
G22 A-D	G2H013 *		Ave TDS (ref year)	1985	335	-24.908	0.000	161.00	3067.00	1141.65	333.02	324.88	790.02	1054.81	934.05	1549.05	1691.07	2318.98	2776.90
			Ave TDS (2000)	2000				161.00	3067.00	1141.65	333.02	324.88	790.02	1054.81	934.05	1549.05	1691.07	2318.98	2776.90
			Stream flow					1.21	0.92	0.92	4.01	11.90	22.91	31.54	35.86	22.76	12.51	6.64	2.82
G22 F-H	G2H002	Eerste	Ave TDS (ref year)	1999	510	-2.555	0.000	420.50	420.00	394.25	309.00	166.00	192.56	261.15	147.00	206.67	270.67	235.25	356.00
			Ave TDS (2000)	2000				420.50	420.00	394.25	309.00	166.00	192.56	261.15	147.00	206.67	270.67	235.25	356.00
			Stream flow					0.57	0.44	0.44	1.89	5.61	10.79	14.86	16.89	10.72	5.89	3.13	1.33
G 22 E	G2H021		Ave TDS (ref year)	1987	365	-2.984	0.000	589.81	667.03	669.83	641.23	549.70	534.95	771.40	384.34	606.61	764.12	622.89	672.69
			Ave TDS (2000)	2000				589.81	667.03	669.83	641.23	549.70	534.95	771.40	384.34	606.61	764.12	622.89	672.69
			Stream flow					0.39	0.30	0.30	1.28	3.81	7.33	10.09	11.47	7.28	4.00	2.12	0.90
G 22 J	G2H029	Lourens	Ave TDS (ref year)	1994	398	-51.564	0.000	242.00	1383.75	2980.50	177.50	354.67	79.00	88.50	84.00	103.33	106.80	153.33	312.00
			Ave TDS (2000)	2000				242.00	1383.75	2980.50	177.50	354.67	79.00	88.50	84.00	103.33	106.80	153.33	312.00
			Stream flow					0.18	0.14	0.14	0.61	1.80	3.46	4.77	5.42	3.44	1.89	1.00	0.43
G 22 K	G2H039	Sir Lowry's pass	Ave TDS (ref year)	1998	298	2.662	0.000	158.40	194.00	194.00	175.33	156.67	184.80	150.50	126.00	145.00	137.00	123.25	145.00
			Ave TDS (2000)	2000				158.40	194.00	194.00	175.33	156.67	184.80	150.50	126.00	145.00	137.00	123.25	145.00
			Stream flow					0.11	0.09	0.09	0.38	1.12	2.16	2.98	3.39	2.15	1.18	0.63	0.27
G 40 A	G4R001	Steenbras	Ave TDS (ref year)	1998	156	0.111	0.000	46.50	48.00	47.00	41.00	35.00	44.00	39.00	34.00	44.00	45.00	53.00	49.75
			Ave TDS (2000)	2000				46.50	48.00	47.00	41.00	35.00	44.00	39.00	34.00	44.00	45.00	53.00	49.75
			Stream flow					0.14	0.15	0.13	0.39	1.01	1.82	2.01	2.33	1.71	1.11	0.64	0.26
G40 B-D	G4H007	Palmiet	Ave TDS (ref year)	1999	997	0.712	0.712	67.50	65.50	62.50	68.25	90.00	77.00	88.00	72.20	90.00	86.75	78.00	94.20
			Ave TDS (2000)	2000				68.21	66.21	63.21	68.96	90.71	77.71	88.71	72.91	90.71	87.46	78.71	94.91
			Stream flow					1.13	1.26	1.10	3.25	8.33	14.98	16.62	19.23	14.15	9.14	5.28	2.16
G 40 E-G	G4R003	Bot	Ave TDS (ref year)	1998	387	-251.258	0.000	4861.00	5265.00	6041.00	10740.00	4148.00	10276.00	13659.00	8669.00	11314.00	12099.00	11663.00	4970.00
			Ave TDS (2000)	2000				4861.00	5265.00	6041.00	10740.00	4148.00	10276.00	13659.00	8669.00	11314.00	12099.00	11663.00	4970.00
			Stream flow					1.75	1.95	1.70	5.04	12.90	23.21	25.74	29.79	21.91	14.16	8.18	3.34
G 40 J-L	G4H006	Klein	Ave TDS (ref year)	1998	309	3.067	0.000	246.00	638.00	730.00	610.50	491.00	834.00	632.00	608.00	584.00	463.50	343.00	246.00
			Ave TDS (2000)	2000				246.00	638.00	730.00	610.50	491.00	834.00	632.00	608.00	584.00	463.50	343.00	246.00
			Stream flow					1.87	2.08	1.81	5.38	13.78	24.80	27.50	31.83	23.41	15.13	8.74	3.57
G 50 A- F, G50J-K	G5H005	Kars	Ave TDS (ref year)	1987	9	-112.563	0.000	1614.00	592.00	592.00	592.00	592.00	592.00	592.00	592.00	592.00	592.00	484.67	484.67
			Ave TDS (2000)	2000				1614.00	592.00	592.00	592.00	592.00	592.00	592.00	592.00	592.00	592.00	484.67	484.67
			Stream flow					1.11	2.26	1.82	4.98	5.93	7.63	7.71	11.54	8.38	9.24	5.85	1.77
G 50 H, G 50 G	G5H008	Salt	Ave TDS (ref year)	1998	259	13.167	0.000	9987.00	6288.50	6288.50	6288.50	2590.00	4863.00	5041.00	4815.00	6473.00	7563.00	1511.50	3222.00
			Ave TDS (2000)	2000				9987.00	6288.50	6288.50	6288.50	2590.00	4863.00	5041.00	4815.00	6473.00	7563.00	1511.50	3222.00
			Stream flow					0.49	1.00	0.80	2.19	6.87	12.36	13.71	15.87	11.67	4.07	2.58	0.78
G 40 H, G40M	G4R004 *		Ave TDS (ref year)	1998	347	-515.617	0.000	26593.00	29527.00	26936.00	29989.00	10929.00	25478.00	20657.00	20455.00	19865.00	23497.00	20754.00	2161.00
			Ave TDS (2000)	2000				26593.00	29527.00	26936.00	29989.00	10929.00	25478.00	20657.00	20455.00	19865.00	23497.00	20754.00	2161.00
			Stream flow					0.93	1.04	0.90	2.68	6.87	12.36	13.71	15.87	11.67	7.54	4.35	1.78

