DEVELOPMENT OF A WATER QUALITY INDEX FOR ESTUARINE WATER QUALITY MANAGEMENT IN SOUTH AFRICA

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DEVELOPMENT OF A WATER QUALITY INDEX FOR ESTUARINE WATER QUALITY MANAGEMENT IN SOUTH AFRICA

Report to the Water Research Commission

by

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Executive Summary

Background and motivation for this study

The National Water Act (NWA) (Act 36 of 1998) for the first time includes estuaries as part of the water resource and as such they are subject to all water resource legislation. In order to set water resource quality objectives for estuaries it is necessary to develop a classification system along the lines of the categories developed for Ecological Reserve determination in freshwater systems (DWAF 1999). At present there are a number of management tools such as importance rating systems and condition or state assessments, which summarise and interpret scientific information into an Assessment Class classification system. Unfortunately most of the available management tools are limited to physical and biological components of estuaries and do not address the assessment of water quality. The need for the development of a classification system for estuaries based on water quality has been raised a number of times (Van Driel 1999) and as a result this study was initiated

Terminology

There is a need for the development of a rationale for the implementation of a risk-based approach to classifying estuaries on the basis of water quality into categories, analogous to the categories implemented in fresh water management.

The NWA provides for a classification system, the Ecological Reserve Assessment Classes. The regulatory endpoint is the loss of "sustainability", with the conditions for each Ecological Reserve Assessment Class expressed in terms of the "risk to the well-being of biota" and therefore the maintenance of "ecological integrity" in the face of adversity. **Ecological integrity** is regarded as "the ability to support and maintain a balanced, integrated, adaptive community of organisms having a full range of elements (genes, species, assemblages) and processes (mutation, demography, biotic interactions, nutrient and energy dynamics, and metapopulation processes) expected in a natural habitat of a region" (Karr 1996). **Sustainability** is seen as "the ability of an ecosystem to support itself despite continuous harvest, removal or loss of some sort" (USEPA 1997).

It is the formulation of the Ecological Reserve Assessment Classes in terms of "likelihood" that allows for the application of a risk-based approach to classifying estuaries into classes. The risk-based approach allows us to relating regulatory endpoints (sustainability) to stressor endpoints (mortality, growth inhibition, etc.). This gives rise to the **Ecological Risk-based Management** (ERBM) approach, which assesses the level of a stressor corresponding to an accepted level of risk. The ERBM approach further requires a formalised structure to realise the experimental level endpoints to regulatory endpoints and then express the aggregate risk through some form of mathematical aggregation of individual stressor risk.

The development of this index is therefore aimed at incorporating the ERBM approach, which requires the development/formulation of a framework in which the regulatory endpoints (as contained in the RDM) are related to experimental endpoints. In addition the index should provide an aggregation technique to integrate the individual stressor risk into a single risk to estuarine sustainability/integrity.

Study Approach

The general hierarchical approach to the development of a Water Quality Index (WQI) was followed. Since this project deals with the development of a specific index that assesses estuarine water quality in terms of a legislative endpoint, it will henceforth be referred to as the Estuarine Water Quality Integrity Index (EWQI). The steps followed to develop the EWQII were:

- Selection of water quality variables
- Transformation of variables into a dimensionless scale
- Formulate and compute the index score
- Ensure accessibility and functionality of the EWQII through incorporation into a Decision Support System (DSS)

Project objectives (as specified in the original contract)

The extent to which the project objectives were met is outlined below. Recommendations or actions as a result of the project findings are given in the text boxes.

1. To develop a water quality index for estuaries, which interprets water quality variables in terms of ecological/biological resource protection.

At a Steering Committee Meeting it was agreed that the index will be referred to as the Estuary Water Quality Integrity Index (EWQII) so that it is not confused with the eWQI used by Harrison et al. (2000). For the purposes of this study, water quality integrity is regarded as the water quality required to maintain estuarine diversity and function. An extensive literature review was undertaken to determine, which WQIs and water quality variables are the most suitable for the development of the EWQII (Mrs L Herbert – PhD student, UniZul). Following the selection of suitable water quality variables, a database containing the relevant stressor-response was compiled for all of the variables by sourcing international dadabases (Mr. A Viljoen – CRUZ, Mr. M Mzimela – UniZul, Mr. P Buthelezi – MSc student, UniZul). For the variable transformation process, a suitable scale or format was required, as well as a classification system to align the EWQII scores with RDM classes. A risk-based approach was selected for the different variables, which were related to a classification system (Dr P. Wade – Phokus Technologies). Transformations of the variables were carried out using the risk-based scales that were selected (Mr G O'Brien – MSc student). The final EWQII, which currently consists of 28 variables have been developed in conjunction with a EWQII Assessment Category classification scheme that interprets the index value in terms of RDM classification. This objective was successfully met.

Recommendation

There is a fair amount of confusion surrounding the use of the correct version of the classification systems used in wtare resource management in South Africa. The Ecological Reserve Studies use the A-F system whereas the River Health Programme uses a Natural to Poor system. Researchers should be updated on the status of the classification revision process regularly.

2. To incorporate the index into a DSS using ARCVIEW as a platform to link to other meta-databases.

Following consultation with persons actively involved in developing and maintaining DSS's using Graphical User Interface (GUI) such as ARCVIEW as platform, it was decided to develop the DSS using web-based HTML and Java-Script. The shell of the DSS, which contains information for a few selected estuaries has been completed and posted on the Department of Zoology, University of Johannesburg website (www.uj.ac.za\zoology). The relevant information (other estuarine index values, links to other estuary information, etc) for all estuaries in South Africa is currently being entered and updated (Mr R Swemmer and Ms M Nyakane – BSc Hons students, UJ). The DSS is not a static tool and it is essential that it is updated regularly.

Recommendation

The DSS must be made available on the WRC and CERM websites. The project leader, Prof. V. Wepener will take the responsibility for the continuous updating of the DSS as information is made available to him.

3. To developed the index in such a way that it will contribute towards the classification in terms of the Ecological Reserve requirements, i.e. different integrity categories as outlined in the RDM procedures.

This has been addressed under Objective 1.

4. To integration of the water quality index with existing estuarine index scores through the DSS.

This has been addressed under Objective 2.

SUMMARY OF FINDINGS

Selection of water quality variables for inclusion in the EWQII

An extensive survey of available literature on water quality classification systems was undertaken to determine, which classification system would be the most suitable for the EWQII and, which water quality variables would be most suitable for inclusion in the EWQII. There was a distinct difference in the ranking of water quality variables based on their importance between estuaries and freshwater systems. Emphasis in most WQIs appears to be on organic loading, with very little attention paid to other forms of pollution. Indeed the eWQI used by Harrison et al. (2000) contained only three variables that reflected biotic responses to water quality (in the form of a stressor-response relationship), i.e. ammonia, DO and AO.

The lack of information on the stressor-response relationships between estuarine organisms and water quality variables is most probably related to the unique physicochemical environment, primarily because of their variable salinity but also because of their strong gradients in other parameters, such as temperature, pH, dissolved oxygen, redox potential, and amount and composition of particles.

As pH and turbidity are strongly controlled by the mixing of marine and fresh water and that the pH of river water entering an estuary will be driven towards 8 by the strong buffering capacity of seawater, an average value for pH probably has little utility. Its importance, however, as an indicator of ionic equilibrium (for example in evaluating the potential for ammonia and metal toxicity) must be taken into account, which was the case for developing a stressor-response curve for ammonia. The water quality significance of turbidity or suspended solids in estuarine water is largely unknown. Turbidity of river water entering estuaries is probably more closely related to the nature of the catchment geology and geomorphology than to other factors. The turbidity will further increase within the estuary as this more turbid water encounters the intruding seawater. This often results in extreme variations in turbidity within an estuary and therefore the concept of mean turbidity for the estuary is meaningless, and thus contributes little to a measure of average estuarine water quality. It is for this reason that these variables were excluded from the EWQII.

The major source of dissolved substances in estuaries is the intruding seawater; hence measurement of TDS (salinity) is a much more important indicator of the extent of seawater mixing than water quality impairment. It is in fact the brackish nature of estuarine water that makes this habitat unique and contributes to its resource value. Therefore salinity was included for investigation as an important variable in the determination of estuarine water quality integrity.

The particular emphasis that was placed on trophic status in the majority of the WQIs warranted the investigation of nutrients as suitable variables for inclusion in the EWQII. Of particular concern in estuarine systems is the influx of inorganic and organic compounds such as trace metals and organic pollutants (e.g. pesticides, petroleum products, etc.) into these systems. Trace metals have previously been included in some of freshwater WQIs, however only one estuarine WQI has incorporated metals as variables. This is probably related to their inherent variability, particularly when linked to increased salinity. Nevertheless, in the South African situation it is imperative that these potentially hazardous substances be included as a reflection of water quality, on condition they meet the requirements mentioned out earlier. Although metals have previously been included in various WQIs, there are no maximum water quality criteria set for Al, Fe and Mn. These three metals were therefore excluded from the list of metal variables. The metals were selected based on the data availability and their inclusion in the South African Marine Water Quality Guidelines. The organic toxicants were selected for inclusion in the EWQII based on their inclusion in the South African Marine Water Quality Guidelines and presence in South African aquatic systems (Heath and Claassen, 1999). The metal toxicants included in the EWQII are: arsenic, cadmium, chromium, copper, cyanide, lead, mercury, tributhyl tin and zinc. The organic toxicants included in the EWQII are: Alachlor, Benzene, Chlordane, Chlorpyrifos, DDT, Dieldrin, Endosulfan, Lindane, Malathion, Phenol, Thiobencarb, Toluene and Total petroleum hydrocarbons.

Transformation of variables

Salinity

This section studies the impacts on estuaries as a result of modification of salinity regimes. Since ecotoxicological investigations popularly use hazard functions incorporating single-species measures, the arguments analysed in this report are based on the ideal of understanding impacts on biota in terms of known ecotoxicological relationships as a function of stress intensity and duration. Variability in environmental conditions, particularly with respect to salinity was considered a critical aspect of this study.

An extensive literature survey revealed that estuaries represent a physicochemically unique environment from a chemical toxicological point of view. Estuaries are characterised by variable salinity, and strong gradients in other critical ecotoxicological parameters, such as temperature, pH, dissolved oxygen, redox potential, and amount and composition of particles. The full range of environmental chemical processes occurs in estuaries, namely adsorption, desorption, coagulation, flocculation, precipitation, biotic assimilation, and biotic excretion. Changing salinity impacts *all* of these chemical processes. There is also a complex relationship between temperature and salinity in estuaries.

Ecotoxicology requires a hazard function which incorporates a measure of the intensity and duration to which the organism assemblage is exposed to a stressor. Estuaries are characterised by many episodic phenomena, and while a proportion of a population may survive a stressor that acts for less than a specific duration, there is a recovery period, during which the surviving organisms are susceptible to ill-effects if struck by another stressor.

Major changes in salinity regime may occur due to anthropogenic modification of estuarine hydrodynamics, and by changing flow-regimes in the upper catchments. In order to understand what might happen if the hydrodynamic quality of an estuary were to be modified; a theoretical analysis was embarked upon. Ecozones were classed into three broad categories –

euhaline (>18 ‰), mesohaline (5-18 ‰) and oligohaline (<5 ‰). Each ecozone, under normal conditions, experiences a sinusoidal modification of salinity, as a result of the influence of tides.

A mathematical analysis of magnitude and duration of salinity changes experienced by organisms in estuaries revealed that the mesohaline ecozone experiences a large fluctuation in salinity, with the extremes of salinity experienced for shorter durations than the salinities of the euhaline or oligohaline ecozones. The euhaline and oligohaline ecozones experience high salinity and low salinity ranges for much longer durations than the mesohaline ecozone does. It is theorised that a modification of an estuary from a mesohaline to an oligohaline or euhaline condition would increase the duration of the stress due to non-optimal salinity for some organisms, and would increase the magnitude of the stress.

The optimal salinity ranges for a large number of estuarine organisms is not known, due to the paucity of ecotoxicological data in public databases. Estuaries are ephemeral phenomena in the context of geological time. Because flow, tidal range and loads of sediments and humic materials are constantly changing, estuaries are far from steady-state systems.

The unstable and unpredictable behaviour of estuarine environmental factors decreases the probability of speciation and increases the probability of extinction of estuarine fauna. Ecologically, there is reduced interspecific (though not intraspecific) biotic competition due to overriding physical-chemical factors, of which salinity is the dominant stressor. In addition, depending on species specific salinity tolerances, in some cases immature organisms may not survive in areas where both mature and immature organisms are deposited. Usage of habitat by different species is actually greater than appears to be the case from snapshot estimates.

The conclusion of the literature survey and the mathematical analysis is that at this stage it is extremely difficult to predict the impact on an estuarine ecosystem, based on hypothesised modifications of salinity regimes, and using the current tools of ecotoxicology. There is simply not enough currently known about the structure of estuarine communities, and the relationship between this structure and macro-variables such as temperature, pH, dissolved oxygen, redox potential, amount and composition of particles, and specific chemical impacts.

It is hypothesised that a promising classification system in terms of salinity may be based directly on the distribution of estuarine fauna or functional groups ("optimal assemblage") that one expects in an unmodified estuary of a particular type.

Optimally, one would be able to empirically assign coefficients to a function of the following form:

$$\Delta_{assemblage} = \sum_i a_i \left| z_i - z_{opt,i} \right| \qquad \text{(Equation 1)}$$

where:

$\Delta_{assemblage}$ = deviation from optimal assemblage for an estuary

a_i = "keystoneness" of species or functional group *i* in the assemblage

z_i = representation of species or functional group *i* in terms of numbers or biomass

$z_{opt,i}$ = optimal representation of species or functional group *i* in terms of numbers or biomass and $|z_i - z_{opt,i}|$ is a measure of scalar deviation from optimum, possibly a modulus, or a quadratic function.

Recommendation

The implementation of the concept of “optimum” assemblages that represent particular types of estuaries particularly in relation to responses to natural variable parameters such as salinity needs to be addressed at research and management level.

Nutrients

The concentrations of nutrients in the water column are not necessarily predictive of the responses by aquatic plants and organisms. Grobelaar (1992) argues that over-simplified models of nutrient loads are inadequate for estuaries and other ecosystems where hydrodynamic factors and high turbidity can mediate the effects of nutrients. It is for these reasons that here are currently no South African nutrient standards for estuarine waters. Furthermore no rating curves based on international standards such as the Australian standards were adopted in the index since virtually all of South Africa’s estuaries would be classified as eutrophic.

A more suitable approach to assessing nutrients in relation to ecosystem integrity is through compiling a nutrient mass balance for an ecosystem, which can often help to identify major sources and sinks of nutrients. A mass balance represents all of the nutrients already present (i.e. water, sediments and biota) plus inputs, less the outputs (i.e. outflows & harvested biota like fish); what is left equals the internal load. Once the internal load is quantified, the external and internal processes which influence the load (e.g. biogeochemical cycling, primary production, etc.) can be identified.

A relatively simple budget model developed by the Land Ocean Interaction in the Coastal Zone Programme of the United Nations (LOICZ) provides both robust estimates of the flux across the coastal zone boundaries and long-term, integrated biogeochemical performance of the entire system. Furthermore, by treating the budget as a first step in the modelling procedure rather than as an end in itself, it is possible to identify the major processes which determine the fluxes and make the important transition from a purely descriptive budget to a predictive process-based model. These characteristics allow for the application of the model to set Reference Conditions or Present Ecological Status conditions. The model can be used to predict the changes in water, salt and nutrient fluxes due to changes in variables (e.g. freshwater inflow volume, increase in nitrogen concentrations in the estuary, etc.). The effect of the altered variable (as a percentage deviation from the reference condition) on ecosystem sustainability is interpreted in terms of a EWQII Assessment Category classification system.

Recommendation

A major stumbling block in the application of the LOICZ mass balance model is the paucity of water quality data for estuaries in South Africa. A National Estuarine Water Quality Monitoring Programme should be initiated.

Interpretation of estuarine water quality modification by discrete chemical discharges

The following variables were selected to form part of the EWQII: organic toxicants (Alachlor, Benzene, Chlordane, Chlorpyrifos, DDT, Dieldrin, Endosulfan, Lindane, Malathion, Phenol, Thiobencarb, Toluene and Total petroleum hydrocarbons.), neutral toxicants (ammonia, chlorine) and metallic toxicants (arsenic, cadmium, chromium, copper, cyanide, lead, mercury, tributhyl tin and zinc). At the start of the revision process, the USEPA ECOTOX databases were accessed to obtain a consistent level of data quality (which included measured concentrations of chemicals, all conditions documented, water quality reported, species used, etc.). Specific data criteria (Table 11) were selected to delimit the data and SSD curves were produced. The protecting concentrations for the toxicants, HC*p*, were estimated by fitting the Burr Type III distribution to the LC_{50} and EC_{50} data using the BurliOz software.

SSD models aim to account for unknown species sensitivities so will only be enhanced by larger datasets. In addition, risk assessments can combine a SSD with chemical exposure data or predicted exposures from simulation models. Therefore, the probability of exceeding an exposure estimate with an unacceptable adverse biological effect can be estimated. These probabilistic estimates of risk are a major strength of the SSD approach over the simpler hazard assessment method. For the development of the EWQII, HC*1* and HC*5* with varying levels of certainty were calculated for all the variables, using both the acute (LC_{50}) and chronic (EC_{50}) data sets. For the purposes of this project the EWQII categories (Table 1) were allocated percentile hazard concentrations (HC*p*'s), or conversely protection concentrations with different levels of certainty for each category. A brief summary of the selection of the different HC*p*'s and corresponding categories is given below:

- The 99% level with 50% certainty (HC*1,*50) was selected to represent conditions in a **"Natural"** system.
- The 95% level of protection and between 75 and 95% certainty (HC*5*,5-25) were chosen to represent a slightly modified system – **"Good"** system. A 95% level of protection, should be sufficient to protect the ecosystem provided keystone species are considered (it should be emphasised that increasing the certainty level from 50% to 95%, i.e. 95,95 results in a guideline value which, in practice, would actually protect considerably more than 95% of species in most cases and frequently over 99%).
- The 95% level of protection and between 50 and 75% certainty (HC*5*,25-50) were chosen to represent a moderately modified system – **"Fair"** system.