n = number of water quality data points available to calculate growth factor

TDS expressed as mg/l

* No guaging station in catchment. Closest guaging satation used

Table B14: Water quality data for drainage region H

Catchment	Guage	River		Year	n	Calculated growth factor	Growth factor used	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
H10, H20,H30,H40 H50,H 60, H70 A-H	H7H006	Bree	Ave TDS (ref year)	1998	841	5.514	0.000	445.00	275.00	562.00	456.00	350.00	242.00	134.00	229.00	417.00	325.00	623.00	212.00
			Ave TDS (2000)	2000				445.00	275.00	562.00	456.00	350.00	242.00	134.00	229.00	417.00	325.00	623.00	212.00
			Stream flow					27.22	31.15	44.08	134.29	244.79	307.34	316.93	296.54	112.43	110.83	76.09	32.23
H 70 J-K	H7H003	Breede	Ave TDS (ref year)	1992	636	-0.744	0.000	72.24	81.19	86.52	106.39	86.94	110.67	114.80	105.80	126.77	60.92	126.40	116.47
			Ave TDS (2000)	2000				72.24	81.19	86.52	106.39	86.94	110.67	114.80	105.80	126.77	60.92	126.40	116.47
			Stream flow					2.23	3.06	3.75	5.39	4.87	3.59	4.06	6.71	5.73	5.51	5.35	2.64
H80	H8H001		Ave TDS (ref year)	1999	774	-1.873	0.000	95.00	111.00	86.00	193.00	211.50	230.00	357.00	70.00	167.00	171.00	472.00	43.00
			Ave TDS (2000)	2000				95.00	111.00	86.00	193.00	211.50	230.00	357.00	70.00	167.00	171.00	472.00	43.00
			Stream flow					4.14	5.21	7.15	9.14	8.08	6.04	6.86	11.07	10.12	10.27	9.92	5.02
H 90 B-C	H9H002		Ave TDS (ref year)	1998	171	0.302	0.000	101.00	51.00	75.00	91.00	66.00	83.33	65.00	78.00	74.00	78.00	71.00	84.00
			Ave TDS (2000)	2000				101.00	51.00	75.00	91.00	66.00	83.33	65.00	78.00	74.00	78.00	71.00	84.00
			Stream flow					0.89	1.11	1.52	2.00	1.75	1.20	1.27	2.11	1.93	2.08	2.12	1.08
H 90 A	H9H005		Ave TDS (ref year)	1999	373	18.108	0.000	264.00	315.50	367.00	237.00	306.50	376.00	589.00	532.00	400.50	532.00	2791.00	1744.00
			Ave TDS (2000)	2000				264.00	315.50	367.00	237.00	306.50	376.00	589.00	532.00	400.50	532.00	2791.00	1744.00
			Stream flow					0.48	0.59	0.81	1.07	0.93	0.64	0.68	1.12	1.03	1.11	1.13	0.58
H 90 D	H9H006 *		Ave TDS (ref year)	1999	221	-0.750	0.000	38.00	49.00	60.00	53.50	47.00	48.50	47.00	40.00	39.00	46.00	44.00	48.00
			Ave TDS (2000)	2000				38.00	49.00	60.00	53.50	47.00	48.50	47.00	40.00	39.00	46.00	44.00	48.00
			Stream flow					2.92	3.63	4.98	6.55	5.72	3.94	4.16	6.88	6.31	6.81	6.91	3.53

n = number of water quality data points available to calculate growth factor

TDS expressed as mg/l

* No guaging station in catchment. Closest guaging sataion used

Table B15: Water quality data for drainage region J

Catchment	Guage	River		Year	n	Calculated growth factor	Growth factor used	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
All	J4H004	Gouritz	Ave TDS (ref year)	1998	356	0.239	0.000	192.00	218.00	185.00	171.00	159.00	170.00	165.00	165.00	220.00	238.00	264.00	223.00
			Ave TDS (2000)	2000				192.00	218.00	185.00	171.00	159.00	170.00	165.00	165.00	220.00	238.00	264.00	223.00
			Stream flow					44.30	59.71	78.51	70.78	53.44	41.39	37.55	55.63	44.79	41.11	55.13	53.37

n = number of water quality data points available to calculate growth factor

TDS expressed as mg/l

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Table B16: Water quality data for drainage region K

Catchment	Guage	River		Year	n	Calculated growth factor	Growth factor used	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
K10 A-B	K1H009	Hartenbos	Ave TDS (ref year)	1997	84	-908.024	0.000	35532.00	35715.00	28246.00	20777.00	33165.00	23718.00	25965.00	27102.00	28239.00	28649.00	29059.00	29635.00
			Ave TDS (2000)	2000				35532.00	35715.00	28246.00	20777.00	33165.00	23718.00	25965.00	27102.00	28239.00	28649.00	29059.00	29635.00
			Stream flow					0.89	0.91	1.53	1.67	1.53	1.02	1.05	1.93	1.88	1.81	1.94	1.05
K10 C-F	K1H014	Little Brak	Ave TDS (ref year)	1992	49	-20.697	0.000	183.00	188.00	175.00	162.00	162.00	176.00	176.50	177.00	196.00	148.00	160.00	175.00
			Ave TDS (2000)	2000				183.00	188.00	175.00	162.00	162.00	176.00	176.50	177.00	196.00	148.00	160.00	175.00
			Stream flow					1.43	1.46	2.46	2.69	2.46	1.65	1.70	3.11	3.03	2.92	3.12	1.69
K20 A	K2H004	Great Brak	Ave TDS (ref year)	1998	140	647.147	0.000	29592.00	33829.00	28229.00	17676.00	24500.00	20213.00	27389.00	3034.00	29025.00	31300.00	30990.00	34543.00
			Ave TDS (2000)	2000				29592.00	33829.00	28229.00	17676.00	24500.00	20213.00	27389.00	3034.00	29025.00	31300.00	30990.00	34543.00
			Stream flow					1.99	1.98	2.79	2.38	2.15	1.46	1.58	2.42	2.86	3.00	2.96	2.21
K30 A	K3H003	Maalgate	Ave TDS (ref year)	1998	381	8.495	0.000	200.00	284.00	147.00	140.00	213.00	241.50	343.00	225.00	249.00	654.00	524.50	395.00
			Ave TDS (2000)	2005				200.00	284.00	147.00	140.00	213.00	241.50	343.00	225.00	249.00	654.00	524.50	395.00
			Stream flow					1.00	0.98	1.19	1.09	1.19	0.93	0.89	1.35	1.48	1.56	1.49	1.09
K30 B	K3H004	Malgas	Ave TDS (ref year)	1998	416	1.327	0.000	89.00	108.00	74.00	75.00	80.00	152.00	101.00	61.00	75.00	89.00	109.00	99.00
			Ave TDS (2000)	2000				89.00	108.00	74.00	75.00	80.00	152.00	101.00	61.00	75.00	89.00	109.00	99.00
			Stream flow					1.84	1.83	2.57	2.18	1.96	1.34	1.44	2.20	2.60	2.74	2.70	2.04
K 30 C	K3H001	Kaaimans	Ave TDS (ref year)	1998	419	0.461	0.000	99.00	98.00	79.00	93.00	80.00	112.00	105.00	77.00	94.25	111.50	109.00	114.00
			Ave TDS (2000)	2000				99.00	98.00	79.00	93.00	80.00	112.00	105.00	77.00	94.25	111.50	109.00	114.00
			Stream flow					2.52	2.50	3.51	2.98	2.68	1.83	1.97	3.00	3.55	3.74	3.69	2.79
K 30 D	K3R006	Tows	Ave TDS (ref year)	1998	225	181.779	0.000	5593.00	7150.00	3528.00	4971.00	11442.00	13324.00	5689.00	3051.00	1186.00	4938.00	5320.00	16977.00
			Ave TDS (2000)	2000				5593.00	7150.00	3528.00	4971.00	11442.00	13324.00	5689.00	3051.00	1186.00	4938.00	5320.00	16977.00
			Stream flow					1.50	1.46	1.78	1.64	1.78	1.39	1.34	2.01	2.22	2.33	2.22	1.63
K 40 A-C	K4R003	Sedgefield	Ave TDS (ref year)	1998	12	-11201.080	0.000	17679.00	13233.00	32002.00	33859.00	26796.00	21088.00	19212.00	17336.00	18141.00	17129.00	17137.00	17366.00
			Ave TDS (2000)	2000				17679.00	13233.00	32002.00	33859.00	26796.00	21088.00	19212.00	17336.00	18141.00	17129.00	17137.00	17366.00
			Stream flow					3.45	3.35	4.11	3.76	4.10	3.19	3.07	4.63	5.10	5.35	5.11	3.75
K 40 E	K4H004	Goukamma	Ave TDS (ref year)	1998	11	317.758	0.000	143.00	243.00	570.00	106.00	192.00	617.00	205.00	192.00	179.00	1705.00	6262.00	128.00
			Ave TDS (2000)	2000				143.00	243.00	570.00	106.00	192.00	617.00	205.00	192.00	179.00	1705.00	6262.00	128.00
			Stream flow					4.59	4.46	5.46	5.01	5.46	4.24	4.09	6.16	6.78	7.13	6.80	4.99
K 50 A-B	K5R001	Knysna	Ave TDS (ref year)	1998	49	583.174	0.000	34906.00	35302.00	34450.00	33375.00	34215.50	35056.00	35149.00	32710.00	34048.75	35387.50	35611.00	36057.00
			Ave TDS (2000)	2000				34906.00	35302.00	34450.00	33375.00	34215.50	35056.00	35149.00	32710.00	34048.75	35387.50	35611.00	36057.00
			Stream flow					5.55	4.93	5.49	6.42	9.72	7.42	7.85	11.70	12.54	12.42	10.72	7.85
K 60 G	K6H014	Piesang	Ave TDS (ref year)	1998	14	-547.849	0.000	24520.00	11368.00	8230.50	5093.00	7412.00	19763.00	19763.00	19763.00	8111.00	15055.00	15055.00	21999.00
			Ave TDS (2000)	2000				24520.00	11368.00	8230.50	5093.00	7412.00	19763.00	19763.00	19763.00	8111.00	15055.00	15055.00	21999.00
			Stream flow					0.73	0.65	0.72	0.85	1.28	0.98	1.04	1.54	1.65	1.64	1.41	1.04
K 60 A-F	K6H006	Keurbooms	Ave TDS (ref year)	1998	14	3129.378	0.000	7293.00	26269.00	16322.00	6375.00	17183.00	24570.00	10781.00	12683.00	14585.00	19822.00	19822.00	25059.00
			Ave TDS (2000)	2000				7293.00	26269.00	16322.00	6375.00	17183.00	24570.00	10781.00	12683.00	14585.00	19822.00	19822.00	25059.00
			Stream flow					5.55	4.93	5.49	6.42	9.72	7.42	7.85	11.70	12.54	12.42	10.72	7.85
K70 A-B	K7H001	Bloukrans	Ave TDS (ref year)	1999	518	0.915	0.000	51.00	52.00	57.67	57.50	47.00	53.33	50.00	53.00	53.50	46.00	51.00	48.00
			Ave TDS (2000)	2000				51.00	52.00	57.67	57.50	47.00	53.33	50.00	53.00	53.50	46.00	51.00	48.00
			Stream flow					2.56	2.34	3.04	2.83	3.82	3.17	3.59	5.22	5.75	5.40	4.53	3.42
K 80 A-C	K9H006	Krom	Ave TDS (ref year)	1998	428	0.700	0.000	50.50	44.00	55.50	67.00	43.00	61.00	55.00	74.00	48.00	53.00	55.00	57.00
			Ave TDS (2000)	2000				50.50	44.00	55.50	67.00	43.00	61.00	55.00	74.00	48.00	53.00	55.00	57.00
			Stream flow					7.00	6.43	8.27	7.77	10.53	9.57	11.00	14.88	15.29	13.45	10.94	8.54
K80 D	K8H006	Groot	Ave TDS (ref year)	1999	428	1.200	0.000	86.00	74.93	94.51	114.10	73.23	103.88	93.66	147.00	95.35	162.31	109.26	113.23
			Ave TDS (2000)	2000				86.00	74.93	94.51	114.10	73.23	103.88	93.66	147.00	95.35	162.31	109.26	113.23
			Stream flow					2.27	2.08	2.68	2.52	3.41	3.10	3.57	4.82	4.96	4.36	3.55	2.77
K80 E-F	K8H004	Tsitsikama	Ave TDS (ref year)	1998	16	-1073.794	0.000	7301.00	12798.00	10809.00	8820.00	10189.50	6081.00	11520.00	810.00	2753.00	3285.00	4457.50	1804.00
			Ave TDS (2000)	2000				7301.00	12798.00	10809.00	8820.00	10189.50	6081.00	11520.00	810.00	2753.00	3285.00	4457.50	1804.00
			Stream flow					6.27	5.76	7.41	6.97	8.47	7.76	9.17	13.42	13.34	13.71	12.06	9.81
K90 A-G	K9H006 *		Ave TDS (ref year)	1998			0.000	7301.00	12798.00	10809.00	8820.00	10189.50	6081.00	11520.00	810.00	2753.00	3285.00	4457.50	1804.00
			Ave TDS (2000)	2000				7301.00	12798.00	10809.00	8820.00	10189.50	6081.00	11520.00	810.00	2753.00	3285.00	4457.50	1804.00
			Stream flow					3.19	3.09	5.61	4.80	8.47	7.76	9.17	13.37	10.87	8.47	4.73	

n = number of water quality data points available to calculate growth factor

TDS expressed as mg/l

* No guaging station in catchment. Closest guaging satation used

Table B17: Water quality data for drainage region L

Catchment	Guage	River		Year	n	Calculated growth factor	Growth factor used	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
All	L9H004	Gamtoos	Ave TDS (ref year)	1982	31	-80.753	0.000	2272.33	2112.67	1583.25	2371.67	1435.46	1435.46	1435.46	1435.46	1435.46	499.25	434.50	689.00
			Ave TDS (2000)	2000				2272.33	2112.67	1583.25	2371.67	1435.46	1435.46	1435.46	1435.46	1435.46	499.25	434.50	689.00
			Stream flow					33.04	50.51	70.41	38.38	42.35	27.39	28.09	45.60	36.00	31.49	37.57	34.71

n = number of water quality data points available to calculate growth factor

TDS expressed as mg/l

Table B18: Water quality data for drainage region M

Catchment	Guage	River		Year	n	Calculated Growth factor	Growth factor used	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
M 20	M2H003	Van Staden	Ave TDS (ref year)	1996	65	-29.686	0.000	212.00	175.00	172.00	185.50	181.50	191.00	108.00	335.00	238.00	210.50	238.00	223.50
			Ave TDS (2000)	2000				212.00	175.00	172.00	185.50	181.50	191.00	108.00	335.00	238.00	210.50	238.00	223.50
			Stream flow					1.70	1.26	5.09	3.86	6.16	5.72	7.31	7.96	8.45	6.23	4.71	3.35
M 10	M1H022	Swartbos	Ave TDS (ref year)	1997	3	16097.163	0.000	33196	27402	26932	29046	28420	29907	16911	52455	34651	35626	37217	34996
			Ave TDS (2000)	2000				33196	27402	26932	29046	28420	29907	16911	52455	34651	35626	37217	34996
			Stream flow					2.95	2.79	6.65	6.00	7.18	4.41	7.68	8.89	10.22	8.84	8.31	4.78
M 30	M1H003 *		Ave TDS (ref year)	1987	67	0.413	0.000	97.59	100.00	97.00	118.00	82.00	78.00	63.00	74.00	103.00	112.15	97.00	95.44
			Ave TDS (2000)	2000				97.59	100.00	97.00	118.00	82.00	78.00	63.00	74.00	103.00	112.15	97.00	95.44
			Stream flow					0.29	0.23	0.88	0.79	0.61	0.22	0.88	1.13	1.99	1.33	1.35	0.68

n = number of water quality data points available to calculate growth factor

TDS expressed as mg/l

* No guaging station in catchment. Closest guaging satation used

Table B19: Water quality data for drainage region N

Catchment	Guage	River		Year	n	Calculated growth factor	Growth factor used	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
All	N4H003	Sundays	Ave TDS (ref year)	1998	375	103.030	0.000	10851.00	3029.00	2624.00	5529.50	10180.50	2271.00	2602.00	7416.67	6567.00	10087.50	10733.00	10430.00
			Ave TDS (2000)	2000				10851.00	3029.00	2624.00	5529.50	10180.50	2271.00	2602.00	7416.67	6567.00	10087.50	10733.00	10430.00
			Stream flow					20.81	30.72	61.23	29.20	19.02	6.50	8.94	19.35	15.83	18.62	24.04	25.78