- The 95% level of protection with less than 50% certainty (HC*5*,>50) was chosen to represent an unacceptably modified system – **"Poor"** system.

Protecting concentrations and different levels of certainty were

Recommendation

Research should be undertaken to study the Burr III optimization with a neural network.

Formulation and computation of the index score

Many different formulae have been used to aggregate variables. The process of aggregation serves to consolidate all variable quality scores obtained from rating curves into a single number. Many regard this process as the most important step in WQI design, due to the potential for loss of information. The composite EWQII category is derived by aggregating the individual categories obtained for each variable. This is achieved through the assignment of a rank value to each category (see Table 13 for HC*p*'s with associated hazard rank scores for the acute-based copper data example once again). Once catecories have been assigned to all 28 individual variables (25 toxicants and 3 nutrient budget components), the hazard rank scores of the individual categories are used to calculate the composite EWQII score and associated EWQII Category. The aggregation method, which is proposed, is the most commonly used aggregation formula in water quality indices, i.e. Solway's unweighted modified mean. The Solway weighted and unweighted sums have been suggested to be sensitive and without bias to changes in water quality variables throughout their range and have being said to provide the "best" results for general water quality indexing (Richardson 1997).

$$I = \frac{1}{100}\left(\frac{1}{n}\sum_{i=1}^{n} q_i\right)^2$$

The resultant hazard rank value obtained is then reinterpreted in terms of an associated EWQII Category.

Incorporation of the EWQII into a DSS

The use of the numerical tools to assist in management decision support is considered the principle method of providing the relevant information. However, all these tools (models) require data to drive their exogenous variables and to derive estimates of their endogenous variables (parameters). A DSS can assist in storing, developing, creating and disseminating the information to general users through a suitable Graphical User Interface. The platform selected for the EWQII DSS is a web-based shell in HTML and Java-Script. The major advantage of this GUI is that it is readily accessible to a wide range of users. The DSS contains links to the software programmes used to calculate the EWQII, nutrient mass balance model and SSD. In addition information on a number of estuarine indices for each estuary is provided.

Technology Transfer

- The products from this project have not been tested outside the project team on other estuarine projects, e.g. EFR's or Reserve studies.
- The SSD approach to setting water resource management objectives has been applied to the Elands River in Mpumalanga with great success and has drawn expression of interest from SAPPI and CSIR (Pretoria). Presentations have been given to individuals from these two organisations.
- The theoretical concepts and application of mass balance models to calculate nutrient fluxes, water quality indices and the SSD approach to ecological risk assessment formed part of theoretical models in the BSc Honours (Aquatic Health) and the tutored MSc in Aquatic Health during 2003 and 2004. A total of 35 honours and 6 MSc students completed the modules successfully.

Further Research

- The implementation of the concept of "optimum" assemblages that represent particular types of estuaries particularly in relation to responses to natural variable parameters such as salinity. Implementation of this function in a management context will entail: a) Classification of morphologically distinct estuaries (which is already available); b) determination of assemblage status (in terms of proportions of species or functional groups) in these estuaries; c) determining the "keystoneness" of the species or functional groups; and d) Assigning classes based on $\Delta_{assemblage}$ calculated from $\Delta_{assemblage} = \sum_i a_i \left| z_i - z_{opt,i} \right|$.
- The EWQII Category classification system for nutrients is not based on any scientific basis. The relevance and applicability of the different Assessment classes need to be verified.
- The "bootstrap" technique used in Burrlioz is initially a simplex routine. The simplex routine is robust to numerical failure, but is not "intelligent" when faced with optimising a function when the response surface is highly wrinkled. Research should be undertaken to study the Burr III optimization with a neural network.

List of publications / Conference presentations

Dissertations

O'Brien, G. C. (2004). An Ecotoxicological investigation into the ecological integrity of a segment of the Elands River, Mpumalanga, South Africa. Unpublished M.Sc Dissertation. Rand Afrikaans University, Auckland Park, South Africa.

Conference presentations

O'Brien, G. C., Wepener, V. and Van Vuren, J. H. J. (2003). "Risk-based approach in assessment of increased salinity in the Elands River, Mpumalanga". *Abstracts, Joint Conference of Southern African Society of Aquatic Scientists and Zoological Society of Southern Africa*, 30 June – 4 July, pp 69-70.

Wade, P. and Wepener, V. (2003). "Towards a risk-based approach to classifying estuaries on the basis of water quality". *Abstracts, Joint Conference of Southern African Society of Aquatic Scientists and Zoological Society of Southern Africa*, 30 June – 4 July, pp 98-90**.**

Wepener, V. and Wade, P. (2003). "The use of species sensitivity distributions (SSD) in estuarine water quality resources directed measures (RDM) determination". *Abstracts, Joint Conference of Southern African Society of Aquatic Scientists and Zoological Society of Southern Africa*, 30 June – 4 July, pp 101.

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Development of a water quality index for estuarine water quality management in South Africa

The Steering Committee responsible for this project consisted of the following persons:

Dr SA Mitchell	Water Research Commission (Chairman)
Ms U Wium	Water Research Commission (Committee Secretary and Coordinator)
Prof DP Cyrus	University of Zululand – Department of Zoology
Dr S Jooste	Resource Quality Services, Department of Water Affairs and Forestry
Dr S Oelofse	Department of Water Affairs and Forestry – Directorate Water Quality management
Ms S Taljaart	CSIR, Environmentek
Dr AK Whitfield	South African Institute for Aquatic Biodiversity
Dr H Waldron	University of Cape Town – Department of Oceanography

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The following persons and organizations are thanked for their input and contributions:

- Students who assisted in data capture, analyses and data input into the DSS: Ms T Ansara, Ms M Nyakane and Mr R Swemmer (Department of Zoology, University of Johannesburg)
- Mr PP Buthelezi, Mr M Mzimela, Mr A Viljoen (Department of Zoology, University of Zululand).

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GLOSSARY OF TERMS

Hazardous	The potential to cause an (undesired) effect
Hazard Concentration (HC_5)	Concentration where 5% of the species are affected
EC_{50}	Concentration that results in a 50% change in the measured endpoint, e.g. 50% reduction in growth or decrease in fecundity
Ecological Risk-based Management (ERBM)	An approach, which assesses the level of a stressor corresponding to an accepted level of risk. The ERBM approach further requires a formalised structure to realise the experimental level endpoints to regulatory endpoints and then express the aggregate risk through some form of mathematical aggregation of individual stressor risk.
EWQII	Estuarine water quality integrity index – not to be confused with the eWQI of Harrison et al. 2000. The index developed during this study that assesses water quality parameters based on the risk that they pose to estuarine ecosystem structure and function.
EWQII category	A category assigned to the EWQII value based on whether the biological template is at severe risk of being altered (Poor category) to being at no risk and approximating natural conditions (Good category).
Integrity	"The ability to support and maintain a balanced, integrated, adaptive community of organisms having a full range of elements (genes, species, assemblages) and processes (mutation, demography, biotic interactions, nutrient and energy dynamics, and metapopulation processes) expected in a natural habitat of a region" (Karr 1996)
LC_{50}	Concentration that causes 50% mortality in test species
Species Sensitivity Distribution	A statistical distribution describing the variation among a set of species in toxicity of a certain compound or mixture. The species set may be composed of a species from a specific taxon, a selected species assemblage, or a natural community.
Sustainability	"The ability of an ecosystem to to support itself despite continuous harvest, removal or loss of some sort" (USEPA 1997)
Stressor	Anthropogenic substance, form of energy or circumstance that may cause a change in ecosystem integrity

LIST OF ABBREVIATIONS

%DO = Percentage dissolved oxygen
ABS = Surfactants
Alk = Alkalinity
BACT = Bacteria
BBM = Building Block Methodology
BOD = Biological oxygen demand
C = Carbon
CDF = Cumulative distribution function
Chl a = Chlorophyll a
Cl = Chloride
COD-Mn = Manganese (mg/l) oxygen
COL = Colour
Coli = Coliforms
COND = Conductivity
DIN = Dissolved inorganic nitrogen
DIP = Dissolved inorganic phosphorous
DO = Dissolved oxygen
DODP = Dissolved oxygen deficit percentage
DS = Dissolved solids
DSS = Decision Support System
E.coli = Escherili coliforms
EC = Electric Conductivity
ERA = Ecological risk assessment
ERBM = Ecological Risk-based Management
EWQII = Estuarine Water Quality Integrity Index
F. coli = Faecal coliforms
GUI = Graphical User Interface
HARD = Hardness of water
LOICZ = Land Ocean Interaction in the Coastal Zone
MAC = Percentage macrophyte area covered
N = Nitrogen
NH_3-N = Ammonia-nitrogen
NH_4 = Ammonium
NOEC = No-observed-effect concentration
NO_2-NO_3 = Nitrite-nitrate
NO_3 = Nitrate
NO_3-N = Nitrate-nitrogen
N_{tot} = Total nitrogen
NWA = National Water Act
OA = Oxygen absorbed
^oC = Temperature
OP = Obvious pollution
P = Phosphorous
PNEC = Predicted no-effect concentration
PO_4 = Phosphate
PO_4-P = Phosphate-phosphorus
P_{tot} = Total Phosphorus
RDM = Resource Directed Measures
SD = Secci depth
SEW = Sewage treatment
SS = Suspended solids
SSD = Species sensitivity distribution
T.coli = Total coliforms
TDS = Total dissolved solids
TIS = Total inorganic substances
TM = Trace metals
T-N = Total nitrogen
TON = Total oxidised nitrogen
TOS = Toxic organic substances
T-P = Total phosphorus
TS = Total solids
TURB = Turbidity
UNEP = United Nations Environmental Programme
WQI = Water quality index

1.0 INTRODUCTION

1.1 ESTUARINE WATER QUALITY WITHIN THE RESOURCE DIRECTED MEASURES (RDM) CONTEXT

The National Water Act (NWA) (Act 36 of 1998) came into effect on 1 October 1998. The central departures of the Act are the concept of resource use being dependent on resource protection and the recognition that the water quality should be extended to resource quality and should include the quantity and quality of the water itself. Quality does not just refer to the physico-chemical components of water but also refers to the integrity of the instream and riparian habitat (and therefore the geomorphological structure of the system), integrity of the instream biota and the associated riparian biota and the assurance of flow (DWAF 1997). For the first time the definition of water resources does not only include the water column of fresh water systems but also the groundwater, sediment, riparian habitat and estuaries.

As far as water quality in estuaries is concerned, resource use involves using resources both to supply water that is 'fit for use' by various user groups and to transport and absorb wastes, particularly using the natural biotic capacity to process organic wastes. In order to protect water resources the NWA allows for the establishment of a classification system. Once a classification system is in place a resource class could be determined, with resource quality objectives associated with each specific class. The resource class and quality objectives permit the determination of the Ecological Reserve. A number of methods have been developed for the determination of water quantity (using the Building Block Methodology – King and Louw 1998) and quality (DAWF 1999) and linking flow and water quality (Malan and Day 2003) to determine the Ecological Reserve for freshwater river systems. The water quality requirement of the NWA prescribes that for a given resource protection level, the concentration of chemical constituents and values of physical variables that should not be exceeded (DWAF 1999). The classification system of water resources that is currently in use varies from resources that are extremely impacted (category E or F) to those that are largely natural (category A). One of the components contributing towards the reserve is the ecological category, which in turn is comprised of a number of different components with their own categories. A system of assessment categories has also been devised for the common water quality variables (e.g. TDS, total inorganic nitrogen) ranging from A to F (DWAF 1999). Concentrations or values typical of natural systems are assigned to an “A” category. As the concentrations of chemicals increase and the values that demarcate the boundary value of specific class are exceeded, the boundary level of a new rating category is entered. The boundary between two categories is relative and the situation may arise where an entity may fall in the boundary and may belong to one of both classes. The degree to which a river, or reach thereof, is protected is dependent on the current state of the river and particularly on the category (Ecological Category) for which it will be managed (Malan et al. 2003). The more protective the category, the more stringent the water quality requirements would be. The River Health Programme makes use of a simplified categorisation of river integrity. The A-F classification system for setting assessment categories for different metrices, including water quality, is replaced with Natural, Good, Fair, and Poor (N-G-F-P) categories (RHP 2005). The new Ecoclassification procedure allows for processes to assign a category (A→F; A = Natural, and F = critically modified) to each component. Ecological evaluation in terms of expected reference conditions, followed by integration of these components, represents the Ecological Status or EcoStatus of a river (Kleynhans et al. 2005). Thus, the EcoStatus can be defined as the totality of the features and characteristics of the river and its riparian areas that bear upon its ability to support an appropriate natural flora and fauna (Kleynhans et al. 2005). This classification procedure emphasises that the boundary between two categories is relative and that the A→F scale represents a continuum. In some cases it may be that there is uncertainty as to which category a particular entity belongs. This situation falls within the concept of a fuzzy boundary where a particular entity may potentially have membership of both classes (Robertson et al. 2004). For practical purposes these situations are referred to as boundary categories and denoted as B/C, C/D, etc.

However, at present no methodolgy exists to classify estuarine integrity in terms of water quality. According to Van Driel (1998) estuarine integrity could be classified by integrating all aspects of estuarine processes, which are represented by individual indices, into a single classification system making use of some existing classification systems (e.g. Botanical Importance Rating – Coetzee et al. 1998; Fish Index – Harrison et al. 1994), modifying others (Habitat Integrity Status – Kleynhans 1996) and developing new indices (e.g. water quality index, benthic invertebrate index, etc.). It is against this background that this project was initiated.

1.2 TOWARDS A RISK-BASED PROTECTION OF ESTUARINE BIODIVERSITY

1.2.1 The risk concept and the NWA

According to Jooste and Claassen (2001) ecological risk has the potential to interpret resource classification, as required in the NWA, on a risk base and can assist in deriving efficient and pragmatic resource quality objectives. Hughes (1999) makes use of a risk-based/assurance modification to the BBM approach in incorporating magnitude-frequency concepts into the determination of ecological management classes. Jooste and Claassen (2001) caution that a risk-based approach requires consideration of the scientific data and its relation to human values since it reduces decisions from a purely mechanical process to one that requires explicit action. It is the NWA, stressor diversity and ecosystems' formulation in terms of likelihood that makes the use of risk-based approach so applicable (Jooste and Claassen 2001). These authors place particular emphasis on the following aspects:

- The NWA requires sustainable use. This implies that use of the resource needs to be balanced against its protection. This is in contrast to the more traditional hazard approach to water resource management, which tends to be inflexible, since only some of the stressor effect information and some of the stressor occurrence information are used to assess resource status. On the other hand, a risk approach allows more of both effect and occurrence data to be used.

• The hazard approach cannot handle the diversity of stressors that impact on the aquatic ecosystem in an integrated fashion. This is because hazards are usually expressed as stressors measured in units such as concentration, flow rate, etc. This approach does not inherently allow for ranking stressors or managing for combined effect. On the other hand a risk-based approach has the advantage integrating different stressors into a common, practically unit less basis.

• The inherent variable and epistemic uncertain nature of ecosystems and our knowledge of it as such, mitigate against making any information regarding the system and its response to stressors redundant. According to Jooste and Claassen (2001) such redundancy is necessarily a part of the hazard approach to resource management, whereas by contrast the approach is wasteful of available data.

Jooste (2001) concludes that both the ecological entity (the ecosystem) and ecological endpoint (sustainability) are fixed for the application of risk-based assessment under the NWA. The risk approach under the NWA follows an ecological risk-based management (ERBM) approach, which assesses the level of a stressor corresponding to an accepted level of risk. As with the traditional ecological risk assessment approach, stressor-response relationships are important in ERBM. According to Jooste (2001) the ERBM further requires a formalised structure for relating the experimental level endpoints to regulatory endpoints. For ERBM under the NWA, it is also necessary to express the aggregate risk through some form of mathematical aggregation of individual stressor risk.

The development of this index is therefore aimed at incorporating the ERBM approach, which requires the development/formulation of a framework in which the regulatory endpoints (as contained in the RDM) are related to experimental endpoints. In addition the index should provide an aggregation technique to integrate the individual stressor risk into a single risk to estuarine sustainability/integrity.

1.2.2 Regulatory endpoints and experimental endpoints

Resource management classification

The classification system that is provided for in the NWA can be linked to risk concepts. In the case of the Ecological Reserve this regulatory endpoint is the loss of sustainability, with the conditions for each Ecological category expressed in terms of the ”risk to the well-being of biota” (MacKay 1999). Table 1 presents the different categories used in Ecological Reserve determination studies, Ecoclassification categories, the RHP River Health categories and the proposed EQII categories and their descriptions of perceived conditions.

For the purposes of this report the EWQII categories will make use of the Natural-Good-Fair-Poor classification system as used in the RHP. Therefore all the water quality variables studied in Section 4 of this report will be interpreted using this classification system. Table 1 can be used to interpret the EWQII in terms of the other categories used in water resource management in South Africa.

Table 1. Ecological categories used in South African water resource management and perceived conditions**.**

Assessment Categories[1]	***Description of Perceived Conditions***	***River Health and EWQII Categories***	***Ecoclassification Categories***
A	Unmodified, or approximates natural condition.	Natural	A
B	Largely natural with few modifications. Although the risk to the well-being and survival of especially intolerant biota, depending on the nature of the disturbance, at a very limited number of localities may be slightly higher than expected under natural conditions, the resilience and adaptability of biota has not been compromised	Good	AB, B, BC
C	Moderately modified. Risks to the well being and survival of intolerant biota depending on the nature of the disturbance may increase substantially with resulting low abundances and frequency of occurrence, and a reduction of resilience and adaptability at a large number of localities.	Fair	C, CD
D	Largely modified. Risks to the well being and survival of intolerant biota depending on the nature of the disturbance increase substantially with resulting low abundances and frequency of occurrence, and a reduction of resilience and adaptability at a large number of localities.	Poor	D, DE
E	Seriously modified. The loss basic physiological and ecosystem functions are extensive.	Poor	E, EF
F	Critically modified. Modifications have reached a critical level and the system has been modified completely with an almost complete loss of ecosystem function.	Poor	F

[1]Current Ecological Reserve Assessment Categories

Stressor-response Relationships in Aquatic Ecotoxicology

The response-concentration ecotoxicological relationship tends to have a log-probability density shape (Figure 1), such as the probit or logit functions, and the response-time relationships (Figure 2) tend to have an inverse power relationship (Newman 1995; Newman and Dixon 1996). These general relationships are used to support the following arguments dealing with the feasibility of applying ecotoxicological analysis in assessing biological responses to water quality variables in estuaries.

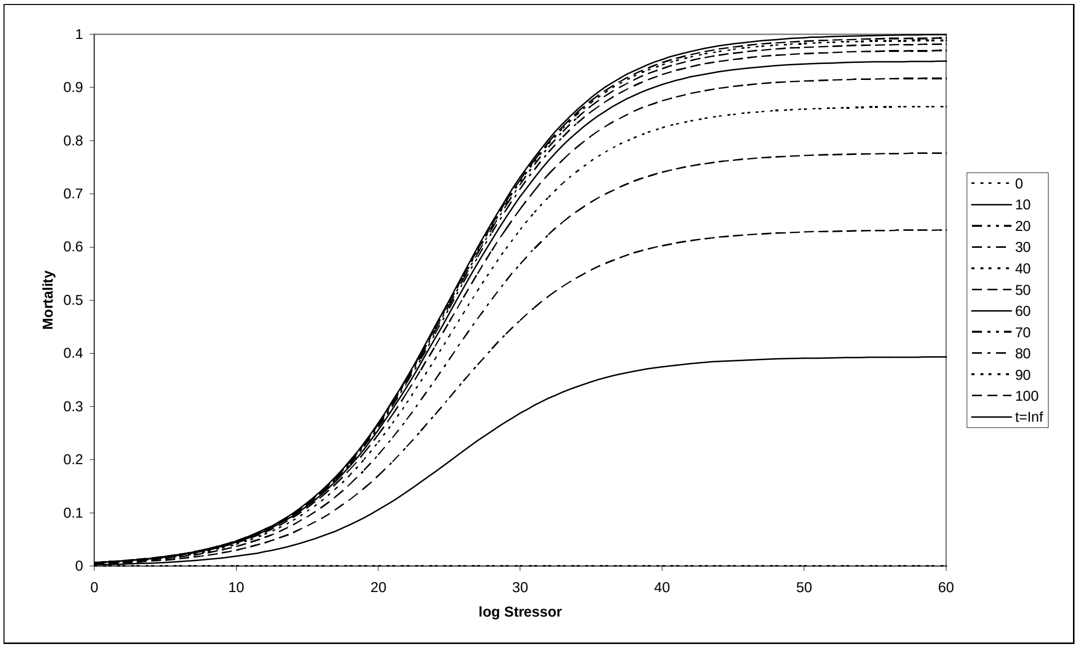

Figure 1. The typical form of log (concentration)-response relationships at different times.

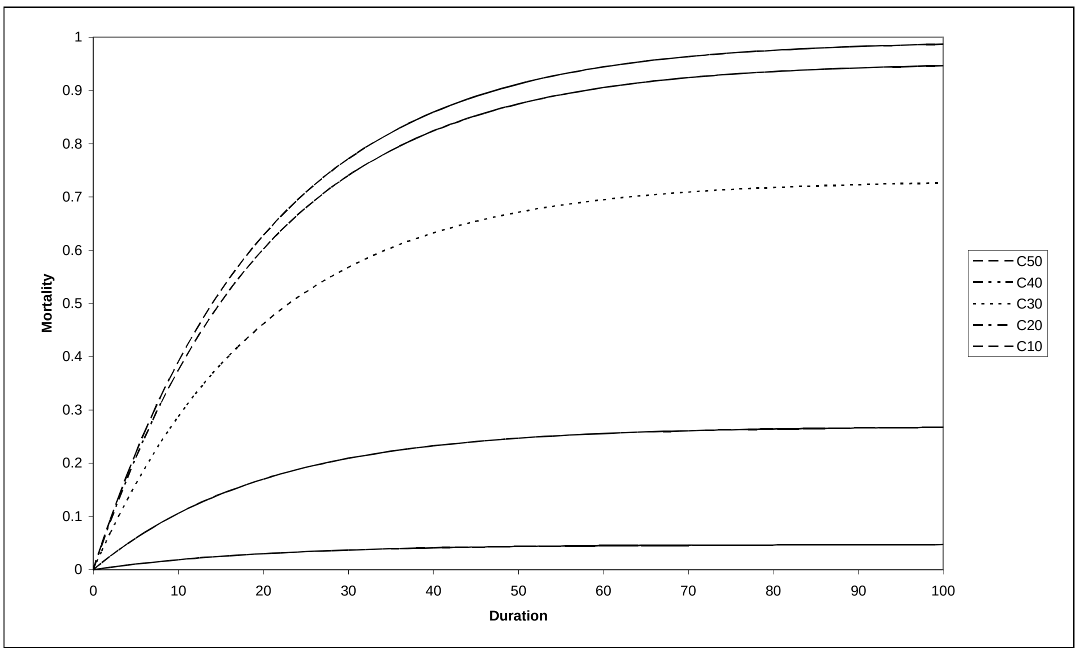

Figure 2. The typical form of duration-response relationships at different concentrations of a chemical (C10 – C50 are relative measures of concentration).

1.2.3 Sources of error

Variability of stressors

The variability of a system can be conceived as the range of values characterising the parameters that describe or determine the system. Estuaries are extremely complex natural systems. There is significant variability in seasonal and spatial aspects of estuaries, including the processes within estuaries, and, indeed, variability within these processes. Little is known about the behaviour of estuaries, and thus, variability of estuaries may be a significant source of error.

Uncertainty

Error due to uncertainty involves lack of knowledge of parameters governing a system. The principal difference between *variability* and *uncertainty* is that error due to uncertainty may be resolved, in principle, by more data gathering, whereas error due to variability is inherent in the system.

Vagueness

Vagueness, or fuzziness, represents a lack of clarity in the definition of the parameters associated with a system (Jooste 2001). Fuzziness is a characteristic of all models of systems, which leads to difficulty in defining ecosystems uniquely at an operational level.

Hazard

Very simply, while *hazard* relates to the magnitude of an undesirable event as a result of a set of circumstances, *risk* relates to the uncertainty of observing the hazardous event. In the context of biodiversity conservation, the hazard would relate to the loss of species from an ecosystem, and risk would relate to the likelihood of loss of species from an ecosystem.

Probability vs possibility

In probabilistic ecological risk assessments, the "likelihood of loss of species" is interpreted as a probabilistic function of ecosystem parameters. Probabilistic treatment of hazards assumes that the events are "crisply" defined, i.e. it is possible to determine whether an event has occurred or not (Jooste 2001). It is important to note (refer back to paragraph on Vagueness) that fuzziness is a property of all ecosystems, and that due effort must be expended in determining the observability of the hazardous event.

Hazard functions

Hazard functions express the (deterministic) relationship between the parameters in a set of circumstances and the hazardous event. Hazard functions greatly assist in explaining events, but are much more useful if applied to the *prediction* of undesirable events. Hazard events in ecotoxicology include loss of species from an ecosystem, and loss of sustainability of an ecosystem. It is important to note that simultaneous stressors are probably present in estuarine dynamics, and it will be necessary to include all stressors in an appropriate hazard function.

Temporal treatment

It is routine in aquatic toxicological investigations to measure, and use, functions that relate effects to stressors. The much-(ab)used LC_{50} is a measure of the probability of loss of 50% of the individuals from a population, as a function of a stressor, or combination of stressors, as is the case in Whole Effluent studies. Estuaries are acknowledged as dynamic systems, and thus stressors may be expected to change magnitude over time. It is known that organisms may tolerate stress for a period of time, before exhibiting the effect deemed significant. Thus, it will probably be important to incorporate a temporal aspect to the hazard function. This is partially discussed in the section 0 "Variation in salinity - ecotoxicological aspects".

Context of biotic assemblage

Ecotoxicological investigations popularly use hazard functions incorporating single-species measures. It is important to bear in mind that in the context of ecosystem protection, the hazard concerned is "loss of species from an ecosystem", meaning that for implementation in Reserve determinations, hazard functions must incorporate descriptions of biotic assemblages.

Exposure

Ecotoxicology requires a hazard function which incorporates a measure of the intensity to which the organism assemblage is exposed to a stressor. There are a number of ways of characterising the intensity of a stressor:

Probabilistic exposure distributions

In the context of chemical hazard, many studies have characterised exposure as the probability of observing a chemical concentration as a function of the chemical concentration itself (see e.g. Maund et al. 2001). This approach has been used in the current study.

Exceedence probability

The "exceedence probability" approach characterises exposure as the probability of a chemical exceeding a particular value, as a function of chemical concentration.

Exceedence-time probability

A third, complimentary approach, possibly very useful in the context of dynamic systems, is the Exceedence-time approach, in which the probability duration of a chemical concentration being exceeded as a function of time.

Cumulative episodic effects

Although not dealt with in the current study, it is worth noting that while a proportion of a population may survive a stressor that acts for less than a specific duration, there is a recovery period, during which the surviving organisms are susceptible to ill-effects if struck by another stressor (see e.g. Morton et al. 2000). Estuaries are characterised by many episodic phenomena, and it may be necessary to incorporate these subtleties into a proper ecotoxicological risk assessment of estuarine organisms.

1.4 STUDY APPROACH

1.4.1 Objectives

The objectives of the study, as indicated in the original project proposal, were as follows:

- The development of a water quality index for estuaries, which interprets water quality variables in terms of ecological/biological resource protection.
- Incorporation of the index into a decision support system (DSS) using ARCVIEW as a platform to link to other meta-databases.
- The index will be developed in such a way that it will contribute towards the classification in terms of the Ecological Reserve requirements, i.e. different integrity classes as outlined in the RDM procedures.
- Integration of the water quality index with existing estuarine index scores through the DSS.

The first two objectives were modified slightly following recommendations by the project Steering Committee members. Therefore the final project objectives were as follows:

- The development of an Estuarine Water Quality Integrity Index (EWQII), which interprets water quality variables in terms of ecological/biological resource protection.
- Incorporation of the index into a decision support system (DSS) using a World Wide Web-based platform to calculate the EWQII and integrate with existing indices.
- The index will be developed in such a way that it will contribute towards the classification in terms of water resourses management in South Africa, i.e. different categories as outlined in the Reserve determination, RHP and EcoStatus.
- Integration of the water quality index with existing estuarine index scores through the DSS.

1.4.2 Format of the report

A detailed literature review was undertaken on the history and development of water quality indices (WQIs). This was seen as being crucial in the development of an estuarine WQI since it allows for the selection of variables, rating curves and aggregation formulae from indices that have already been developed. This literature review is presented in **Section 2** of the report. As part of the general review a specific section relating to the classification of estuaries was included **Section 3**. From this review it will be possible to select the water quality parameters that are regarded as essential components in the assessment of water quality integrity of estuaries. These selected parameters will be assessed for suitability for inclusion in the EWQII.

In **Section 4** the selected water quality parameters are interpreted within the context of WQIs and ERBM. This includes the selection of existing rating curves and the development of new rating curves to relate regulatory endpoints to experimental endpoints, followed by the aggregation and interpretation of rating curves in terms of ERBM.

Section 5 provides a brief description of the method followed to incorporate the EWQII and other existing estuarine indices into a decision support system (DSS). Through the DSS the EWQII is applied to selected estuaries in South Africa. In **Section 6** the conclusions and recommendations for future research are provided.

2.0 LITERATURE REVIEW ON WATER QUALITY INDICES

2.1 INTRODUCTION

Accelerated population growth throughout the world has led to an increased demand for water (Melloul and Collins 1998). This, combined with the increased pollution of water bodies has created a need for monitoring of many of these systems in order to be able to quantify pollution (Joung et al. 1979; Miller et al. 1986). WQIs may be used to bridge the gap between monitoring and reporting of water quality data (Couillard and Lefebvre 1985; Richardson 1997), by providing a means to assimilate and effectively convey results from a vast quantity of data in a simple and effective manner (Couillard and Lefebvre 1985; Miller et al. 1986).

The aim of this section is to critically review the history and development of WQIs. The long-term objectives being the development of a WQI, drawing from a review of indices already developed.

2.1.1 Definition of WQI

WQIs are generally considered as part of a subset of indices used to "measure" environmental quality (Richardson 1997). Various authors have defined them as follows:

- "A form of average derived by relating a group of variables to a common scale and combining them into a single number." (Scottish Development Department 1976 in House and Ellis 1980).
- "Summarising information by combining several different variables (constituents) into a univariate expression" (Landwehr 1979 in Richardson 1997).
- "A quantitative expression of the degree of water quality impairment of a given water body." (Dunnette 1979).
- "An algorithm that expresses a measurement of an assessment of qualitative state of water. It is a simplified expression of a complex combination of several factors and its relevance depends on its reliability and the quantity of information it provides." (Couillard and Lefebvre 1985).
- "A summary statistic derived from water quality data that summarises the water quality state of that water" (Moore 1990 in Richardson 1997).
- "Integrating complex data and generating a single number reflecting the overall status of water quality in a given water body " (Cude 1997 in Richardson 1997).
- "A mathematical instrument used to transform large quantities of water quality data into a single number which represents the water quality level while eliminating the subjective assessments of water quality and biases of individual water quality experts." (Štambuk-Giljanovic 1999).

A water quality index is therefore, in essence, a function used to simplify large quantities of data into a more useful form in order to convey an image of overall quality to a variety of different users (Richardson 1997). All WQIs therefore follow the same basic principle in that they require some form of simple quality vector to synthesise analytical data (Couillard and Lefebvre 1985). WQIs are also communication tools for the transmission of information either to scientists or the general public (Couillard and Lefebvre 1985).

2.1.2 History

The need to monitor water quality was already recognised in Germany in 1850, where efforts were made to make some connection between purity of water and the presence of certain organisms. In 1912 the Royal Commission on Sewage disposal used a river classification system (Bolton et al. 1978) based on the visible condition of a watercourse incorporating such characteristics as smell, turbidity, presence/absence of fish, suspended matter and algal growth. Several countries later followed suit, instituting classification systems looking at either the pollution level or the presence and absence of certain macro and micro-organisms (Couillard and Lefebvre 1985). These early classification systems were largely of a descriptive nature.

Horton (1965) was the first to suggest the integration of different water quality variables into an overall numerically based index (Couillard andLefebvre 1985). Numerous numerically based indices have since been developed and further modified, some of which are: Prati et al. (1971), Moore (1973), Harkins (1974), Landwehr (1974), Walski and Parker (1971, 1974), Inhaber (1975), Ross (1977), Bolton et al. (1978), Yu and Fogel (1978), Dunnette (1979), Joung et al. (1979), House and Ellis (1980), Porcella et al. (1980), Steinhart et al. (1982), St.-Louis and Legendre (1982), Bharagava (1983), Couillard and Lefebvre (1985), Poch et al. (1986), Dinius (1987), House (1990), Smith (1989, 1990), Wepener et al. (1992), Erondu and Nduka (1993), Dojilido et al. (1994), Cooper et al. (1994), Gray (1996), Karydis (1996), Richardson (1997), Melloul and Collins (1998), and Štambuk-Giljanovic (1999).

There have been a number of different trends in the evolution of WQIs. The first is perhaps the emphasis on the development of a large diversity of indices for specific uses (Lohani and Todino 1984; Richardson 1997). Couillard and Lefebvre (1985) recognised a number of different phases. In the 1960s it was the development of general indices, the 1970s specific-use, planning indices and statistical approaches, and in the 1980's the development of trophic state indices. Many more WQIs have been developed since the reviews by Couillard and Lefebvre (1985). Once again the emphasis appears to be on the development of general use indices.

The second trend is the shift from the emphasis on freshwater systems to estuarine and marine systems. Most of the indices developed to date focus on fluvial water quality, such as lakes (Steinhart et al. 1982), general waterways (Smith 1989,1990; Walski and Parker 1974), freshwater (Dinuis 1987), and the remainder relate in particular to rivers. Only recently have indices been developed which are applicable to estuaries (Cooper et al. 1994; Richardson 1997) and two, which are applicable to the marine environment (Karydis 1996; Vollenweider et al. 1998).

The third and final trend is the transformation of the expression of the final results (Couillard andLefebvre 1985). Most WQI scores are expressed in a single numerical value.

Some authors have replaced this value with a combination of numerical or alphanumerical values for example the GLNI (Schierow and Chesters 1988). These extra values provide additional information about the reliability of the value obtained and whether any standards have been exceeded (Couillard and Lefebvre 1985).

2.2 DEVELOPMENT OF WQIS

There are generally four basic steps involved in the development of WQIs. They are; (a) the selection of water quality variables; (b) transformation or the comparison of variables on a common scale through the development of rating curves; (c) weighting of variables based on their importance to overall water quality; and (d) formulating and computing of the overall index.

2.2.1 Variable Selection

A major limitation in earlier indices was the method of variable selection. It is not possible to monitor all water quality variables; hence the most important ones need to be selected. The exclusion of some variables may however lead to the loss of important information. An additional concern has been the fact that the interrelationships between variables are usually ignored (Lohani and Todino 1984).