n = number of water quality data points available to calculate growth factor

TDS expressed as mg/l

Table B20: Water quality data for drainage region P

Catchment	Guage	River		Year	n	Calculated growth factor	Growth factor used	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
P10	P1H005	Boesmans	Ave TDS (ref year)	1994	1		0.000	608.49	461.88	409.43	423.78	423.27	411.72	414.30	403.33	395.57	409.00	457.10	386.84
			Ave TDS (2000)	2000				608.49	461.88	409.43	423.78	423.27	411.72	414.30	403.33	395.57	409.00	457.10	386.84
			Stream flow					1.55	1.87	6.29	3.48	4.40	2.90	4.96	5.95	7.84	7.08	6.19	3.45
P30	P3H001	Kariega	Ave TDS (ref year)	1999	306	65.011	65.011	2974.00	3358.50	3362.00	3483.50	3605.00	3629.00	3676.00	3625.00	3506.00	2874.00	3212.00	3038.00
			Ave TDS (2000)	2000				3039.01	3423.51	3427.01	3548.51	3670.01	3694.01	3741.01	3690.01	3571.01	2939.01	3277.01	3103.01
			Stream flow					0.49	0.82	2.46	1.56	1.81	1.08	1.59	1.68	2.34	2.01	2.46	1.21
P40 A-D	P3H001	Kowie	Ave TDS (ref year)	1999	278	27.055	27.055	1004.00	1100.00	1122.00	1711.00	1759.00	1884.67	1896.00	2152.00	2576.00	3039.50	3110.00	933.00
			Ave TDS (2000)	2000				1031.05	1127.05	1149.05	1738.05	1786.05	1911.72	1923.05	2179.05	2603.05	3066.55	3137.05	960.05
			Stream flow					1.24	1.98	5.75	3.84	4.33	2.87	3.87	4.03	5.84	4.95	5.76	2.89
P20 A-B	P1H003 *		Ave TDS (ref year)	1998	528	-5.017	0.000	3312.50	3340.50	2993.33	2937.00	2662.00	2719.50	2783.00	2868.33	2838.00	2892.33	2916.50	2965.50
			Ave TDS (2000)	2000				3312.50	3340.50	2993.33	2937.00	2662.00	2719.50	2783.00	2868.33	2838.00	2892.33	2916.50	2965.50
			Stream flow					1.15	1.14	4.20	2.54	4.11	3.24	4.28	4.49	6.34	5.40	4.41	2.56

n = number of water quality data points available to calculate growth factor

TDS expressed as mg/l

* No guaging station in catchment. Closest guaging satation used

B21

Table B21: Water quality data for drainage region Q

Catchment	Guage	River		Year	n	Calculated growth factor	Growth factor used	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
Q92	Q9H001		Ave TDS (ref year)	1999	393	-32.555	0.000	1077.50	1205.00	1028.00	1035.83	1043.67	1466.50	1210.50	1221.50	1329.00	919.50	1238.00	978.00
			Ave TDS (2000)	2000				1077.50	1205.00	1028.00	1035.83	1043.67	1466.50	1210.50	1221.50	1329.00	919.50	1238.00	978.00
			Stream flow					4.35	7.32	15.90	7.86	4.68	2.56	2.63	4.09	3.29	6.15	9.09	7.76
Q11-Q14,Q21-Q22, Q41-Q44,Q50, Q60,Q70,Q80	Q9H013	Great Fish	Ave TDS (ref year)	1989	56	-37.330	0.000	202.00	636.00	1070.00	694.50	319.00	709.00	600.00	300.00	200.00	164.00	183.00	461.00
			Ave TDS (2000)	2000				202.00	636.00	1070.00	694.50	319.00	709.00	600.00	300.00	200.00	164.00	183.00	461.00
			Stream flow					31.71	47.40	87.81	37.37	15.27	5.32	5.30	9.05	8.42	17.32	32.29	35.02
Q94 + Q93	Q9H029		Ave TDS (ref year)	1998	92	3.905	0.000	389.50	237.50	121.00	292.00	334.00	417.50	501.00	455.00	409.00	479.00	314.25	149.50
			Ave TDS (2000)	2000				389.50	237.50	121.00	292.00	334.00	417.50	501.00	455.00	409.00	479.00	314.25	149.50
			Stream flow					6.99	9.54	18.61	10.15	6.12	2.80	2.87	6.12	5.62	9.82	15.28	12.00

n = number of water quality data points available to calculate growth factor

TDS expressed as mg/l

Table B22: Water quality data for drainage region R

Catchment	Guage	River		Year	n	Calculated growth factor	Growth factor used	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
R10,R40	R1H015	Kieskamma	Ave TDS (ref year)	1998	397	-9.767	0.000	381.00	236.00	165.50	187.00	207.00	205.00	283.00	284.00	284.00	183.00	284.00	172.00
			Ave TDS (2000)	2000				381.00	236.00	165.50	187.00	207.00	205.00	283.00	284.00	284.00	183.00	284.00	172.00
			Stream flow					11.66	15.05	33.20	24.54	18.76	9.04	11.81	24.65	21.43	27.13	37.46	20.72
R20	R2H002	Buffalo	Ave TDS (ref year)	1979	14	-44.429	0.000	1144.00	85.00	49.00	0.00	773.60	802.25	90.00	90.00	90.00	90.00	90.00	90.00
			Ave TDS (2000)	2000				1144.00	85.00	49.00	0.00	773.60	802.25	90.00	90.00	90.00	90.00	90.00	90.00
			Stream flow					4.54	6.05	11.78	8.60	6.23	2.98	4.66	9.38	7.92	9.57	15.70	8.11
R30E-F	R3H002	Nahoon	Ave TDS (ref year)	1997	198	-10.321	0.000	144.00	220.00	233.00	287.00	245.00	212.00	186.00	229.00	154.00	187.00	194.00	223.00
			Ave TDS (2000)	2000				144.00	220.00	233.00	287.00	245.00	212.00	186.00	229.00	154.00	187.00	194.00	223.00
			Stream flow					3.29	4.32	7.82	5.79	3.69	1.63	3.06	5.56	4.75	6.26	9.52	4.84
R30 A-D	R3H001	Gqunube	Ave TDS (ref year)	1999	169	-7.200	0.000	222.50	268.00	246.00	298.00	289.00	380.00	141.00	380.00	512.00	351.00	286.00	221.00
			Ave TDS (2000)	2000				222.50	268.00	246.00	298.00	289.00	380.00	141.00	380.00	512.00	351.00	286.00	221.00
			Stream flow					7.10	9.33	16.90	12.51	7.97	3.52	6.61	12.01	10.27	13.53	20.57	10.47

n = number of water quality data points available to calculate growth factor

TDS expressed as mg/l

Table B23: Water quality data for drainage region S

Catchment	Guage	River		Year	n	Calculated growth factor	Growth factor used	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
S31-S 32, S20	S7H004	Great Kei	Ave TDS (ref year)	1999	125	-3.015	0.000	204.50	164.00	0.00	203.00	285.00	394.00	394.00	405.67	387.00	322.50	397.00	230.00
S10, S40, S50			Ave TDS (2000)	2000				204.50	368.50	164.00	203.00	488.00	679.00	788.00	799.67	792.67	709.50	719.50	627.00
S60, S70 AB			Stream flow					82.58	118.64	169.34	84.61	38.02	20.48	27.37	35.40	38.12	56.83	94.38	86.39
S70 C+D+E	S7H001		Ave TDS (ref year)	1999	37	61.426	0.000	227.00	288.33	246.00	250.00	370.00	588.00	618.50	686.00	691.00	533.00	598.00	412.50
			Ave TDS (2000)	2000				227.00	288.33	246.00	250.00	370.00	588.00	618.50	686.00	691.00	533.00	598.00	412.50
			Stream flow					4.74	7.79	16.98	13.58	9.65	4.66	7.83	9.02	8.65	11.89	15.44	7.15