Horton (1965) used a subjective method that of a committee debate process, for variable selection, as did Dinius (1972). This was suggested by Joung et al. (1979) to limit these indices usefulness. Brown et al. (1970) based their index on that of Hortons, except for variable selection which was done by the Delphi opinion assessment process. This technique formed the basis of numerous subsequent indices. Other authors have suggested that the selection of variables by a panel of experts still incorporates subjective opinion or a method of rank order observation for variable selection (Lohani et al. 1984). However, Landwehr and Deininger (1974) stated that this method correlated least with that of the experts, and the basis of this WQI method would require the recalculation of this index whenever new data became available. Bharagava (1983) also stated that although this index was sensitive, the models on which the index was based made calculations cumbersome. As an alternative Joung et al. (1979) suggested the use of factor analysis not only to determine the interrelationships between variables but also to select which variables to include in an index. Lohani and Todino (1984) also used factor analysis, since it " seeks to express a large number of variables in terms of a smaller, more manageable number of factors based on linear relationships between the original variables". Other indices applied principle component analysis to develop the WQI, with the intention that this may enable them to improve geographical identification of problem areas and develop more appropriate water quality standards (Lohani and Todino 1984). Richardson (1997) suggested that the use of these alternate methods is uncommon. The tendency is towards the use of a combination of the Delphi technique for variable selection with the use of multivariate statistics to test for interrelationships between variables.

Nevertheless, the main cause of differences between indices is still the method of variable selection, since this varies greatly. Dunnette (1979) tested six indices to see how well they correlated. He suggested that correlations between indices should be interpreted with care since poor or marginal correlations between indices are not necessarily indicative of what could constitute a good or bad WQI. In addition some of the indices are poorly developed or not scientifically defensible. He concluded that the selection and combining of variables is not as critical as first thought, as long as variables are selected from the five commonly recognised impairment categories: oxygen status, eutrophication, health aspects, physical characteristics, and dissolved substances.

The categories suggested by Dunnette (1979) were based on perceived freshwater requirements. These categories are not really appropriate for estuarine and marine systems. Therefore Cooper et al. (1994) and later Harrison et al. (2000) proposed a revision of these five categories into three categories for "suitability of use" based on requirements for marine or estuarine systems (Table 2).

Dunnette (1979) suggested that special water impairments such as toxicity and radioactivity should not be included in a WQI. Rather, areas found to have these problems should be noted and dealt with separately. The reason being that only in this way would a WQI be valid for use over an extended geographical area. Three WQI's have been developed including toxicity data, namely: the near-shore quality index of the Great Lakes (Steinhart 1982 in Couillard and Lefebvre 1985 and Schierow and Chesters 1988), consumers WQI for recreational water quality (Walski and Parker 1974) and the aquatic toxicity index for rating ecosystem health (Wepener et al. 1992). Generally these WQIs are more locally specific than generally applicable (Richardson 1997). The index of Brown et al. only included toxicity data in the NSF index, when toxicity levels exceeded the maximum set by regulatory standards (Brown et al. in Richardson 1997). House (1989) demonstrated that the use of an aquatic toxicity index in conjunction with a generalised WQI provided a more complete assessment of water quality (Richardson 1997).

Table 2. Suitability of use categories and variables proposed by Cooper et al. (1994) with reasons for the inclusion of selected variables.

Category	Variable	Reason for inclusion
Suitability for aquatic life	Dissolved Oxygen	Essential to aquatic life
	Oxygen absorbed	Measure of organic loading
	Ammonia nitrogen	Toxicity to aquatic fauna
Suitability for human contact	*E. coli*	Evidence for human pathogens
Trophic status	Nitrate nitrogen	Aquatic plant growth stimulant
	ortho-phosphate	Aquatic plant growth stimulant
	Chlorophyll-a	Indicator of algal growth

2.2.2 Transformation of Variables

The purpose of variable transformation is to eliminate concentration units to produce a dimensionless scale with two end-points (Couillard and Lefebvre 1985), defined by acceptable and unacceptable limits within a range on an ordinate scale (Richardson 1997). Water quality may therefore be rated for example between 0 and 100, 0 being poor and 100 being pristine (Richardson 1997). Numerous other rating scales have been used, namely: between -100 and 100 (Stoner 1978 in Richardson 1997), -50 and 100 (Beron et al. 1979 in Richardson 1997), 10 and 100 (Dunnette 1979; House 1989), 0 and 25 (Gray 1996), 0 and 14 (Prati et al. 1971), 0/1 and 10 (Cooper et al. 1994, Melloul and Collins 1998; Ross 1977), 0 and 5 (Dinius 1987), and 0 and 1 (St.-Louis and Legendre 1982). House (1989) suggested that water would always be of some economic value even if it were purely for navigation or effluent transport purposes and should therefore have a value greater than 0. This however depends on the purpose for the index; specific use indices should be 0 since water may be of such a quality that it is not feasible for use (House 1989). Erondu and Nduka (1993) also suggested that having an upper limit of a 100 is not very relevant, since this would not be attainable in a natural environment. There is as yet no consensus on which is the best rating scale to use. Nevertheless a scale between 0 and 100 is the most common.

There are a number of different methods of variable transformation. The most common of these is rating curves, which may be based on either empirical information (Walski and Parker 1974) or environmental standards (House 1989). Most indices rate conditions with reference to some kind of standard (Schierows and Chesters 1988). They link variable concentration to that variable's desired value or standard (Melloul and Collin 1998; Štambuk-Giljanovic 1999). In this case, each variable is therefore represented by a rating curve based on criteria inherent to that variable where their scores vary proportionally with an improvement or deterioration in the quality of the water (Couillard and Lefebvre 1985). There are various different ways of representing rating curves, for example; transforming scale with discrete steps as in Horton's (1965) index, segmented linear or non-linear (Prati *et al.* 1971), continuous curve line (majority of indices) or expressed as a mathematical function (Dinius 1987; Joung *et al.* 1979).

Some of the other methods of variable transformation are the use of; a logarithmic transformation (Dunnette 1979; Karydis 1996; St.Louis and Legendre 1982; Vollenweider *et al.* 1998), rating tables (Gray 1996), non-parametric multivariate ranking procedures (Harkins 1974) and multiple regression analysis (Lohani and Todino 1984). Dunnette (1979) suggested that the logarithmic transformation of variables has a number of advantages over other methods of transformation, namely: that when low concentrations are transformed they are recognised as having greater impact than higher concentrations; variables which vary inversely proportional to water quality result in negative exponential curves (Walski and Parker 1974); curves are simple to reproduce and, negative exponential curves may be represented as a straight line on a semi-log scale making it easy to read-off values for calculation of the index (Walski and Parker 1974).

Rating curves are still, however, the most frequently used method of variable transformation (Harrison *et al.* 2000).

2.2.3 Weighting of Variables

The weighting of variables aims to assign relative importance to each variable and elucidate interrelations between the different variables. Allocated weights normally add up to 1, with the most important variable having the highest rating (Couillard and Lefebvre 1985). Weights may be determined based on a variable's relative importance (Bolton *et al.* 1978; Melloul and Collin 1998; Ross 1977), accepted standards (Inhaber 1975), Delphi technique or a statistical method such as principal component analysis (Lohani and Todino 1984), discriminate analysis (St.-Louis and Legendre 1982), regression analysis (Joung *et al.* 1979) or a combination of these. Of these the Delphi technique is probably the most frequently used (Harrison et al. 2000).

The applicability of weightings assigned to variables and the criteria on which these were based should be continually assessed (Richardson 1997). It is almost inevitable that continued research and acquisition of new information might alter information on which weights were based. Inhaber (1976) stated "A weighting system needs to take into account the varying emphasis between parameters, but also reflect non-linearity in pollutant-effect relationship, and importance of thresholds and peaks as against averages" (Richardson 1997).

Dojlido et al. (1994) suggested that it is better not to weight variables. The weighting of variables may lead to improper evaluation of rivers due to different variables having varying importance in different systems. Weighting eliminates the possibility of comparison between different systems since a particular variable's importance differs from system to system (Dojlido et al. 1994). Weighting variables also indicates that there is prior knowledge of that variable's importance in the system and its interaction with other variables and, that the relative importance of one variable over another is known (Wepener et al. 1992). Bolton et al. (1978) suggested that weighting variables is not essential. However, Inhaber (1976) stated that despite there being no consensus on which is the best method to use "not doing so may be regarded as an abdication of responsibility" (Richardson 1997).

2.2.4 Formulating and Computing

Many different formulae have been used to aggregate variables (Couillard and Lefebvre 1985). Table 2 contains a list of the most frequently used formulations. The process of aggregation serves to consolidate all variable quality scores obtained from rating curves into a single number. Many regard this process as the most important step in WQI design, due to the potential for loss of information (Richardson 1997). As with any simplification process the potential for distortion of the information provided by the original data is great. The two most common types of data distortion are referred to as ambiguity and eclipsing (Ball et al. 1980). Ambiguity is when the value of an index exceeds a limit value when none of the individual quality scores do (Couillard and Lefebvre 1985). This is particularly true for non-standardised indices

(Richardson 1997). On the other hand eclipsing is when an overall index score is acceptable but one or more of the variables exceed acceptable limits (Couillard and Lefebvre 1985). This is seen when using a weighted sum (Richardson 1997).

Brown et al. (1970, 1972) and Dinius (1987) all made use of a weighted arithmetic mean to aggregate variables. This method as well as the modified arithmetic mean, lacks sensitivity, in that a single bad parameter does not allow sufficient lowering of the index (Bharagava 1983; Walski and Parker 1974). It is generally agreed that a weighted product is better than a weighted sum (Couillard and Lefebvre 1985). Brown et al. (1973) and Landwehr (1974) put forward two additional methods, namely: the weighted multiplicative index, and the unweighted multiplicative or geometric index. Walski and Parker (1974) found the geometric mean to be a good alternative. Joung et al. (1979) and Landwehr (1974) suggested that this form was an unbiased and viable method. However, Gray (1996) found that the geometric mean was not adequate since if one or more of the values scored zero the WQI became zero. Walski and Parker (1974) see this as an advantage. This may however lead to an underestimation of the final value (Richardson 1997). On the other hand, the weighted multiplicative index despite being responsive to low water quality scores, consistently overestimates water quality, the only exception being when concentrations are in excess of accepted limits (Richardson 1997). This is contrary to Couillard and Lefebvre (1985) suggestion that it serves to eliminate such overestimation. Richardson (1997) suggested that this was due to its nonlinearity especially when weights are small. However, Landwehr (1974) described this form to be both excellent in describing water quality trends and in distinguishing between different field situations.

Dojlido et al. (1994) made use of the square root of the harmonic mean, since it gave a high statistical value to those variables with the least favourable value. It also eliminated weighting of variables which is advantageous should different systems be compared with one another.

Smith (1990) advocated the use of the minimum operator since it "avoids eclipsing" and did not exhibit ambiguity. The usefulness of this aggregation is questionable because of the lack of information it conveys and its basis on the poorest quality parameter (Couillard and Lefebvre 1985). This method of aggregation is probably of greater use in combination with another method of aggregation, as seen in Wepener et al. (1992).

The Solway weighted and unweighted sums have been suggested to be sensitive and without bias to changes in water quality variables throughout their range and have being said to provide the "best" results for general water quality indexing (Richardson 1997).

2.3 LIST OF WQIS

Table 3 contains a list of various WQIs developed to date. It consists of three columns which describe in detail the development of these indices, i.e. the variables selected and method of selection used, variable transformation and weighting if any, and variable aggregation. The fourth column indicates applicability in relation to the particular use, the aquatic system and the region it was developed for.

2.4 LIMITATIONS OF WQIS

The possible danger in the use of an index is that it may be misused or valuable information maybe lost or hidden due to aggregation of data (Dunnette 1979; Ross 1977). Three main areas of concern are the "subjectivity" related to selection of variables and variable weightings, whether variables should be weighted at all and the most effective method of aggregation with out unnecessary loss of information or on the other hand to complex to be effective. There is also, as may be deduced from the above discussion, no generally accepted method for the assessment of water quality (Gavrishova 1979). For these reasons, WQIs have tended to be under utilised (Couillard and Lefebvre 1985). Despite these limitations, the fact that a large amount of effort has been expended on the development and improvement of water quality indices is itself indicative of their intrinsic value (Richardson 1997).

To increase their utilisation, a balance must be achieved between oversimplification and excessive complexity in addition to them being used in their proper context (Bharagava 1983; Ross 1977). WQIs should therefore meet some basic requirements if they are to be useful. These are:

1. They should be readily derived from available monitoring data;
2. Impart an understanding of the significance of the data represented; and
3. Objectively designed but comparable with expert judgment in order that validity can be assessed (Dunnette 1979).

Table 3. Most frequently used aggregation functions.

Method	Equation	Reference
Arithmetic unweighted sum	$I = \frac{1}{n} \sum_{i=1}^{n} q_i$	Couillard and Lefebvre 1985; Landwehr and Deininger 1976
Arithmetic weighted sum	$I = \sum_{i=1}^{n} q_i w_i$	Couillard and Lefebvre 1985; Landwehr and Deininger 1976; House and Ellis 1980
Modified Arithmetic mean	$I = \frac{1}{100} (\sum_{i=1}^{n} q_i w_i)^2$	Richardson 1997
Unweighted geometric mean or unweighted product or unweighted multiplicative index	$I = (\prod_{i=1}^{n} q_i)^{1/n}$	Bhargava 1983; Couillard and Lefebvre 1985; Landwehr and Deininger 1976; House and Ellis 1980
Weighted geometric mean or weighted product or weighted multiplicative index	$I = \prod_{i=1}^{n} q_i^{w_i}$	Couillard and Lefebvre 1985; Landwehr and Deininger 1976; Smith 1990; House and Ellis 1980
Solway modified unweighted sum	$I = \frac{1}{100} (\frac{1}{n} \sum_{i=1}^{n} q_i)^2$	Couillard and Lefebvre 1985; House and Ellis 1980; Wepener et al. 1992
Solway modified weighted sum	$I = \frac{1}{100} (\sum_{i=1}^{n} q_i w_i)^2$	Couillard and Lefebvre 1985; Smith 1990; House and Ellis 1980
Harmonic square mean	$I = \sqrt{\frac{n}{\sum_{i=1}^{n} \frac{1}{q_i^2}}}$	Dojlido et al. 1994; Richardson 1997.
Minimum operator	$I = \min(q_1, q_2, ...q_n)$	Couillard and Lefebvre 1985; Smith 1990; House and Ellis 1980
Maximum operator	$I = \max(q_1, q_2, ...q_n)$	Couillard and Lefebvre 1985; House and Ellis (1980)

Table 4. List of Water Quality indices (update from Couillard and Lefebvre 1985).

Authors	Selected Variables	Variable transformation and weighting	Variable aggregation	Applicability
Beron et al. (1979; 1980, 1982) [+] Groupe de recherche sur l'eau en milieu urbain Index	Numerous parameters depend on use; Number of uses considered: potable water, aquatic life, pollution sensitive and pollution tolerant spp., recreation, and agriculture. Three sets of variables; primary, accessory and supplementary, the latter includes mainly toxic substances and is optional.	Weighting dependant on intended use; Rating curves vary according to use; Scale between -50 and 100.	Weighted sum	Developed for multiple uses; Rivers
Bharagava (1983) Integrated WQI	9 variables, ^{o}C, SD, DO, BOD, Cl, COND, HARD, Coli, NH_3-N.	Equal weighting of relevant variables	Geometric weighted mean and inclusion of a sensitivity function	Various uses; Rivers, India
Bolton et al. (1978)	10 variables DO, BOD, NH_3, E.coli, pH, TON, PO_4, SS, COND, ℃	Rating curves used to produce dimensionless scale between 0 and 100; variables weighted to a total weighting of 1, based on importance of variable.	Weighted geometric or weighted Solway mean	No specific use considered; Rivers , UK
Brown et al. (1970, 1973) [+] National Sanitation Foundation WQI	9 variables selected by Delphi type technique; faecal coliform, pH, BOD, NO_3, PO_4, ^{o}C, TURB, TS and %DO	Delphi technique used for unequal weighting of variables; Rating curves to produce dimensionless scale 0-100	Weighted product	No specific use considered; Rivers, USA
Cooper et al. (1994) WQI	Authors selected 7 variables from 3 estuarine impairment categories, DO, OA, NH_4, F.coli, NO_3-N, PO_4-P	Use of rating curves to produce dimensionless scale range between 0 and 10., weighted impairment categories equally, and unequal weighting of variables.	Solway modified weighted sum	No specific use considered; Estuaries, South Africa
Dinius (1987) Index of Water Quality	Delphi type technique used to select 12 variables, DO, BOD_5, Coli., E. coli., pH, Alk, HARD, Cl, COND, ^{o}C, COL.	Four-round Delphi evaluation using a seven member panel used to weight variables; importance rated on a scale of 0 to 5	Multiplicative aggregation function	Several uses considered; Freshwater, USA
Dojilido et al. (1994) WQI	7 basic variables, BOD_5; SS; PO_4; NH_3; DS; COD-Mn; DO.	Dimensionless scale; variables not weighted , values of 0-100 based on government standards	Unweighted harmonic mean of squares	General use and speci-fic use by variation in variables selected; Rivers, Poland
Dunnette (1979) WQI	6 variables selected by Delphi type technique; DO, BOD, NO_2-NO_3, TS, pH, F. coli.	Log transformation of variables to produce a dimensionless scale between 10-100; weighting of variables by Delphi technique	Weighted arithmetic mean	No specific use considered; Rivers, USA
Erondu and Nduka (1993) WQI	8 variables, ^{o}C, pH, DO, BOD, NH_3-N, Sulphide, Silica, HARD.		Exponential model of the Geometric Mean which is as follows: WQI= exp Σ^{i}_{n} f_i (P_i) x 100 Where f_i is sensitivity function of parameter index i, and n is number of relevant observations	Includes specific uses such as bathing, public water supply, fish culturing and industrial uses; Rivers, Nigeria
Gray (1996) Acid Mine Drainage Index	7 variables, pH, SO_4, Fe, Zn, Al, Cu, CD	Variables weighted and water quality rating table used to obtain WQ scores between 0 and 25	Modified weighted arithmetic mean	Use in acid mine drainage contamination
Harkins (1974) [+]	Selection and number of variables used, up to user.	No weightings and no rating curves used.	Kendall's non-parametric multivariate ranking procedure. Aggregation formula:	Lake, river or discharge

Table 4. continued

Authors	Selected Variables	Variable transformation and weighting	Variable aggregation	Applicability
Horton (1965) Quality Index	10 variables, SEWAGE., pH, COND, %DO, T.coli, CCE, ALK, Cl, ^{o}C, OP.	parameter's weightings interrelated; rating curves used to produce dimensionless scale 0-100	Weighted sum multiplied by two coefficients	No specific use considered; Rivers, USA
House (1989,1990) WQI	A number of selection criteria used to select 9 variables, DO; NH_3-N, BOD, SS, NO_3, pH, ℃, Cl, T.coli	Delphi technique used to determine weightings; rating curves based on accepted standards used to produce dimensionless scale of 10 to 100,	Solway modified weighted sum	No specific use considered; Rivers, UK
Ibbotson (1977) +	Author suggests T.coli/ F.coli, DO, TN, TP, pH, ^{o}C, TDS, TM and TURB.	All variables of equal weighting in calculating subindices, subindices are weighted; Rating curves developed from accepted standards ranging between 1 and 10.	Final calculation is weighted sum	Various uses considered, potable water, recreation, agricultural and aquatic life; Rivers
Inhaber (1975)	Two subindices: (1) general quality - consists of trace metal subindex (Cd, Li, Cu, Zn, Cr, HARD); turbidity and effects on potable water subindex; and commercial fishing subindex. (2) Subindex for punctual discharges (BOD, SS, NH_3, TP, Phenols, Cyanide)	(1) No weighting for parameters or uses; use of rating curves; (2) special weighting for some variables not for uses, rating curves included but not clear.	(1) Root mean square; (2) Weighted sum. Combined aggregation formulae is: $ICQE=I^2_{AMB}+I^2_{RT}/2$	More of a general environmental quality index. Lake, river or discharge
Joung *et al.* (1979), Miller *et al.* (1986) WQI for Nevada	10 variables selected particular to Nevada and common to 5 freshwater impairment cate-gories, ^{o}C, BOD, TP, PO_4-P, TN, NO_3-N, EC, TURB, pH, DODP.	Combination of PCA and multiple regression analysis used to weight variables; Rating equations were developed by polynomial regression analysis to produce a dimensionless scale of 0 to 100.	Weighted sum	Rivers specific to Nevada, USA
Karydis (1996)	4 variables of measures of eutrophication; PO_4, NO_2; NO_3; NH_3	Log transformation and standard-isation of variables using the following formula: $Z_{ij} = \frac{X_{ij} - Y_i}{\sigma_i}$ Scale 0-100;		Coastal/Marine
Keilani *et al.* (1974)+ National Water Quality Economic Index	Delphi technique used determine five variables for each of eight uses; User selects use with regards to particular area	Delphi technique used to determine weightings (add up to 1) and rating curves for the different variables. Scale ranges between 0 and 100.	Aggregation formula is a weighted sum with two different weightings; one for the variable *i* of use *j*, and one for the use *j* itself.	Applicable to eight different uses; Lakes and rivers of specific region
Lohani and Todino(1984) WQI	Authors selected 13 variables, pH, ^{o}C, DO, TURB, SS, Cl, NO_2, NO_3, TN, PO4, BOD, T.coli, COND	Principal component analysis was used to determine variable weights; multiple regression was used to produce a scale of 0-100;	Aggregation formula is: $I(i) = \sum_{j=1}^{n} \frac{a(ji)\gamma(j)}{\lambda(i)}$ Where *a(ji)* = factor loading on variable *j* on factor *i*; ϒ(*j*)= standardised form of variable; λ(*i*) = eigenvalue of factor *i*	Very data specific, Chao Phraya River, Thailand
Melloul and Collin (1998) Index of Aquifer Water Quality	Authors selected 2 variables Cl, NO_3 (for preliminary testing of index) use of additional variables up to the user.	Use of rating curves based on accepted standards to produce a dimensionless scale 0 to 10; Weighted according to relative importance.	Modified weighted sum	Aquifers, particular interest in salinisation and pollution

Table 4. continued

Authors	Selected Variables	Variable transformation and weighting	Variable aggregation	Applicability
Padgett and Stanford (1973)[+] Industrial Water Pollution Index	Variable selection is up to the user.	Normalised values reflect scores for the different observations; Weight-ing is optional;	Weighted or unweighted sum of the normalised values	Particularly to indust-rial use; discharge
Porcella *et al.* (1980) Lake Evaluation Index	Authors selected 6 variables SD, TP, TN, Chl-a, DO, MAC; Empirical functions used to aggregate each of the variables	Use of rating scale between 0 (not polluted) and 100 (polluted); variables weighting not clear.	Weighted Sum	Assumption main source of pollution is nutrient enrichment; Lakes, Canada
Prati *et al.* (1971) Implicit Index of Pollution	Authors selected 13 variables; pH, %DO, BOD, COD, SS, NH_3, NO_3, Cl, Fe, Mn, ABS, CCE, C.KUB;	equal weighting; dimensionless scale of 0-14 based on standards (for potable water) from various organisations, value greater than 8 = heavily polluted	Unweighted arithmetic mean	Specific use - potable water; Rivers, Canada
Richardson (1997)	Author selected 8 variables; DO, NH_3, pH, F.coli, TURB, NO_3-N, OP, Chl-a.	Use of rating curves based on water quality guidelines; dimensionless scale of 0 to 100; user decides on weighting	Unweighted harmonic square mean	Estuaries, New South Wales, Australia
Ross (1977)[+] WQI System	Author selected 4 variables based on those being indicative of pollution, SS, BOD, DO, NH_3.	Scale 0 to 10; 0= polluted and 10= pristine; relative weighting of variables incorporated in rating curves; descending order of importance; NH_3 and BOD, SS, DO and %DO.	Aggregation method - summation of trans-formed values divided by the total weight of all the variables	No specific use considered; River, UK.
Smith (1989, 1990) WQI System	Delphi method of variable selection 9 variables; DO, pH, SS, TURB, ^{o}C change, BOD_5, NH_3, F.coli.	Delphi method and accepted standards were used to produce rating curves on a scale of 0-100	Initially used weighted multiplicative, latter re-placed with minimum operator	Considered the following uses general, bathing, water supply and fish spawning; Waterways, New Zealand
St.Louis and Legendre (1982) Microbial WQI	Only bacteriological variables were included, T.coli, Fecal, Streptococci	Data log-transformed and dis-criminate analysis done to determine weightings and rating curves on a scale between 0 and 1	Aggregation method is the discriminate score less the min. value obtained for a sample divided by the max. less the min. for the same sample.	Lakes Beaches
Stambuk-Giljanovic (1999) WQI	9 variables, ℃; Mineralisation, Corrosion coefficient, %DO, BOD_5; T-N; Protein N; T.coli	Weighted on a dimensionless scale of 0-100;	Weighted sum	Ground water for use as drinking water, Dalmatia
Steinhart *et al.* (1982) Great Lakes Nearshore Index	9 variables from 4 different categories, chemical, COND, Cl, P_{tot}; physical, SS, OP; biological, F.coli, Chl. a; and toxic, TOS, TIS.	Rating curves vary according to variable category; to produce a dimensionless scale between 0 and 100; Categories or subindices have different weightings	Weighted sum	General use index, Lakes, USA
Stoner (1978)[+]	Variable selection according to use; generally two groups: (I) toxic substances, (II) health or aesthetic parameters; 21 parameters used for irrigation and 39 for potable water.	(I) no weighting, step function rating curves; (II) parameters weighted, National Academy of Sciences standards used as basis for rating curves; Scores range between -100 and 100.	Aggregation formulae is: $I = \sum T_i + \sum w_i q_i$	Specific use considered, namely: irrigation and potable water; Rivers

Table 4. continued

Authors	Selected Variables	Variable transformation and weighting	Variable aggregation	Applicability
Truett *et al.* (1975)+ Prevalence duration Intensity	3 parameters selected; (P) spatial extent; (D) duration and (I) intensity of effect. (I) consists 3 subparameters: ecological, practical and aesthetic scopes.	(P) no rating curves, (D) score is that proportion of the year that a standard is not stateside, (I) score is the sum of 3 subparameters of impact levels. Weighting is according to use	Aggregation formula: $\mathrm{PDI} = (\mathrm{P} \times \mathrm{D} \times \mathrm{I}) / \mathrm{M}$ Where M = miles in the covered administrative unit set by state/county	To assess general water quality of rivers
Walski and Parker (1974) Consumers WQI	Authors selected 12 variables,	Sensitivity functions based on negative exponential equations, user give own weightings for variables rating between 0 and 1; no weighting for different uses,	Geometric mean (weighted product);	Developed for recreational use; Waterways, USA
Wepener *et al.* (1992) Aquatic Toxicity Index	14 variables, DO, pH, TURB, TDS, F, K, OP, Zn, Mn, Cr, Cu, Pb, Ni;	No weightings used; scale Use of existing and modified rating curves using WQ standards to produce a scale between 0-100,	Solway modified unweighted additive aggregation function and a minimum operator	No specific use considered, Rivers, South Africa
Yu and Fogel (1978) Combined WQI	Two components were used (a) 5 water quality variables, SS, ABS, T.coli, NO_3, PO_4, and (b) an economic variable		Index is an absolute value	Water treatment, USA

Refer List of abbreviation for symbols ; + from Couillard and Lefebvre (1985)

3.0 ESTUARINE WATER QUALITY REQUIREMENTS

3.1 INTRODUCTION

Estuaries are highly variable systems, characterised by complex interactions indicative of the mixing of fluvial and marine water (Branch and Branch 1981; Richardson 1997). They are controlled by the fundamental variables of water quantity, quality and movement (Richardson 1997; Whitfield 1998). The biotic and abiotic gradients that are established by the cycles of disturbance fundamental to all estuaries are central to the distribution and abundance of all organisms in these systems (Whitfield 1998).

The nature of an estuary is also directly related to its catchment and the coastline. This is particularly evident in SA where the Orange River Estuary is separated by some 3100 km of coastline from Kosi Estuary, the Atlantic Ocean running along the west coast and the Pacific Ocean along the east and south coasts. The West Coast is characterised by the sporadic upwelling of cool nutrient rich waters typical of the Benguela current. From the south coast, just east of Cape Point to the east coast there is a marked increase in temperature from warm-temperate water to warm subtropical water, consistent with the Agulhas current. These differences have a profound influence on the inland climate and vegetation, where the Northwest coast is characteristically a low rainfall area and is therefore semi-arid, the Southwest coast has winter rainfall, south coast has summer and winter rainfall, and the east coast has high summer rainfall. The geomorphology of these coastal areas further influences the type of estuary. The rivers of KwaZulu Natal are typically short with steep gradients, this combined with the high rainfall characteristic of this region result in rivers with high velocity, greater cutting action and greater silt loads. South coast rivers although also characteristically short with steep gradients, drain sandstone/quartzite and therefore carry relatively low silt loads. West Coast rivers on the other hand are normally little more than dry riverbeds only connecting to the sea during times of exceptional rainfall. The number of estuaries in South Africa depends on the definition of an estuary.

3.2 DEFINITION OF AN ESTUARY

Pritchard (1967 in Whitfield 1998) defined an estuary as "a semi-enclosed body of water which has a free connection with the open sea and within which sea water is measurably diluted with freshwater derived from land drainage". This definition is not really appropriate to many of estuaries in South Africa, which are characterised by frequent closure and only opened due to high discharge from rivers. Day (1981) defined an estuary as " a partially enclosed coastal body of water which is either permanently or periodically open to the sea and within which there is a measurable variation of salinity due to the mixture of sea water with freshwater derived from land drainage" (Whitfield 1998). Heydorn more recently defined estuaries as " that portion of a river system entering the sea where there is within boundaries of the land, a gradual transition in physical, chemical and biological characteristics from fresh to sea water". However, since most

SA estuaries are closed for most of the year, resulting in reversed salinity gradients this is also not an appropriate definition (Whitfield 1998). The definition according to Day (1981) is thought to be the most appropriate since it encompasses most estuaries in southern Africa. However it does not account for the variety of different types of estuaries found in this region (Whitfield 1998). This variety has lead to the classification of these systems.

3.3 CLASSIFICATION OF ESTUARIES

According to Whitfield (1992) there are 117 subtropical, 123 warm-temperate and 10 temperate estuaries in SA (from Whitfield 1998). Estuaries may be classified based on a particular characteristic such as salinity or a combination of a number of different criteria (Whitfield 1998). Salinity is a key factor in characterisation of estuaries. The Venice system of classification divides estuaries into oligohaline (0.5-4.9), mesohaline (5.0-17.9), polyhaline (18.0-29.9), euhaline (30.0-39.9) or hypersaline (salinity greater than 35) based on the salinity of each system. The classification according to Day (1981) is also based mainly on the salinity of estuaries:

(a) Normal / positive estuaries increase in salinity form head (river) towards the sea and net flow seaward over a full tidal cycle. Divided in turn according to extent of stratification into saltwedge, highly stratified, partially mixed and vertically homogenous;
(b) Hypersaline/ negative estuaries where salinity gradient increases from the sea towards the head (river), water level is below sea level and net flow is therefore inward;
(c) Closed/ Blind estuaries, temporarily closed by a sandbar, have no tidal range and no tidal currents.

Freshwater input from the river and extent of overtopping and evaporation determine the salinity. On the other hand, the classification according to Whitfield (1998) is based on a combination of physiographic, hydrographic and salinity characteristics and are divided into; (a) permanently open; (b) temporarily open/closed; (c). river mouths; (d) estuarine lakes; and (e) estuarine bays. Harrison et al. (2000) classification was based on the main forms of morphological variation in SA estuaries (Figure 3).

This is the conceptual basis of this classification. However, very little data is available on certain of the criteria used for this classification. In addition to this, variations in processes operative in each type of system do not account for potential variations in habitat that may arise due to variations in size. The more practical classification based on available data and accounting for size variations is therefore presented in Figure 4. This figure is basically the same as the previous figure as far as the open/closed division thereafter only the non-barred type is fully identified. The closed systems are subdivided on the basis of their surface area into three groups, one comprising those systems smaller than 2ha, a second between 2 and 150ha, and lastly those over 150ha. The open systems were divided into non-barred and barred. The barred open estuaries were divided according to mean annual runoff (MAR) values. The mouths of the smaller estuaries are most probably maintained by freshwater discharge and are therefore river dominated. On the other hand, the larger estuaries probably comprise a combination of tide and river dominated systems, some of which will oscillate between the two depending on the season (Harrison et al. 2000).

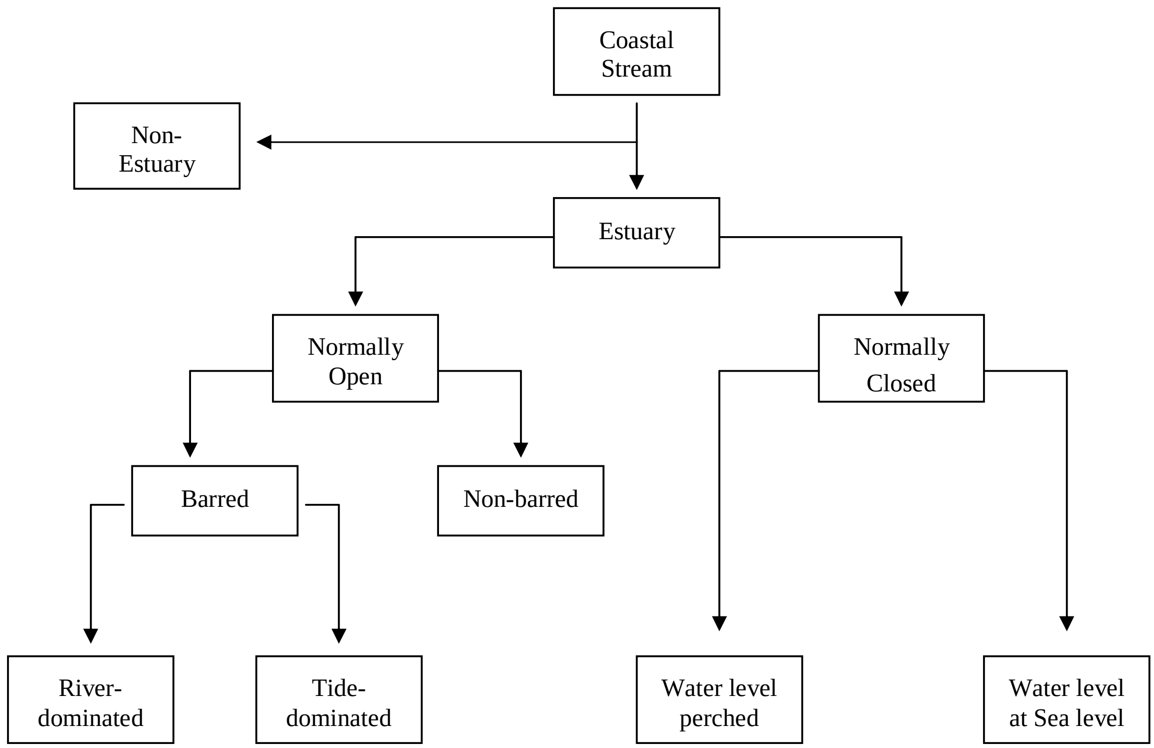

Figure 3. A conceptual classification for South African estuaries based on the range of estuaries present (Harrison et al. 2000).