n = number of water quality data points available to calculate growth factor

TDS expressed as mg/l

B23

Table B24: Water quality data for drainage region T

Catchment	Guage	River		Year	n	Calculated growth factor	Growth factor used	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
T60 J,K	T6H001	Mntafufu	Ave TDS (ref year)	1999	24	-0.334	0.000	145.00	135.00	135.00	139.00	143.00	144.00	141.00	158.00	163.00	167.00	171.00	158.00
			Ave TDS (2000)	2000				145.00	135.00	135.00	139.00	143.00	144.00	141.00	158.00	163.00	167.00	171.00	158.00
			Stream flow					6.21	8.00	11.32	7.97	4.86	3.74	3.66	2.74	4.04	7.46	11.89	9.04
T60 H	T6R001	Mkozi	Ave TDS (ref year)	1996	2		0.000	89.71	83.53	83.53	86.00	91.50	97.00	94.98	106.43	112.13	112.49	115.19	106.43
			Ave TDS (2000)	2000				89.71	83.53	83.53	86.00	91.50	97.00	94.98	106.43	112.13	112.49	115.19	106.43
			Stream flow					3.73	4.81	6.80	4.79	2.92	2.25	2.20	1.65	2.42	4.48	7.14	5.43
T60 E	T6H002		Ave TDS (ref year)	1981	3		0.000	293.00	307.12	324.77	337.13	318.00	322.00	310.95	339.36	342.52	326.74	350.41	329.89
			Ave TDS (2000)	2000				293.00	307.12	324.77	337.13	318.00	322.00	310.95	339.36	342.52	326.74	350.41	329.89
			Stream flow					2.29	2.96	4.18	2.95	1.79	1.38	1.35	1.01	1.49	2.76	4.39	3.34
T60 F	T6H004		Ave TDS (ref year)	1999	24	9.182	0.000	166.00	174.00	184.00	191.00	198.00	204.00	197.00	215.00	217.00	207.00	222.00	209.00
			Ave TDS (2000)	2005				166.00	174.00	184.00	191.00	198.00	204.00	197.00	215.00	217.00	207.00	222.00	209.00
			Stream flow					5.37	6.93	9.80	6.90	4.20	3.24	3.17	2.38	3.49	6.46	10.30	7.83
T60 A-D,G	T6H003	Mtentu	Ave TDS (ref year)	1981			0.000	202.00	211.73	223.90	214.15	222.00	199.00	192.17	209.73	211.68	201.93	216.56	203.88
			Ave TDS (2000)	2000				202.00	211.73	223.90	214.15	222.00	199.00	192.17	209.73	211.68	201.93	216.56	203.88
			Stream flow					25.62	33.03	46.75	32.92	20.05	15.46	15.11	11.33	16.66	30.81	49.10	37.34
T40	T4H001	Mtamvuna	Ave TDS (ref year)	1999	386	0.635	0.635	63.00	50.00	49.50	66.00	76.00	86.00	89.47	90.20	90.00	100.00	90.00	61.00
			Ave TDS (2000)	2000				63.64	50.64	50.14	66.64	76.64	86.64	90.11	90.83	90.64	100.64	90.64	61.64
			Stream flow					29.35	32.40	41.54	26.94	16.58	12.95	10.28	7.67	14.60	26.28	41.16	38.01
T70 A,B	T7H001	Mngazi	Ave TDS (ref year)	1999	42	3.029	0.000	120.50	144.00	182.50	182.50	195.50	216.00	211.00	454.50	234.50	242.00	240.00	77.00
			Ave TDS (2000)	2000				120.50	144.00	182.50	182.50	195.50	216.00	211.00	454.50	234.50	242.00	240.00	77.00
			Stream flow					3.57	4.98	10.70	7.90	3.93	3.22	3.71	2.72	3.85	5.21	7.62	5.88
T70 C-F	T7H003	Mgazana	Ave TDS (ref year)	1981	3		0.000	304.00	328.50	328.50	353.00	299.50	246.00	258.00	258.00	270.00	285.00	285.00	300.00
			Ave TDS (2000)	2000				304.00	328.50	328.50	353.00	299.50	246.00	258.00	258.00	270.00	285.00	285.00	300.00
			Stream flow					6.18	8.62	18.53	13.68	6.81	5.58	6.43	4.72	6.68	9.03	13.21	10.20
T52 K-L	T5H012	Mzimkhulu	Ave TDS (ref year)	1996	310	2.532	2.532	233.00	234.00	200.60	245.00	268.25	278.00	202.00	278.00	328.00	279.00	230.00	107.00
			Ave TDS (2000)	2000				243.13	244.13	210.73	255.13	278.38	288.13	212.13	288.13	338.13	289.13	240.13	117.13
			Stream flow					11.19	12.18	14.38	8.28	5.00	3.67	2.91	2.25	4.72	7.18	12.37	13.71
T52 E-H	T5H002		Ave TDS (ref year)	1999	40	0.845	0.000	73.00	74.00	74.00	70.00	84.50	91.00	93.00	104.67	105.00	93.50	83.25	73.00
			Ave TDS (2000)	2000				73.00	74.00	74.00	70.00	84.50	91.00	93.00	104.67	105.00	93.50	83.25	73.00
			Stream flow					19.31	21.01	24.81	14.29	8.62	6.34	5.03	3.88	8.15	12.38	21.34	23.66
T51, T52 A-B	T5H001		Ave TDS (ref year)	1997	3		0.000	54.40	55.15	55.15	52.17	62.97	67.82	69.31	78.00	78.25	69.68	62.04	54.40
			Ave TDS (2000)	2000				54.40	55.15	55.15	52.17	62.97	67.82	69.31	78.00	78.25	69.68	62.04	54.40
			Stream flow					116.42	129.90	128.31	59.26	28.45	17.13	12.35	11.53	22.45	34.38	60.39	93.89
T31-T36	T3R002	Mzimvubu	Ave TDS (ref year)	1997	5		0.000	86.11	87.29	87.29	82.57	99.67	107.34	109.70	123.46	123.85	110.29	98.20	86.11
			Ave TDS (2000)	2000				86.11	87.29	87.29	82.57	99.67	107.34	109.70	123.46	123.85	110.29	98.20	86.11
			Stream flow					267.20	354.06	383.00	177.27	80.90	58.27	55.64	46.51	80.97	113.62	180.72	213.18
T20,T70 G, T80	T2H005 *		Ave TDS (ref year)	1981	10		0.000	210.00	189.00	189.00	168.00	139.00	110.00	64.00	104.00	144.00	112.00	161.00	161.00
			Ave TDS (2000)	2000				210.00	189.00	189.00	168.00	139.00	110.00	64.00	104.00	144.00	112.00	161.00	161.00
			Stream flow					39.23	49.91	85.39	62.89	34.58	21.72	26.06	23.98	33.14	45.28	66.65	48.27
T11-T13, T90	T1H004	Bashee	Ave TDS (ref year)	1999	33	-0.433	0.000	74.50	59.00	77.00	95.00	113.00	115.00	114.50	121.33	123.00	177.00	128.00	98.00
			Ave TDS (2000)	2000				74.50	59.00	77.00	95.00	113.00	115.00	114.50	121.33	123.00	177.00	128.00	98.00
			Stream flow					67.24	84.67	138.17	86.99	46.33	25.69	31.84	31.08	49.08	65.91	97.25	77.53

n = number of water quality data points available to calculate growth factor

TDS expressed as mg/l

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Table B25: Water quality data for drainage region U