According to Harrison et al. (2000) the classification revealed that much of the available knowledge on SA estuaries is restricted to a limited range of system types. However, no one system is more valuable than another. It also therefore follows that if a system does not necessarily mimic a view of what is a pristine estuary, it does not necessarily mean that it is polluted. The natural variability inherent in estuaries therefore needs to be taken into accounted in the development of a water quality index (Harrison et al. 2000).

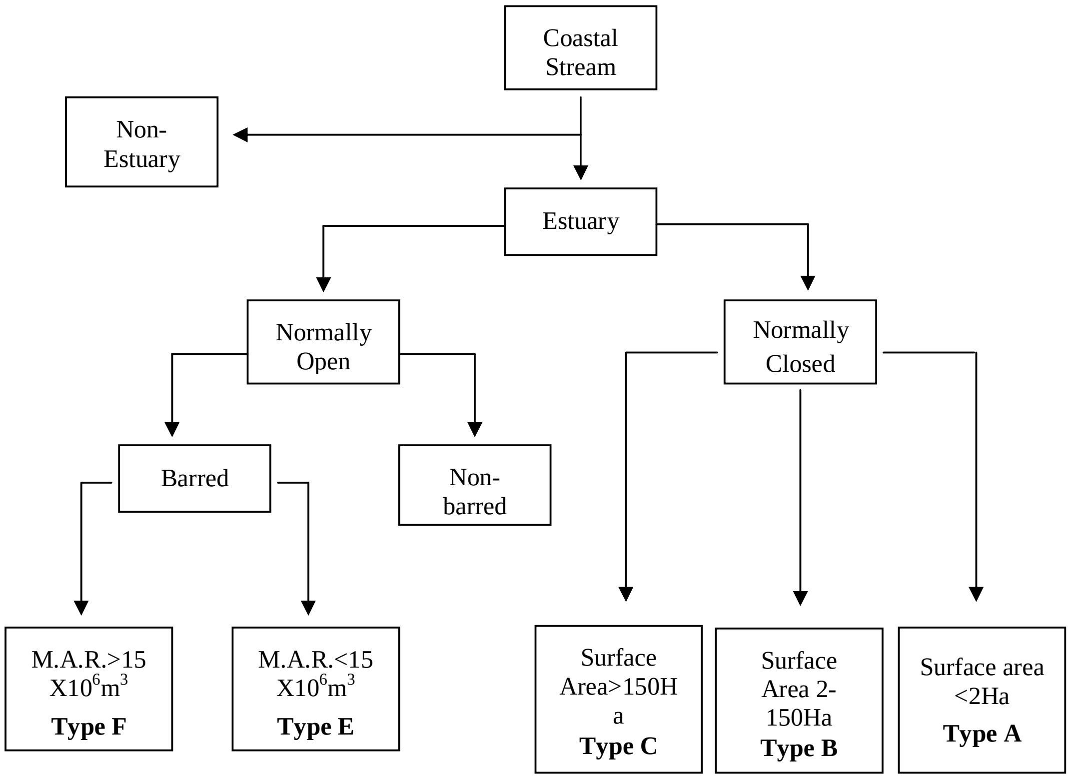

Figure 4. A classification of estuaries in South Africa according to available data, taken from Harrison et al. (2000).

3.4 THE UNIQUE ECOTOXICOLOGICAL NATURE OF ESTUARIES

From a chemical toxicological point of view, estuaries represent a physicochemically unique environment, primarily because of their variable salinity but also because of their strong gradients in other parameters, such as temperature, pH, dissolved oxygen, redox potential, and amount and composition of particles (Chapman and Wang, 2001). Salinity varies spatially (laterally, vertically) and temporally and is the controlling factor for partitioning of contaminants between solution and particulate phases. Salinity also controls the distribution and types of estuarine biota.

3.4.1 The ecotoxicological context of estuarine sediments

Chapman and Wang (2001) reviewed chemical, toxicological, and community-level assessment techniques for estuarine sediments, including chemistry (grain size effects, background enrichment, bioavailability, sediment quality values, and interstitial water chemistry), biological surveys, and whole sediment toxicity testing (single-species tests, potential confounding factors, community level tests, laboratory-to-field comparisons). They concluded that there is currently a clear need to tailor such assessment techniques specifically for estuarine environments. For instance, current bioavailability models in wide use including equilibrium partitioning may have little applicability to estuarine sediments, appropriate reference comparisons are difficult in biological surveys, and there are too few full-gradient estuarine sediment toxicity tests available. It is surmised that these may be applicable to aquatic organisms.

3.4.2 Unique physicochemical aspects of estuaries

Estuarine chemical processes

From a chemical point of view, an estuary is a continuously, slowly agitated reaction vessel in which fresh water and saline water, each with different trace chemical compositions, are drastically mixed. Contaminants in estuaries are mainly transported from rivers and/or from direct effluents located on or near estuaries. Processes affecting contaminants fall into the general category of transport and transformation. The full range of environmental chemical processes occurs in estuaries, namely adsorption, desorption, coagulation, flocculation, precipitation, biotic assimilation, and biotic excretion. Changing ionic strength (0.0 – 0.7 moles/litre, through changes in salinity) impact all the above chemical processes.

Solid particles in the water column and in the sediments can act as a sink of hydrophobic contaminants, and a source of metals. Metal flux into the aqueous column can be counteracted by flocculation processes including particulate organic matter, the rate of which is high at high ionic strengths. Only those metals that form very strong complexes (Turekian 1977) and organic chemicals that are less hydrophobic (Zhou et al. 1998) may be transported out of estuaries to the ocean. This natural mechanism renders estuaries more susceptive to contamination.

While the overlying water in estuaries can be heterogeneous because of different mixtures of fresh and saline water, a much higher degree of heterogeneity and variability exists within estuarine sediments not only because of the salinity differences in the pore waters but also because of the diverse and complicated composition of the sediments. Different sediments can have significantly different capacities for collecting contaminants. For instance, the grain size distribution of sediment is probably the most important factor controlling sediment metal concentrations; correlations commonly exist between decreasing grain size and increasing metal concentrations.

3.5 SELECTION OF WATER QUALITY VARIABLES FOR USE IN WQIS

The great variation in the different types of estuaries found in SA and the different abiotic influences on them make it difficult to select only a handful of variables for inclusion in a water quality index. Variables have previously been selected according to those that are most indicative of pollution, and those for which data is readily available (Dojlido et al. 1994). Variables have more recently been selected in order to be representative of the five impairment categories put forward by Dunnette (1979). However, Harrison et al. (2000) suggested that due to the highly variable nature of physical characteristics and dissolved substances in estuaries, their inclusion in a water quality index must be carefully considered. As mentioned in Section 2.2.1, Dunnette's original five impairment categories were reduced to three. Therefore although an impairment category which includes indicators such as temperature, salinity, pH and turbidity may still be necessary, the applicability of their inclusion needs to be explored further (Harrison et al. 2000).

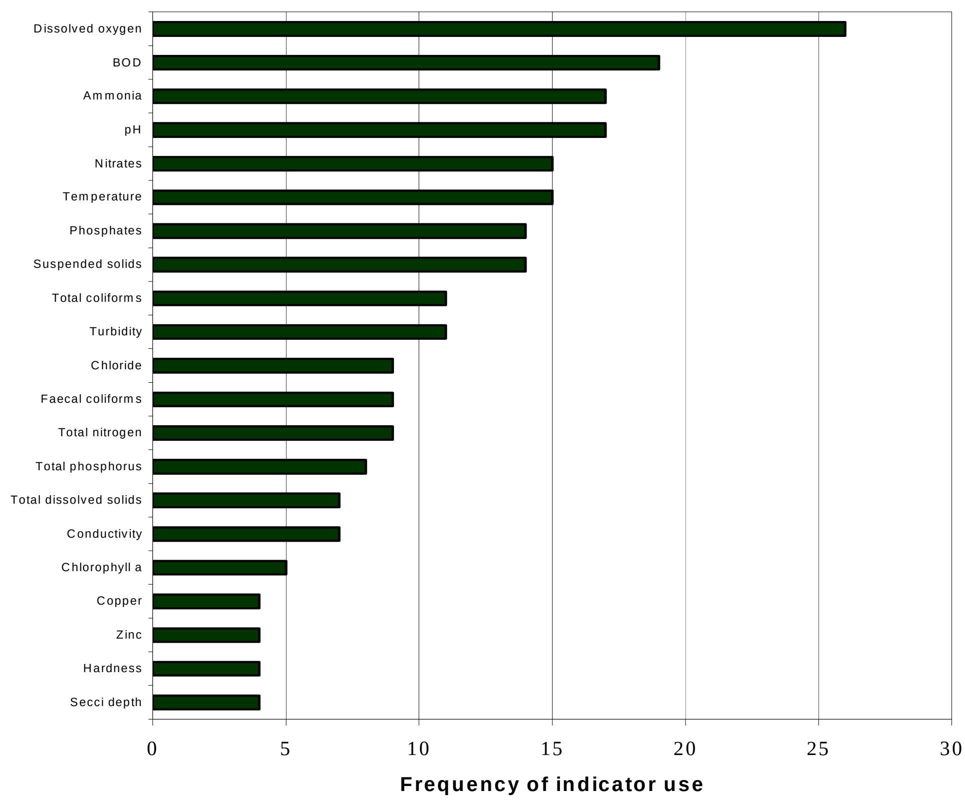

Figure 5. Graphic representation of the frequency of use of variables from a literature review of water quality indices developed to date. Indicates only those variables used more than three times.

Wepener et al. (1992) and House (1989) suggested that there are three criteria that a variable should fulfill in order to be selected; namely, (a) readily available data on the variable; (b) should be an important indicator of water quality change or pollution (Ross 1977); and (c) there should be maximum water quality criteria set for the variable selected. From a review of the literature, an indication of those variables used most often in WQIs may be obtained. This is represented graphically in Figure 5. However when presenting those variables selected for estuarine WQIs a different picture arises (Figure 6). Richardson (1997) suggested that only the first ten variables are really relevant since to date most WQIs have an average of 9 variables. From the review done during this study the average number of variables is 8. For convenience, the first ten will be considered in conjunction with other related parameters.

From Figure 5, dissolved oxygen (DO) is the most frequently used variable. This variable primarily indicates the status of higher aquatic life (Walski and Parker 1974) and is essential for maintaining aquatic ecosystems and the characteristics of clean water. Figure 6 only rates DO as fourth on the list of importance. This may however be related to the reluctance of researchers to include physical characteristics in estuarine WQIs due to the inherent variability of these parameters in estuaries. Perhaps the solution to the inclusion of this variable is in the two different methods of measuring DO, namely, percentage saturation (%DO) and in milligrams per litre. The prior is probably the most meaningful since it varies with changes in salinity, temperature and altitude (Dunnette 1979). %DO therefore includes the effects of temperature on oxygen concentrations and indicates if there is supersaturation that is harmful to some organisms. Percentage DO also fluctuates diurnally due to aquatic plants, and semi-diurnally as a result of tidal mixing, turbulence and chemical oxidation (Richardson 1997). However measuring %DO may over estimate standards needed at high temperatures and under estimate those needed at low temperatures for example. The influence of physical factors on %DO therefore make it inappropriate as a variable for an estuarine WQI. However, the use of milligrams per litre DO would possibly be just as effective while excluding the effects of physical parameters on the readings.

Biological oxygen demand (BOD) is the second most frequently used variable, but not rated at all for estuarine WQIs. Although BOD is perhaps more relevant and easier to measure than COD as a measure of oxygen depletion by bacterial processes, its relevance is questionable (Richardson 1997). Its practical value is not known, in addition to the fact that its relationship to actual biological oxidation are not fully understood (Dunnette 1979). DO measurements are far more appropriate at a given point and time, and far easier to measure (Prati et al. 1971; Walski and Parker 1974). Although, Harrison et al. (2000) preferentially measured oxygen absorption (OA) as opposed to BOD or DO, very little data is available on this variable. In addition, there has been no maximum water quality criteria set for both BOD and OA measurements. It is therefore again suggested that DO be used since it meets all the necessary requirements mentioned earlier.

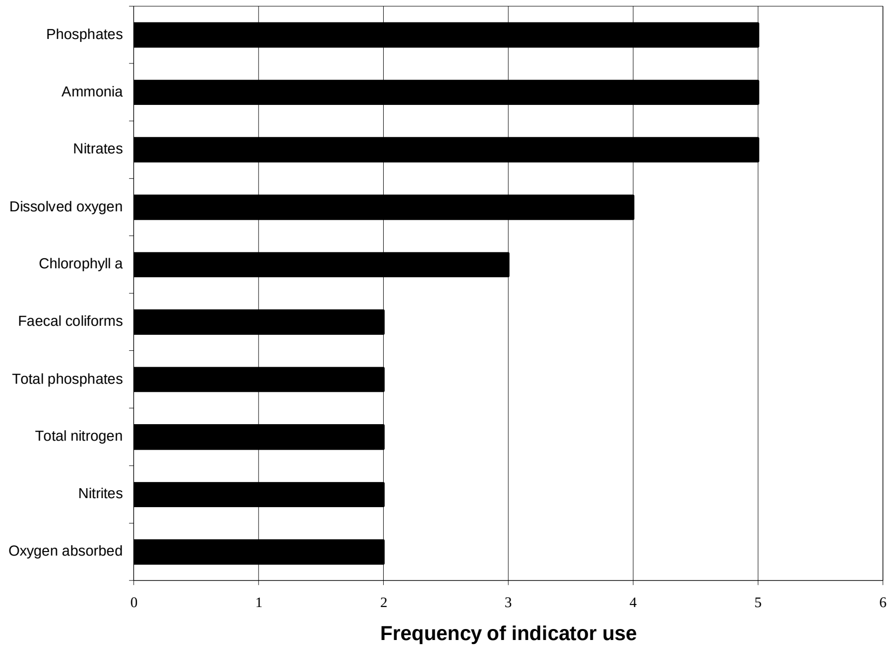

Figure 6. Graphic representation of the frequency of use of variables from a literature review of estuarine water quality indices developed to date. Indicates only those variables used more than twice.

Ammonia is the third most important variable according to reviewed literature (Figure 6). From purely estuarine water quality indices it is viewed as one of three most important variables, the other two being nitrates and phosphates. Total nitrogen has often been suggested as a conservative estimate of all nitrogen that may be available in a fluvial system (Richardson 1997). However, nitrate-nitrogen remains the most common and important inorganic form of nitrogen with regards to potential for eutrophication. Further, both ammonia and nitrate may be utilised by microorganisms (Dunnette 1979). High concentrations of ammonium are highly toxic to fish, and therefore may be a useful indicator of organic pollution (Richardson 1997). Both these variables fulfill the requirements mentioned earlier and therefore should be included in the WQI.

The next two variables are that of pH and temperature respectively (Figure 5). Both these variables are lumped together with a number of other variables of apparent minimal importance when considering the estuarine WQIs only. Once again, both these physical variables are known to vary considerably between and even within estuaries (Harrison et al. 2000). Despite this, pH may still be a useful indicator of for example the discharge of acidic or basic pollutants, the potential for changes in ammonia toxicity (Harrison et al. 2000) or intense photosynthetic activity by plankton when used as a measure of ionic equilibria. Further, pH is widely monitored and has known maximum water quality criteria (Richardson 1997), therefore fulfilling the requirements mentioned earlier. The use of temperature, on the other hand, is more difficult to warrant since it influences most aquatic processes and crosses all impairment categories (Richardson 1997).

Phosphates are rated seventh for general WQIs (Figure 5) and as one of the top three for estuarine WQIs (Figure 6). Phosphorus as a whole is primarily found in the form of dissolved inorganic ortho-phosphate or bound to fine and coarse particulate material, usually transported in rivers by soil particles. Eutrophication has been observed to occur when total phosphorus increases to between 40 and 60mg/l. However only when phosphorus occurs in solution as phosphate, is it bioavailable. On the other hand, ortho-phosphates are known to be a limiting factor for algal growth in freshwaters, becoming problematic in waters where levels of river flow and turbidities are low and good light penetration encourages plant growth. It is therefore suggested that soluble phosphates should preferentially be used to indicate trophic status (Richardson 1997).

The next variable is suspended solids (SS) (Figure 5). This is once again not rated for estuarine WQIs. SS reduces light penetration and is therefore a measure of the "cloudiness" of the water (Richardson 1997; Walski and Parker 1974). Total solids include both the dissolved (TDS) and the above-mentioned suspended (SS) fraction. However, TDS is much more indicative of intruding marine water in an estuarine system than of a source of pollution (Cooper *et al.* 1994). Walski and Parker (1974) have suggested that there is sufficient correlation between SS and turbidity to suggest that SS maybe eliminated from WQIs. However, both these parameters are poorly rated in the literature which is not at first evident from Figure 5. Both turbidity and SS may be more related to geomorphology and geology, or to the mixing of fresh and marine waters than to changes in water quality itself (Cooper et al. 1994). As with the other physical variables, a mean SS or turbidity may have little relevance to an estuarine system having dramatic variations in these variables both horizontally and vertically (Harrison et al. 2000). Further, the large variation in geomorphology between the different estuaries in SA, which is known to influence especially turbidity, may result in a skewed view of water quality at any given locality should these variables be included.

The last variable is that of Total coliforms (T.coli). Although T.coli are not rated for estuarine WQIs, faecal coliforms (F.coli) are rated as sixth (Figure 6). House (1989) and Walski and Parker (1974) suggested that some measure of bacterial count needs to be included in a WQI if water is for potable or recreational use. Some studies have placed strong emphasis on the inclusion of F.coli (Bolton et al. 1978). However, indications are that this may be redundant, since it has been shown that viruses and parasitic protozoa are often present when F.coli are absent (Richardson 1997). Nevertheless, F.coli remain the easiest to measure of the presence of bacteria and in the absence of better alternatives they should still be included.