Catchment	Guage	River		Year	n	Calculated growth factor	Growth factor used	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
U10	U1h006	Mkomazi	Ave TDS (ref year)	1999	619	-0.600	0.000	57.00	77.00	68.00	98.00	126.00	137.00	187.95	177.00	210.00	195.00	116.50	61.00
			Ave TDS (2000)	2000				57.00	77.00	68.00	98.00	126.00	137.00	187.95	177.00	210.00	195.00	116.50	61.00
			Stream flow					137.01	144.31	136.38	65.32	28.93	16.97	11.71	12.65	27.11	39.48	75.50	110.82
U20	U2H008	Mgeni	Ave TDS (ref year)	1988	24	-0.507	0.000	102.00	60.00	85.00	110.00	168.00	148.00	179.40	188.20	197.00	148.00	99.00	100.50
			Ave TDS (2000)	2000				102.00	60.00	85.00	110.00	168.00	148.00	179.40	188.20	197.00	148.00	99.00	100.50
			Stream flow					80.53	88.44	92.58	53.37	29.51	18.93	13.01	12.25	23.77	27.91	44.31	62.89
U70	U7H008	Nungwana	Ave TDS (ref year)	1995	233	6.277	5.000	109.37	114.39	110.82	88.79	94.75	90.41	93.81	94.75	102.72	101.91	104.99	103.91
			Ave TDS (2000)	2000				134.37	139.39	135.82	113.79	119.75	115.41	118.81	119.75	127.72	126.91	129.99	128.91
			Stream flow					10.74	12.89	17.78	11.60	6.60	5.21	3.44	2.71	5.96	6.08	9.72	9.80
U40, U50 *	U4H007	Mvoti	Ave TDS (ref year)	1996	337	4.646	2.000	206.67	107.00	214.50	111.00	204.75	204.75	298.50	316.00	252.50	189.00	160.33	156.00
			Ave TDS (2000)	2000				214.67	115.00	222.50	119.00	212.75	212.75	306.50	324.00	260.50	197.00	168.33	164.00
			Stream flow					62.15	71.34	82.67	48.35	32.95	23.21	15.42	15.49	34.88	39.50	52.86	61.07
U80 A-F	U8H002	Mtwalume	Ave TDS (ref year)	1992	60	4.560	4.560	160.00	137.00	133.50	144.00	149.00	163.00	166.00	167.50	184.00	175.00	170.00	187.00
			Ave TDS (2000)	2000				196.48	173.48	169.98	180.48	185.48	199.48	202.48	203.98	220.48	211.48	206.48	223.48
			Stream flow					15.09	22.26	30.33	19.82	10.88	11.81	8.80	5.86	10.62	13.89	15.84	15.69
U 80G	U8R001	Mzinto	Ave TDS (ref year)	1998	151	0.555	0.400	162.00	155.00	162.00	168.00	175.00	177.00	200.91	164.00	174.00	165.00	167.00	153.00
			Ave TDS (2000)	2000				162.80	155.80	162.80	168.80	175.80	177.80	201.71	164.80	174.80	165.80	167.80	153.80
			Stream flow					2.13	3.14	4.27	2.79	1.53	1.66	1.24	0.83	1.50	1.96	2.23	2.21
U 80 K+L	U8H008	Mpambanyon	Ave TDS (ref year)	1998	82	-51.485	0.000	219.00	473.00	286.00	311.00	357.00	391.00	552.82	594.30	441.00	493.00	492.00	220.00
			Ave TDS (2000)	2000				219.00	473.00	286.00	311.00	357.00	391.00	552.82	594.30	441.00	493.00	492.00	220.00
			Stream flow					8.20	12.10	16.49	10.78	5.92	6.42	4.78	3.19	5.77	7.55	8.61	8.53
U30 C-E*	U8H001	Tongati	Ave TDS (ref year)	1992	363	-0.357	0.000	91.00	76.00	80.50	82.00	83.00	90.00	92.00	98.50	99.00	96.00	103.00	79.00
			Ave TDS (2000)	2000				91.00	76.00	80.50	82.00	83.00	90.00	92.00	98.50	99.00	96.00	103.00	79.00
			Stream flow					9.81	13.62	17.28	11.16	7.24	6.13	3.89	3.33	6.85	9.07	12.46	9.47
U 30 A-B	U3H005	Mdloti	Ave TDS (ref year)	1995	468	3.939	3.000	129.46	131.99	137.65	207.13	123.57	121.32	121.97	121.97	123.62	122.33	125.73	126.12
			Ave TDS (2000)	2000				144.46	146.99	152.65	222.13	138.57	136.32	136.68	136.97	138.62	137.33	140.73	141.12
			Stream flow					7.20	10.00	12.69	8.20	5.32	4.50	2.86	2.45	5.03	6.66	9.15	6.95

n = number of water quality data points available to calculate growth factor

TDS expressed as mg/l

* No guaging station in catchment. Closest guaging satation used

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Table B26: Water quality data for drainage region V

Catchment	Guage	River		Year	n	Calculated growth factor	Growth factor used	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
All	V5H002	Tugela	Ave TDS (ref year)	1999				144.00	97.00	115.00	130.00	172.00	266.00	283.00	294.00	311.00	298.00	336.00	152.00
			Ave TDS (2000)	2000	875	0.407	0.407	144.41	97.41	115.41	130.41	172.41	266.41	283.41	294.41	311.41	298.41	336.41	152.41
			Stream flow					611.15	636.92	523.01	245.07	106.32	57.82	49.39	58.96	126.63	183.80	331.79	449.56

n = number of water quality data points available to calculate growth factor

TDS expressed as mg/l

Table B27: Water quality data for drainage region W

Catchment	Guage	River		Year	n	Calculated growth factor	Growth factor used	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
W51-WW57, W60	W5H023	Great Usutu	Ave TDS (ref year)	1988	151	-7.049	0.000	101.00	101.00	112.99	138.00	240.33	255.00	186.00	272.00	184.00	127.72	120.00	55.00
			Ave TDS (2000)	2000				101.00	101.00	112.99	138.00	240.33	255.00	186.00	272.00	184.00	127.72	120.00	55.00
			Stream flow					481.23	470.60	338.06	207.66	123.70	82.24	68.40	60.28	66.25	131.86	287.08	397.97
W41-W45	W4H009	Pongola	Ave TDS (ref year)	1998	207	-8.916	0.000	391.00	345.00	331.00	325.00	327.00	238.00	368.00	375.00	334.00	312.00	290.00	340.50
			Ave TDS (2000)	2000				391.00	345.00	331.00	325.00	327.00	238.00	368.00	375.00	334.00	312.00	290.00	340.50
			Stream flow					129.56	127.28	100.75	54.09	27.53	18.83	19.62	16.63	24.36	50.52	92.70	106.39
W11-W13, W21-W23	W2H032 *		Ave TDS (ref year)	1998	29	-	0.000	239.00	271.00	183.00	386.00	367.00	657.00	964.00	919.00	794.00	554.50	315.00	198.00
			Ave TDS (2000)	2000				239.00	271.00	183.00	386.00	367.00	657.00	964.00	919.00	794.00	554.50	315.00	198.00
			Stream flow					210.21	258.08	231.75	124.87	80.52	57.71	61.73	45.29	94.72	112.05	159.35	181.65
W31-W32, W70	W3H018	Mkuze	Ave TDS (ref year)	1987	8	-	0.000	358.00	358.00	274.00	274.00	322.00	424.67	424.67	424.67	424.67	424.67	424.67	424.67
			Ave TDS (2000)	2000				358.00	358.00	274.00	274.00	322.00	424.67	424.67	424.67	424.67	424.67	424.67	424.67
			Stream flow					86.07	85.85	76.56	45.49	25.68	21.03	22.65	18.09	28.92	41.31	61.29	68.33

n = number of water quality data points available to calculate growth factor

TDS expressed as mg/l

* No guaging station in catchment. Closest guaging satation used

Table B28: Water quality data for drainage region X

Catchment	Guage	River		Year	n	Calculated growth factor	Growth factor used	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
X31-X33, X40*	X3H015	Sabie	Ave TDS (ref year)	1998	634	2.903	2.900	85.50	86.50	77.60	87.00	85.67	86.00	91.00	106.63	101.50	91.00	95.00	90.25
			Ave TDS (2000)	2000				91.30	92.30	83.40	92.80	91.47	91.80	96.80	112.43	107.30	96.80	100.80	96.05
			Stream flow					77.29	103.55	89.25	48.62	24.92	17.78	14.26	12.15	11.30	12.90	25.23	48.60
X21-X24, X11-X13	X1H042	Komati	Ave TDS (ref year)	1999	343	3.133	3.100	156.25	185.67	192.00	236.00	275.25	358.50	60.20	462.67	427.20	287.67	238.33	204.00
			Ave TDS (2000)	2000				159.35	188.77	195.10	239.10	278.35	361.60	63.30	465.77	430.30	290.77	241.43	207.10
			Stream flow					299.88	346.54	266.93	158.82	100.38	75.08	61.76	53.19	49.59	66.41	146.92	230.07

n = number of water quality data points available to calculate growth factor

TDS expressed as mg/l

* No guaging station in catchment. Closest guaging satation used

Table B29: Summary of river quality data

Drainage Region		Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec	TOTAL	%
A	Flow	424.07	480.40	357.22	189.35	95.88	68.17	56.01	46.85	40.39	52.83	123.60	219.68	2154	4.89
	TDS load	93394.68	93152.54	71097.44	43703.95	21818.01	15845.67	14256.27	12237.79	10956.99	15194.37	35432.73	47690.65	475381	1.36
B	Flow	439.50	510.05	392.48	195.44	99.10	69.34	55.44	46.63	42.38	63.99	188.49	256.13	2359	5.35
	TDS load	102151.63	172712.88	140202.68	42574.56	28830.59	25001.91	23490.84	19285.91	21325.93	49930.85	199645.37	62283.14	887436	2.54
C	Flow	769.97	764.17	628.98	314.10	123.76	50.54	40.05	40.64	119.42	271.33	537.41	506.17	4167	9.46
	TDS load	793454.09	680620.75	306942.24	291013.65	93356.29	37652.30	34189.44	31179.34	112376.73	265170.33	466284.56	376610.59	3490850	9.97
D	Flow	901.50	1141.65	1376.06	804.81	368.23	183.90	152.35	177.14	272.40	454.00	569.77	566.70	6969	15.82
	TDS load	304296.63	478743.12	555218.72	285872.58	115675.44	51770.60	50378.04	68730.72	54825.30	112879.28	175357.61	172855.81	2426604	6.93
E	Flow	6.15	5.39	5.44	23.94	45.32	115.61	97.92	100.15	67.06	36.75	20.98	10.29	535	1.21
	TDS load	2267.96	2220.38	3361.83	13460.06	22811.19	57718.70	27819.47	24015.35	19028.30	11254.47	9215.70	4472.23	197646	0.56
F	Flow	0.09	0.20	0.20	0.86	1.97	9.48	4.49	3.96	1.48	0.38	0.49	0.41	24	0.05
	TDS load	201.43	602.40	703.00	2760.00	5923.68	29420.62	14098.52	14756.36	4431.69	1531.90	1954.53	1129.58	77514	0.22
G	Flow	15.94	16.13	15.30	55.59	164.16	318.66	374.60	424.18	283.90	169.23	92.62	36.30	1967	4.46
	TDS load	186319.22	152261.26	180565.73	768037.06	636886.40	1044986.00	832191.32	869616.43	665698.36	1261433.28	1050133.77	240284.85	7888414	22.54
H	Flow	37.88	44.75	62.30	158.44	266.14	322.75	333.97	324.42	137.55	136.60	101.52	45.07	1971	4.47
	TDS load	12994.26	9812.96	26426.02	64358.61	88477.73	76694.82	46062.25	70427.76	50102.13	39175.52	56365.18	8619.62	549517	1.57
J	Flow	44.30	59.71	78.51	70.78	53.44	41.39	37.55	55.63	44.79	41.11	55.13	53.37	636	1.44
	TDS load	8506.22	13016.36	14524.85	12103.63	8496.43	7036.85	6196.02	9178.35	9854.47	9783.02	14553.52	11901.38	125151	0.36
K	Flow	52.35	49.15	64.11	61.99	79.71	65.05	71.08	103.44	109.32	103.22	90.18	65.12	915	2.08
	TDS load	483395.05	581159.76	689788.19	578049.28	927935.56	705232.36	740326.27	733193.74	933139.45	1050060.63	989666.41	728064.95	9140012	26.11
L	Flow	33.04	50.51	70.41	38.38	42.35	27.39	28.09	45.60	36.00	31.49	37.57	34.71	476	1.08
	TDS load	75072.80	106705.38	111471.76	91018.84	60796.89	39318.08	40324.46	65456.60	51670.46	15722.14	16324.53	23914.40	697796	1.99
M	Flow	4.94	4.28	12.62	10.65	13.95	10.35	15.87	17.98	20.66	16.40	14.37	8.81	151	0.34
	TDS load	98315.50	76694.99	180060.09	175085.76	205221.89	133000.83	130720.85	469076.89	356349.29	316394.42	310525.20	168095.58	2619541	7.48
N	Flow	20.81	30.72	61.23	29.20	19.02	6.50	8.94	19.35	15.83	18.62	24.04	25.78	280	0.64
	TDS load	225809.31	93050.88	160667.52	161461.40	193633.11	14761.50	23261.88	143512.50	103955.61	187829.25	258021.32	268885.40	1834850	5.24
P	Flow	4.43	5.81	18.70	11.43	14.65	10.10	14.71	16.16	22.36	19.45	18.82	10.11	167	0.38
	TDS load	7521.24	9703.27	30190.59	21175.36	27190.41	19512.57	27373.52	30272.61	44642.37	39617.48	41804.65	15461.96	314466	0.90
Q	Flow	43.05	64.26	122.32	55.38	26.07	10.68	10.80	19.26	17.33	33.28	56.66	54.78	514	1.17
	TDS load	138310.65	41229.67	112556.55	37060.54	11800.45	8699.22	7804.00	10492.71	8351.05	13196.83	21961.35	25527.18	312490	0.89
R	Flow	26.59	34.75	69.70	51.43	36.64	17.17	26.13	51.60	44.37	56.49	83.25	44.14	542	1.23
	TDS load	11690.45	7518.01	12050.79	9976.05	11907.94	5928.50	5261.92	13683.11	12788.23	11746.88	19781.83	7687.03	130021	0.37
S	Flow	87.32	126.43	186.33	98.20	47.67	25.14	35.20	44.42	46.78	68.72	109.82	93.54	970	2.20
	TDS load	17963.17	45966.09	31949.90	20572.79	22124.98	16644.41	26410.45	34493.82	36200.25	46656.27	77141.76	57115.55	433239	1.24
T	Flow	602.92	753.44	923.68	513.03	265.02	180.65	179.74	153.46	251.74	371.24	583.54	587.32	5366	12.18
	TDS load	58870.81	72802.95	97999.46	58618.07	32911.25	22525.97	21401.07	20953.90	34800.26	51584.52	76058.87	60380.78	608908	1.74
U	Flow	332.86	378.12	410.48	231.39	128.89	94.83	65.16	58.75	121.49	152.10	230.69	287.44	2492	5.66
	TDS load	37848.34	39001.66	51848.12	29482.30	22142.83	16991.40	15094.66	13776.58	26748.48	29153.63	33798.89	31812.32	347699	0.99
V	Flow	611.15	636.92	523.01	245.07	106.32	57.82	49.39	48.96	126.63	183.80	331.79	449.56	3380	7.67
	TDS load	88254.87	62040.39	60358.99	31958.53	18329.73	15403.04	13996.77	17358.33	39433.50	54848.56	111616.24	68515.84	582115	1.66
W	Flow	907.08	941.81	747.12	432.11	257.43	179.80	172.40	140.29	214.24	335.75	600.42	754.34	5683	12.90
	TDS load	180318.69	192114.25	134931.10	106900.61	76551.86	72297.43	89069.25	71936.24	107812.49	112282.24	137556.91	123097.34	1404868	4.01
X	Flow	377.16	450.09	356.18	207.44	125.30	92.86	76.02	65.35	60.90	79.31	172.15	278.67	2341	5.31
	TDS load	54841.43	74973.58	59521.95	42485.68	30220.60	28779.76	5289.45	26142.55	22552.70	20559.43	38014.93	52315.18	455697	1.30
TOTAL	Flow	5743.1	6548.7	6482.4	3799.0	2381.0	1958.2	1905.9	2014.2	2097.0	2696.1	4043.3	4388.4	44057.3701	100
	Load	2857898.4	3006103.5	3032437.5	2887729.3	2663043.2	2445222.5	2195016.7	2769777.6	2727044.0	3716005.3	4143215.9	2556721.4	35000215	100
	Concentration	0.498	0.459	0.468	0.760	1.118	1.249	1.152	1.375	1.300	1.378	1.025	0.583		