Although not rated in either of the reviews, Chlorophyll a (Chl-a) was included by both Richardson (1997) and Cooper et al. (1994). Richardson (1997) viewed this variable as an important addition to the other two soluble nutrients, namely; nitrate and phosphates. However it was excluded by Harrison et al. (2000). For the purpose of this study it is perhaps pertinent to exclude Chl a as well. The reasons for this are related to difficulties in sampling accurately, the lack of data and the lack of maximum water quality criteria for this variable.

3.6 VARIABLE SELECTION FOR THE EWQII

Due to the dynamic nature of estuarine water masses under "normal" conditions, physical characteristics and dissolved substances content of estuarine water are highly variable (Harrison et al. 2000). The pH and turbidity are strongly controlled by the mixing of marine and fresh water. Given the buffering capacity of seawater, the pH of river water entering an estuary will be driven toward 8. Thus, the pH of estuarine water generally increases towards the mouth, and an average value for the estuary probably has little utility. Its importance, however, as an indicator of ionic equilibrium (for example in evaluating the potential for ammonia and metal toxicity) must be taken into account, which was the case for developing HC's for ammonia (see Section 4.4). The water quality significance of turbidity or suspended solids in estuarine water is largely unknown. According to Harrison et al. (2000) the turbidity of the river water entering estuaries is probably more closely related to the nature of the catchment geology and geomorphology than to other factors. The turbidity will further increase within the estuary as this more turbid water encounters the intruding seawater. This often results in extreme variations in turbidity within an estuary and therefore the concept of mean turbidity for the estuary is meaningless, and thus contributes little to a measure of average estuarine water quality. It is for this reason that these variables were excluded from the EWQII.

The major source of dissolved substances in estuaries is the intruding seawater; hence measurement of TDS (salinity) is a much more important indicator of the extent of seawater mixing than water quality impairment. It is in fact the brackish nature of estuarine water that makes this habitat unique and contributes to its resource value (Harrison et al. 2000). Therefore **salinity was included** for investigation as an important variable in the determination of estuarine water quality integrity **(see Section 4.1)**.

Emphasis in most WQIs appears to be on organic loading, with very little attention paid to other forms of pollution. The Integrated pollution and waste management white paper identified six areas of concern with regard to aquatic pollution, namely: salinisation, enrichment, microbial pollution, sedimentation (high suspended solids), inorganic and organic compounds, diffuse water pollution and marine exploitation. Although, not all are appropriate to estuaries, these problems should be considered during variable selection. Enrichment and microbial pollution have already been accounted for by the inclusion of ammonia, nitrates and ortho-phosphates; and faecal coliforms respectively. **Nutrients were therefore also selected as variables** to be investigated for suitability for inclusion in the EWQII **(see Section 4.2)**.

Of particular concern in estuarine systems is the influx of inorganic and organic compounds such as trace metals and organic pollutants (e.g. pesticides, petroleum products, etc.) into these systems. Trace metals have previously been included in some of the freshwater WQIs, however only one estuarine WQI has incorporated these variables. This is probably related to their inherent variability, particularly when linked to increased salinity. Nevertheless, in the South African situation it is imperative that these potentially hazardous substances be included as a reflection of water quality, on condition they meet the requirements mentioned earlier. Although metals have previously been included in various WQIs, there are no maximum water quality criteria set for Al, Fe and Mn. These three metals were therefore excluded from the list of metal variables. The metals were selected based on the data availability and their inclusion in the South African Marine Water Quality Guidelines. The organic toxicants were selected for inclusion in the EWQII based on their inclusion in the South African Marine Water Quality Guidelines and presence in South African aquatic systems (Heath and Claassen, 1999). The metal toxicants included in the EWQII are: arsenic, cadmium, chromium, copper, cyanide, lead, mercury, tributhyl tin and zinc. The organic toxicants included in the EWQII are: Alachlor, Benzene, Chlordane, Chlorpyrifos, DDT, Dieldrin, Endosulfan, Lindane, Malathion, Phenol, Thiobencarb, Toluene and Total petroleum hydrocarbons. **Section 4.4 deals with the inclusion of discrete chemicals in the EWQII**.

4.0 INCORPORATION OF SELECTED WATER QUALITY PARAMETERS INTO THE EWQII

4.1 SALINITY

4.1.1 Physicochemically based classification of hydrodynamics of estuaries

On a physicochemical basis, estuaries may be broadly divided into two types – vertically stratified or vertically homogeneous. Vertically stratified estuaries are classified into salt wedge, shallow, partially mixed estuaries and fjords. In vertically homogeneous estuaries tidal currents predominate, and vertical salinity differences are less than 1 ‰ because of intense vertical mixing. Shallow, well-mixed estuaries exhibit intense coupling between benthic and pelagic systems. There is, as for all estuaries, a horizontal gradient of salinity, increasing from the head to the mouth. However, lateral variation can occur where the ratio of width to depth is sufficiently large, such that the one side of the estuary (looking to sea) will contain lower-salinity water than the other side.

4.1.2 Anthropogenic Modification of estuarine hydrodynamics

The hydrodynamics of an estuary may be modified in a number of ways – the water flow down a river may be reduced by abstraction; the periodicity and intensity of river discharges may be influenced by damming, or by enhanced runoff by urbanization, deforestation and draining of wetlands; the estuary mouth may be deliberately opened or closed.

4.1.3 Disturbances in salinity and coupled variables – an attempted analytical approach

In order to understand what might happen if the hydrodynamic quality of an estuary were to be modified; a theoretical analysis was embarked upon. The example of salinity is explored. Discussions in terms of salinity also apply to pH modification, since salinity is correlated with pH in estuaries where the pH of the river water differs greatly from that of seawater.

Natural variation in salinity - magnitude and duration

It may be seen from the previous section that there is significant complexity in salinity regimes in estuaries. Within a single estuary, one may encounter many different ecozones, typified by salinity ranges. For the purposes of this highly analytical discussion, ecozones in estuaries are classed into three broad categories – euhaline (>18 ‰), mesohaline (5-18 ‰) and oligohaline (<5 ‰). The ecozones will be discussed in terms of magnitude and duration of fluctuations salinity fluctuations, and in terms of impacts on species of changes in ecozones. Figure 7 depicts the salinity regime as a function of time that the three ecozones may experience, if tides influence the ecozones. These are permanently open (represented by mostly open on figure), temporary open-closed (represented by half-open on figure) and closed estuary (represented by mostly closed on figure).

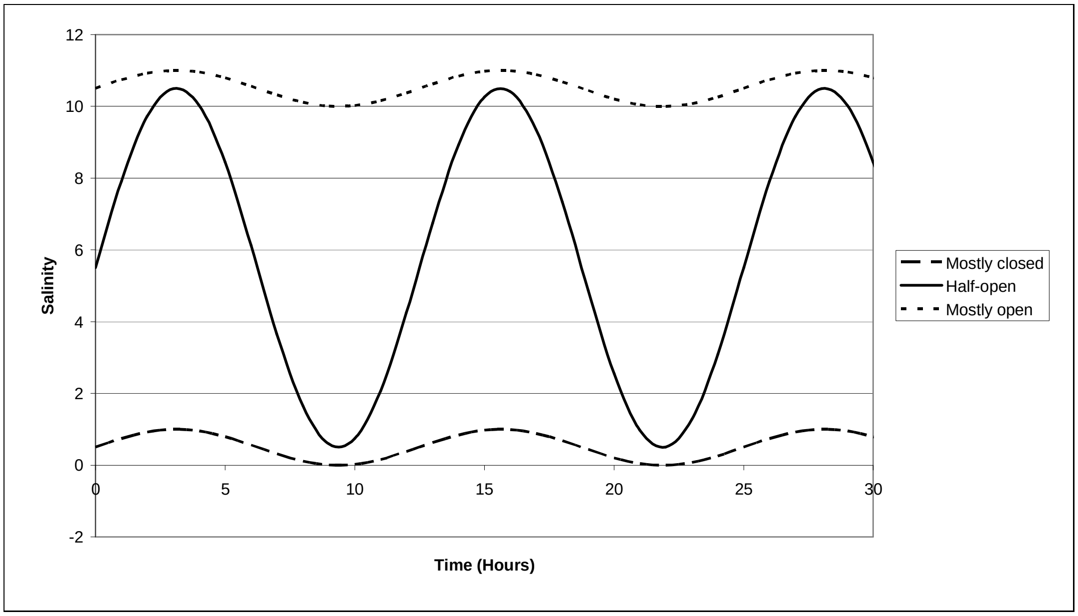

Figure 7. Salinity versus time for three types of ecozones subject to tidal periodicity.

Variation in salinity - ecotoxicological aspects

Many organisms are sensitive to changes in salinity. Thus, a change in salinity may be viewed as a stressor. It is known that for a large number of organisms, the response to a stressor is dependent not only on the magnitude of the stressor, but on the duration of the impact of the stressor. Thus, it may be important to consider the magnitude and duration of salinity changes experienced by organisms in estuaries.

Figure 8 depicts the dependence of the magnitude of salinity (within a narrow range) experienced by an organism in each of the three ecozones as mentioned in the previous paragraph. The mesohaline ecozone experiences a large fluctuation in salinity, with the extremes of salinity experienced for shorter durations than the salinities of the euhaline or oligohaline ecozones. The euhaline and oligohaline ecozones experience high salinity and low salinity ranges for much longer durations than the mesohaline ecozone does.

Consequences of Anthropogenic Modification of estuarine hydrodynamics

It is theorised that a modification of an estuary from a mesohaline to an oligohaline or euhaline condition would increase the duration of the stress due to non-optimal salinity for some organisms, and would increase the magnitude of the stress (Figure 9). The optimal salinity ranges for a large number of estuarine organisms is not known, due to the paucity of ecotoxicological data in public databases, such as ECOTOX. Thus, it is probably necessary to base the resource management classification of estuaries in terms of directly observable biotic assemblages, characteristic of the estuary type that one is attempting to manage the estuary towards.

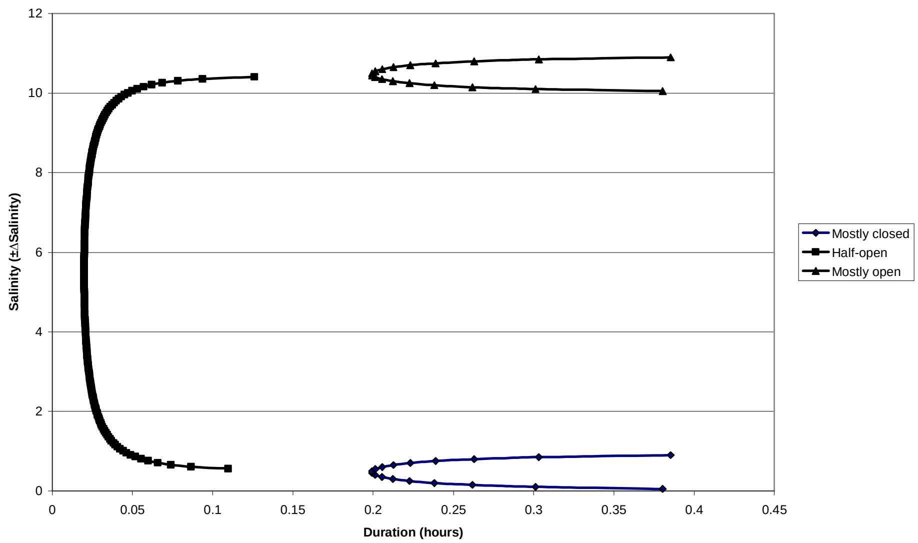

Figure 8. Magnitude of salinity (±δ) versus duration of salinity for the three ecozones

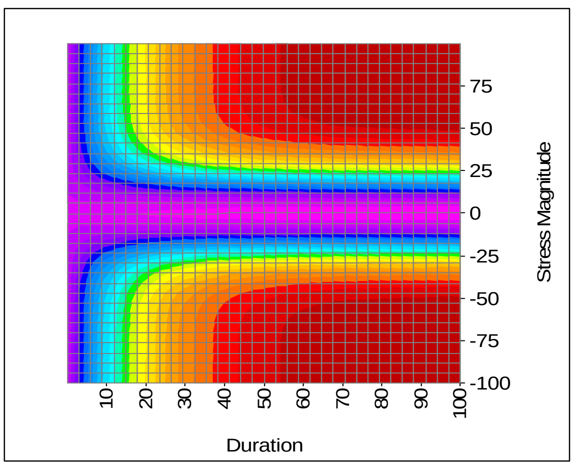

Figure 9: Abundance of species adapted to a particular salinity regime, when stressed by decreased or increased salinity (+ve or –ve stress), as a function of duration of stressor. The maximum abundance occurs at zero stress, and at zero duration for all stresses.

4.1.4 Classification of Estuaries in terms of biotic assemblages

Estuaries as Darwinian challenging environments

Estuaries are ephemeral phenomena in the context of geological time. Because flow, tidal range and loads of sediments and humic materials are constantly changing, estuaries are far from steady-state systems (Chapman and Wang 2001). In the case of salinity, the greatest number of species occurs in fresh and in marine waters, with fewer numbers of species at intermediate salinities (Figure 10). This apparent paradox (the “paradox of brackish waters” of Remane (Chapman and Wang 2001)) can be explained in terms of Darwinian evolutionary mechanics. Estuaries are transitional areas where conditions are challenging to both residents and immigrants.

The unstable and unpredictable behaviour of estuarine physicochemical environmental factors decreases the probability of speciation and increases the probability of extinction of estuarine fauna, while excluding most marine and freshwater species, which thrive by comparison. It has been suggested that it takes approximately 12 million years for all niches in an ecosystem to be adapted to properly – estuaries do not persist for even a fraction of this duration (Chapman and Wang 2001). Ecologically, there is reduced interspecific (though not intraspecific) biotic competition due to overriding physical-chemical factors, of which salinity is the dominant stressor.

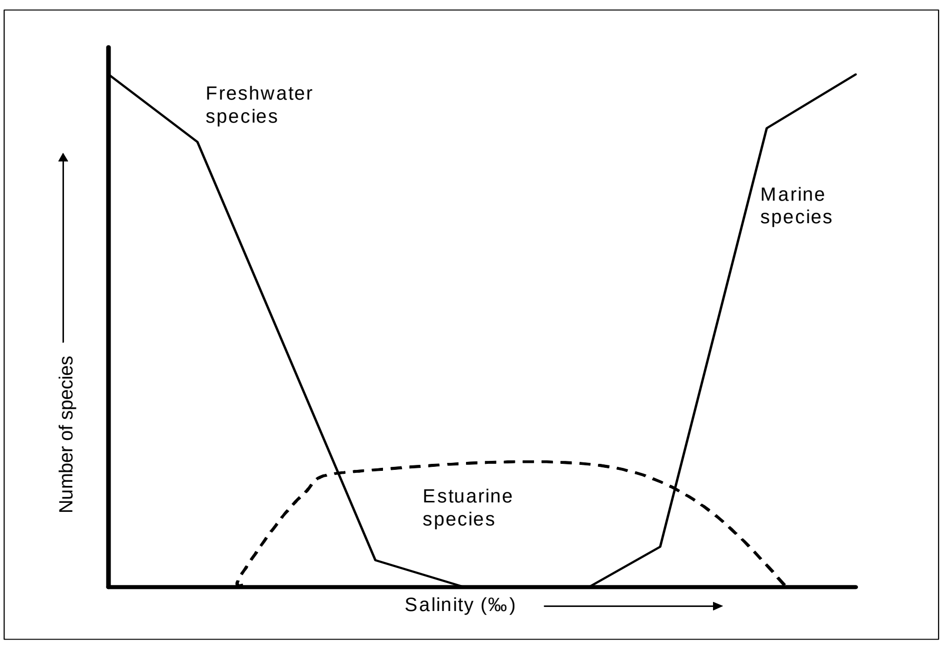

Figure 10. Illustration of the “paradox of brackish water” of Remane. (Adapted from Chapman and Wang 2001).

Influences changing the relative proportion of estuarine species

Estuarine salinities are generally considered to be above about 1 and below about 30 ‰. Freshwater organisms can generally survive, grow, and reproduce in a few ‰ salinity. Salinities of 30 ‰ are not challenging to most marine organisms. Estuarine species richness or diversity are least within a critical salinity range of about 5 to 8 ‰, which reflects the inabilities of many organisms to tolerate salinity stress and to undergo extensive cell volume regulation (Chapman and Wang 2001).

Faunal distributions in estuaries are controlled primarily by salinity and secondarily by factors such as substrate, temperature, dissolved oxygen, and anthropogenic pollution. Organisms can survive in estuaries by one or a combination of the following strategies: avoiding estuarine conditions (e.g., saltwater organisms remaining within the salt wedge in salt wedge estuaries, freshwater organisms remaining above), reducing contact with inimical environments, adaptation (e.g., ion regulation, volume regulation, or osmoregulation), or acclimation. Thus, the *behaviour* of organisms contributes greatly to their prevalence in estuaries under conditions of stress.

Estuarine organisms in constant bioenergetic stress

However, not all organisms living in estuaries live under optimal conditions, which results in natural bioenergetic stress to those organisms (Vernberg and Piyatiratitivoraku 1998). For example, periodic seasonal cycles of anoxic and oxic conditions in bottom waters of partially stratified estuaries (e.g., in Chesapeake Bay) result in a corresponding cycle of mortality and recolonization by benthic macrofauna (Riedel et al. 1997). Estuarine organisms living in such stressful natural conditions may be more (or less) susceptible to anthropogenic stress.

Depending on species specific salinity tolerances, in some cases immature organisms may not survive in areas where both mature and immature organisms are deposited. Because of these species shifts in salt wedge estuaries, usage of habitat by different species is actually greater than appears to be the case from snapshot estimates. Hypoxia is also a feature of some estuaries, related to circulation of bottom waters, which are primarily saline (Kuo and Neilson 1987; Dauer et al. 1992). Effects of hypoxia on estuarine benthos, independent of other stresses (e.g., variable salinity, anthropogenic inputs), will change community composition and reduce diversity and biomass (Dauer et al. 1992; Harper et al. 1981; Holland et al. 1987).