Flow in million m³/month
Load in kg/month
Concentration in kg/m³

TableB30: Summary of river quality for all monitored quality parameters

Drainage region	Conductivity mS/cm	TDS mg/l	pH	Sodium mg/l	Magnesium mg/l	Calcium mg/l	Flouride mg/l	Chloride mg/l	Nitrite/Nitrate mg/l	Sulphate mg/l	Phosphate mg/l	Alkalinity mg/l as CaCO3	Silica mg/l
A	53.72	342.49	7.74	37.46	20.81	33.57	0.37	43.53	0.55	40.13	0.12	149.76	4.75
B	77.23	553.02	8.16	56.42	41.34	37.37	0.73	58.29	1.56	150.93	0.03	159.21	6.48
C	137.46	894.75	7.55	151.79	61.51	51.80	0.68	192.59	0.03	263.09	0.01	147.87	1.15
D	47.48	346.14	8.44	36.78	17.71	32.03	0.32	34.09	0.13	40.45	0.04	147.63	4.00
E	62.01	354.09	7.22	96.58	18.06	19.43	0.22	185.73	0.21	39.82	0.02	36.68	2.79
F	119.28	768.85	8.33	152.48	35.07	48.95	0.43	271.41	0.37	82.14	0.04	138.93	6.35
G	615.22	4191.18	7.07	1382.25	168.04	70.81	0.40	2505.87	0.97	338.55	0.36	64.53	2.85
H	42.86	234.41	6.44	57.02	8.60	6.54	0.14	92.19	0.12	22.89	0.03	28.78	2.06
J	39.78	204.56	6.77	56.90	7.89	5.17	0.11	100.21	0.18	15.00	0.02	15.32	3.55
K	537.98	3822.95	5.77	1422.78	168.06	61.09	0.23	2578.32	0.09	348.80	0.04	36.31	2.02
L	201.88	1206.00	7.27	289.38	54.15	52.70	0.30	484.39	0.97	186.92	0.01	105.66	3.35
M	129.52	959.16	7.13	315.10	38.17	17.41	0.16	578.12	0.10	78.55	0.03	21.74	3.81
N	441.17	2993.48	8.40	805.66	102.09	68.81	0.88	1003.85	1.65	422.19	0.05	497.96	8.53
P	358.68	2176.53	8.05	545.64	92.66	75.07	0.48	982.75	0.27	141.00	0.05	235.42	2.11
Q	170.92	1161.65	8.20	284.38	43.78	37.68	0.77	315.24	0.69	165.66	0.08	273.08	8.87
R	54.50	327.25	7.69	59.35	14.24	21.45	0.29	85.78	0.61	17.37	0.09	102.14	6.26
S	48.46	344.96	8.27	47.07	17.58	25.20	0.37	54.29	0.50	13.66	0.05	150.07	5.70
T	21.51	143.28	7.62	19.96	8.78	10.32	0.18	25.34	0.36	7.13	0.02	65.14	7.17
U	20.91	131.92	7.36	27.35	6.40	8.64	0.43	33.63	0.50	8.22	0.02	46.24	8.45
V	24.77	187.38	7.66	20.70	9.75	19.23	0.27	17.06	0.36	17.37	0.05	90.31	5.79
W	46.91	308.63	7.53	51.56	16.25	22.07	0.35	63.40	0.36	15.42	0.02	123.36	9.29
X	24.48	172.87	7.75	18.75	10.31	12.74	0.21	17.48	0.22	11.74	0.02	81.30	7.27
Total Load(kg/m)	4087756.7	27639741.8		6634004.0	13740644.4	1234489.5	15906.9	10611421.4	17456.8	3466146.5	2085.3	4827486.8	240957.2
Ave Concentration(kg/m3)	92.78	627.36		150.58	31.19	28.02	0.36	240.85	0.40	78.67	0.05	109.57	5.47
Common ions (% of TDS)				24.00	4.97	4.47		38.39		12.54			

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APPENDIX C

GROUNDWATER QUALITY DATA

The data presented in this appendix was taken from the electronic atlas provided by the Department of Water Affairs and Forestry, from the project "An assessment of groundwater quality at a national scale in the Republic of South Africa". Map A1 shows the distribution of groundwater monitoring sites, and Map C1 shows the total dissolved solids concentration distribution.

APPENDIX D

HYDROSALINITY MODEL STRUCTURE AND PROGRAM CODE

The equations used in the environmental fate model are given in **Chapter 4**. The general structure of the software program is shown in Table B1, and the program code is given in Pages Form1-1 to Form1-28.

Table B1: Structure of environmental fate model program.

Model calculations	Model inputs	Equations
Set initial conditions	• River depth • Soil moisture salt concentration • Observed groundwater flow • Surface salt storages (all surfaces) • Erodible and loose soil depths (rural) • Catchment area • Fraction urban area • Fraction rural area under irrigation • Catchment length	
Start of Annual loop	• Year simulation starts • Year simulation ends	
Start of monthly loop	• Number of days in month	
Calculate monthly deposition velocities	• Summer deposition velocity • Winter deposition velocity	
Start of daily loop		
Calculate daily emissions	• Total mass of salt released into each compartment	
Calculate daily aerosol generation	• Anthropogenic aerosol generation rates (natural and agricultural)	[4-8] - [4-9]
Calculate daily wind velocities	• Monthly wind velocities	
Calculate daily evaporation	• Monthly evaporation • Evaporation factors	
Calculate daily rainfall	• Monthly rainfall	[4-17] – [4-20]
Start of hourly loop		
Calculate hourly rainfall and interception loss	• Rainfall duration coefficients	[4-17] – [4-20]
Calculate surface runoff, interflow and infiltration	• Minimum infiltration rate • Maximum infiltration rate • Maximum proportion of surface runoff derived from interflow	[4-21] – [4-27]
Calculate hourly evaporation		
Calculate hourly soil moisture and evaporation using Newton-Raphson technique	• Soil moisture capacity • Soil moisture below which no evaporation occurs • Power of soil moisture – percolation relationship	[4-43] – [4-46b]

Calculate daily totals	• Coefficient of soil moisture-evaporation relationship • Percolation at soil moisture capacity	

Calculate aerosol concentrations and deposition rates (urban and rural)	• Dry deposition factors (winter and summer) • Occult deposition factor • Atmospheric mixing height • Wash ratio • Fraction salt in aerosol • Natural aerosol generation rates	[4-1] – [4-16]
Calculate groundwater storage, loss and flow to river using the Newton-Raphson technique	• Recession constant for groundwater depletion • Proportion of groundwater entering deep groundwater	[4-58] – [4-61b]
Attenuate and lag surface runoff and groundwater flow	• Lag period	
Calculate sediment generation from natural surfaces	• Catchment cover density • Sediment detachment coefficient • Erosivity factor • Loose soil density • Sediment particle diameter • Sediment specific gravity • Coefficients of suspended sediment-river flow relationship	[4-28] – [4-29]
Calculate salt storage, infiltration, interflow and surface runoff salt load from all surfaces	• Langmuir constants • Surface wash-off parameters • Salt solubility limit • Salt leach rate • Soil void fraction • Soil density • Anthropogenic salt generation rates	[4-30] – [4-42d]
Calculate the salt concentration in the soil moisture, the mass of salt adsorbed, and the mass of salt precipitated		[4-47] – [457b]
Calculate the salt concentration in the groundwater		[4-56]
Mix/adsorb/desorb and route surface runoff		[4-63] – [4-65]

Route river flow using Newton-Raphson technique	• River width • River length • Proportion of catchment runoff draining to the upstream end of the river • River slope • Manning factor • River evaporation factor • River bedloss	[4-66] – [4-75]
Route river salt		

End of daily loop

End of monthly loop

End of annual loop