Towards an estuarine classification system

All of the preceding comments indicate that it may be extremely difficult to attempt to regulate impacts on estuarine structure, with concomitant changes in salinity regimes, by classifying estuaries in terms of salinity. A possibly more promising classification system in terms of salinity may be based directly on the distribution of estuarine fauna or functional groups (“optimal assemblage”) that one expects in an unmodified estuary of a particular type.

It is here hypothesised that it is possible to empirically assign coefficients to a function of the following form:

$$\Delta_{assemblage} = \sum_i a_i \left| z_i - z_{opt,i} \right| \qquad \text{(Equation 1)}$$

where:

$\Delta_{assemblage}$ = deviation from optimal assemblage for an estuary

a_i = "keystoneness" of species or functional group *i* in the assemblage

z_i = representation of species or functional group *i* in terms of numbers or biomass

$z_{opt,i}$ = optimal representation of species or functional group *i* in terms of numbers or biomass

and $|z_i - z_{opt,i}|$ is a measure of scalar deviation from optimum, possibly a modulus, or a quadratic function.

Implementation of this function in a management context will entail:

1. Classification of morphologically distinct estuaries
2. Determination of assemblage status (in terms of proportions of species or functional groups) in these estuaries
3. Determining the "keystoneness" of the species or functional groups
4. Assigning classes based on $\Delta_{assemblage}$ calculated from the above formula.

Determination of "keystoneness"

"Keystoneness" is a measure of the importance of the species or functional group to the integrity of the estuarine ecosystem. A sufficiently rigorous method of determining "keystoneness" is system dynamics modelling (Campbell et al. 2001; Bossel 2001), applied to the bioenergetics of the estuarine ecosystem (cf Kooijman 1993). An alternative method of determining "keystoneness" may be by empirically determining the assemblages of a related system of estuaries, and by optimising the coefficients of Equation 1 by a regression (or probably more sensibly a neural network) algorithm.

4.2 NUTRIENTS: CARBON, NITROGEN AND PHOSPHORUS FLUXES IN FOUR SUB-TROPICAL ESTUARIES OF NORTHERN KWAZULU-NATAL: CASE STUDY IN THE APPLICATION OF A MASS BALANCE APPROACH

4.2.1 Introduction

The chemistry of estuaries is dependent on a combination of tidal pulses, riverine flow and hydrodynamic and autochthonous biological processes. The total concentrations (i.e. µg per litre) of nitrogen (N) and phosphates (P) in the water column are useful measures of the potential for nuisance plant growths but they can often overestimate what is actually bioavailable for plant growth. Moreover, only measuring the concentration of nutrients in the water column does not take into account the fact that polluted waterbodies will have significant stores of N and P in the sediments and associated with suspended particulate matter (SPM). Plants can derive their nutrients from sources other than in the water column, e.g. seagrass beds meet their high nutrient demands by trapping nutrients and by uptake and recycling in the beds, not in the water column (Erftemeijer and Middleburg 1995). Thus the concentration of nutrients in the water column will not necessarily be predictive of the response by biota. Grobelaar (1992) argues that over-simplified models of nutrient loads are inadequate for estuaries and other ecosystems (such as in South Africa) where hydrodynamic factors and high turbidity can mediate the effects of nutrients.

It is for these reasons that here are currently no South African nutrient guideline values for estuarine waters. If the available standards from other countries (e.g. Australia) were adopted, then virtually all of South Africa's estuaries would be classified as eutrophic (Harrison et al. 2000). According to Harrison et al. (2000) the Australian standards reflect systems which are intrinsically different to those in South Africa, where fluvial effects naturally produce relatively higher nutrient concentrations. KwaZulu-Natal is a good example where nutrient concentrations, derived from detrital sources, result in relatively high background nutrient levels (Harrison et al. 2000). A more suitable approach to assessing nutrients in relation to ecosystem integrity would be through compiling a nutrient mass balance for an ecosystem, which can often help to identify major sources and sinks of nutrients. A mass balance represents all of the nutrients already present (i.e. water, sediments and biota) plus inputs, less the outputs (i.e. outflows & harvested biota like fish); what is left equals the internal load (Ekholm et al. 1997). Once the internal load is quantified, the external and internal processes which influence the load (e.g. biogeochemical cycling, primary production, etc.) can be identified. Information from the mass balance model will permit the locations where management actions can be targeted, which may include reduction of nutrient loads going into the system, preventing the release of nutrients from the sediments, or harvesting biota as a way to remove nutrients (ANZECC 2000a). This sort of approach is invariably more complicated that the traditional approach of dealing with issues like nutrient pollution in isolation of other factors, but ecosystems are complex and if they are to be understood and managed sustainably a more sophisticated approach is required where whole ecosystem dynamics are taken into account (ANZECC 2000a).

This chapter reports on the interpretation of chemical data from four sub-tropical estuaries in KwaZulu-Natal within the United Nations Environmental Program (UNEP) biogeochemical modeling framework. One of the central concerns of UNEP's "International Geosphere-Biosphere Program: A Study of Global Change" (IGBP) is an improved understanding of the global carbon cycle and the likely changes which, might occur as a consequence of global changes, both systemic and cumulative. The Land Ocean Interactions in the Coastal Zone (LOICZ) Core Project of the IGBP, established in 1993, is concerned with understanding the role of the coastal sub-system in the functioning of the total earth system, including the role of the coastal zone in the disturbed and undisturbed cycles of carbon, nitrogen and phosphorus (Gordon et al. 1996). The key objectives of LOICZ are to: gain a better understanding of the global cycles of the key elements carbon (C), nitrogen (N) and phosphorus (P); understand how the coastal zone affects material fluxes through biogeochemical processes; and characterize the relationship of these fluxes to environmental change, including human intervention (Pernetta and Milliman 1995). In order to achieve these objectives it was necessary to develop horizontal and, to a lesser extent, vertical material flux models. These models provide insight into flux dynamics from the continental basins through regional seas to continental oceanic margins, based on the understanding of biogeochemical processes and data for the coastal systems, habitats and human dimension (Dupra et al. 2002).

For LOICZ it is essential to identify and quantify the major net fluxes in representative parts of the world's coastal seas. This information will indicate whether the coastal seas are a net importer or exporter of carbon, nitrogen and phosphorus and indicate what the dominant processes are likely to be. There are several advantages to developing simple models of fluxes, often thought of simply as nutrient budgets (Gordon et al. 1996). They are both simple and comprehensive so they give an overall picture of the system very quickly. In addition, their computation requires only the summation of the boundary fluxes of the system. A consequence of their simplicity is that limitations on the availability of data rapidly become evident. As a result, budget models provide both robust estimates of the flux across the coastal zone boundaries and long-term, integrated biogeochemical performance of the entire system. Furthermore, by treating the budget as a first step in the modeling procedure rather than as an end in itself, one can proceed to identify the major processes which determine the fluxes and make the important transition from a purely descriptive budget to a predictive process-based model.

Recently there has been a move to develop budgets that link several variables using known relationships, for example building linked CNP budgets using stoichiometric relationships such as Redfield ratios (Gordon et al. 1996). The use of known stoichiometric relationships allows linked budgets to be applied in new areas, with limited data availability in order to infer underlying fluxes. The objective of this chapter was to apply the LOICZ biogeochemical model to data from the Mhlathuze, Mvoti, Nhlabane and Thukela estuaries in KwaZulu-Natal. Furthermore, the nutrient mass balance approach was used to develop "reference conditions" and it was demonstrated how a classification of estuarine water quality could be based on deviations from the nutrient mass balance reference conditions.

4.2.2 Materials and Methods

The LOICZ approach is an ideal model for the South African situation where water quality data for most estuaries are extremely limited. The advantages of the LOICZ model are that one can work minimal and secondary data. These attributes make the model robust and provide a widely applicable, uniform methodology to provide information on processes of CNP flux in estuaries. Within the context of LOICZ biogeochemical modeling, the primary questions to be addressed concern the role of the coastal zone as a source or sink for carbon, nitrogen, and phosphorus.

Conservation of mass is one of the most fundamental concepts of ecology and geochemistry and the LOICZ budget procedure assumes that materials are conserved. The difference (Σ [sources – sinks]) of imported (Σ inputs) and exported (Σoutputs) materials may be explained by the processes within the system (Figure 11). This section will only briefly refer to the formulae used to derive the mass balance equations and for a detailed description on the mathematical structure of the LOICZ biogeochemical budgeting procedure; the reader is referred to Gordon et al. (1996).

To construct a budget model, it is necessary to define the spatial domain to be modeled. The definition of the land boundary is usually relatively easy; it is likely to be defined by the shoreline or the limit of tidal excursion. However in order to understand CNP processes in a system it is essential to provide background on the physical and biological characteristics of the particular system. Stoichiometrically linked water-salt-nutrient budgets actually comprise a series of budgets, which are solved in a prescribed order. In general terms, the sequence of budgets for use in stoichiometrically linked CNP budgets follows four steps: water budgets, salt budgets, non-conservative materials and stoichiometric linkages among non-conservative budgets. The following methodological descriptions were summarized from Gordon et al. (1996).

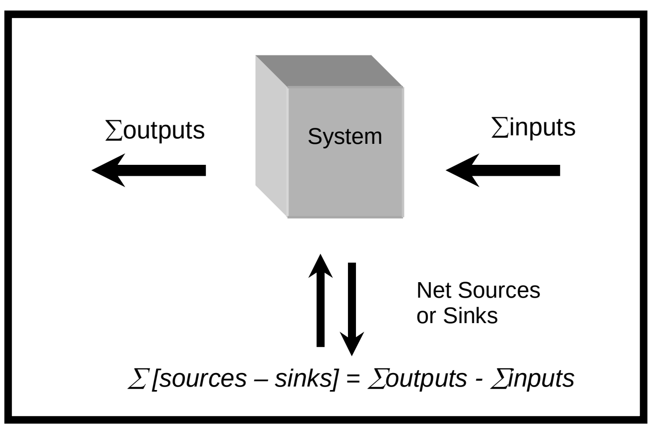

Figure 11. Generalised diagram indicating the components of the LOICZ budget procedure. (Adapted from Gordon et al. 1996).

Biophysical description of the estuaries:

In order to assess the water quality of a system it is essential to establish the extent of natural variation and the fate of substances entering the system. However, this is not possible unless the character of the estuary is understood. Essential biophysical information required includes system area and volume, river runoff, precipitation, evaporation, salinity gradient, nutrient loads (dissolved inorganic phosphorus (DIP), dissolved inorganic nitrogen (DIN), and if available – dissolved organic phosphorous and nitrogen and dissolved inorganic carbon. A brief overview of information requirements for describing the characteristics of an estuary using the LOICZ model is presented in Table 5.

Water Budgets:

The concept of the hydrological cycle is well established, and is often presented (both globally and locally) in terms of water budgets. A simple diagram (Figure 12A) represents this conceptual model. Freshwater inflows to a coastal marine system (such as runoff, precipitation, groundwater) and evaporation from the system are often rather easy to account for. The fundamental concept behind the budgets remains the conservation of water mass. Therefore, if it is assumed that either water volume remains constant or that the change of water volume through time is known, then net water outflow from the system can be estimated by difference. This flow is known as "residual flow;" and although there are likely to be other flows, the difference between inflows and evaporative outflow must be balanced by this residual flow. As examples of judgment about individual systems, it is often (but not always) legitimate to assume that the system volume remains constant. Groundwater, sewage discharge, and other freshwater sources may often, but not always, be ignored. Often, but not always, runoff overwhelms the direct meteorological fluxes of precipitation and evaporation.

Table 5. Factors relating to the definition of the coastal zone areas for the development of coastal budget models (Adapted from Gordon et al. 1996).

Physical Description	Shelf edge, bay mouth, estuary, coastal lagoons
Topography/bathymetry	Tidal excursion, boundary of residual circulation
Current system	Frontal structure
Gradient of material concentration	Tidal or river dominated, waves, currents, closed, etc.
Energy regime	Soil type, runoff, input of dissolved and particulate
Catchment	material
Biological Description	Coral reef, seagrass, mangrove, salt marshes
Habitat type	Length of growing season, production
Biological production	
Chemical Description	
Nutrients	CNP concentration and flux
Socio-Economic Description	Population density, growth
Demographics	Land cover, crop type, human activity, etc.
Land use	

Since water is conserved, the water volume entering a system must equal water volume storage within the system minus the water volume flowing out of the system (Figure 12A). Inflows include stream runoff (V_Q), direct precipitation (V_P), and groundwater (V_G). There might be other inflows (V_O) such as sewage. Removals include evaporation (V_E). Whilst most coastal aquatic systems have inflows and outflows forced by winds and tides, the difference between inflows and outflows will tend towards 0 when averaged over periods progressively longer than a single tide cycle. The residual volume (V_R) remains as the "residual flow" required to balance the water budget (i.e. conserve volume). Note that V_R is positive only in systems when evaporation exceeds precipitation and river inflow; that is, residual flow is into the system. The more usual case where freshwater input predominates, a negative value for V_R is found.

Therefore water storage may be represented by the change in system with time (dV_{sys}/dt): $dV_{Sys}/dt = V_Q+V_P+V_E+V_G+V_O+V_R$ and at steady state flows equal or approximating 0 can be eliminated to simplify the equation to:

$$V_R = -(V_Q+V_P+V_E+V_G+V_O) \qquad \text{(Equation 2)}$$

Salt Budgets:

Coastal marine systems have flows across the system boundaries in addition to the residual flow. For example, these systems have water inflow and outflow associated with tides, winds, density, and large-scale circulation patterns. If the salinity of the system of interest as well as that of adjacent systems exchanging water with that system is known, then it may be possible to construct a salt budget (Figure 12B), which includes these exchange flows in addition to residual flow. "Salinity", as defined by oceanographers, could be regarded as the sum of all salts and is readily measured. Because salt is not being either produced or consumed in the system, salinity is said to be "conservative" with respect to water within the system.

The primary equation representing the salt budget states that the salt flux is equal to each of the volume fluxes multiplied by the salinity (S) of each water type. In the case of the residually advecting water, the salinity is taken at the system boundary. Water in the system of interest (i.e. the estuary) is designated by S_{Sys}, whilst S_{Ocn} designates water outside the system. The salt flux not accounted for by the salinities used to describe the freshwater flow in the water budget must be balanced by mixing. The average salinity at the system boundary (S_R) is calculated as $(S_{Ocn}+ S_{Sys})/2$. The salt flux carried by the residual flow could therefore be represented by V_RS_R. Since salt must be conserved the residual salt flux is brought back to the system through the mixing of salt flux across the boundary (V_XS_X) via tides, wind and general circulation pattern. Therefore $V_XS_X= -V_RS_R$, with $S_X=(S_{Ocn}-S_{Sys})$. By rearrangement the mixing flux (V_X) can be calculated as:

$$V_X=-V_RS_R/(S_{Ocn}-S_{Sys}) \qquad \text{(Equation 3)}$$

Total water exchange time is given by the ratio of the system volume to (V_R + $|V_X|$). A point to note in this derivation of circulation from a combined water and salt budget is that there must be a salinity difference between S_{Ocn} and S_{Sys}.

Budgets of non-conservative materials:

The next step in the budgeting exercise is to consider materials, which may not behave conservatively with respect to salinity (Figure 12C). These budgets may be termed budgets of non-conservative materials. While this might be done with any reactive material (for example, Si, which is actively involved in both biotic and abiotic reactions), the particular interest here is in the balance among the essential plant nutrient elements C, N, and P. All dissolved elements will exchange between the system (estuary) and the adjacent ocean according to the criteria established in the water and salt budgets. Deviations are attributed to net non-conservative reactions of N and P in the system. This residual for each element is a measure of the net internal fluxes (that is, sources minus sinks) of these materials. The derivation of the equations used to calculate N and P fluxes in the systems is presented below. Since N and P are calculated similarly, they are represented by ΔY in the equations below. The residual nutrient fluxes (Y_R) are calculated as (Y_{Ocn}+ Y_{Sys})/2. Thus: $d(VY)/dt = V_QY_Q + V_GY_G + V_OY_O + V_PY_P + V_EY_E + V_RY_R + V_X(Y_{ocn} - Y_{syst}) + \Delta Y$. Through eliminating the terms that are equal to or near 0 the equation can be rewritten as:

$$0 = V_QY_Q + V_GY_G + V_OY_O + V_RY_R + V_X(Y_{ocn} - Y_{syst}) + \Delta Y$$

$$\Delta Y = -V_QY_Q - V_GY_G - V_OY_O - V_RY_R - V_X(Y_{ocn} - Y_{syst}) \qquad \text{(Equation 4)}$$

Stoichiometric linkages among non-conservative budgets:

The next step involves developing the stoichiometric linkages among non-conservative budgets. According to Gordon et al. (1996) the basic assumptions for the LOICZ model are that net biogeochemical processes in coastal marine systems are dominated by a few specific chemical reactions; that the biogeochemical cycles of C, N, and P are intimately linked; and that the approximate stoichiometric relationships among these elements for the dominating reactions can be written. Much of the flux of C, N, and P in coastal waters is attributed to production and consumption of organic matter, and the composition of organic matter tends to be relatively constant within the ocean. If plankton metabolism dominates, then the well-established “Redfield Ratio” (Redfield 1934) is likely to be a reasonable approximation of the C:N:P ratio of locally produced (or consumed) organic matter. If the system metabolism is dominated by seagrass or benthic algal metabolism, then some other composition may be more appropriate (Atkinson and Smith 1983). For systems in which sedimentary materials apparently dominate the local reaction, or in which particle inputs and outputs can be assumed to be small, then the sediment composition may be an appropriate compositional ratio to consider. In any case, some estimate can be made of the local organic matter composition (Gordon *et al.* 1996).

For the sake of linking the C, N, and P budgets, P may be considered to have the simplest chemical pathways. All phosphorus in the system can be considered to be in either the dissolved phase or the particulate phase, and phosphorus reactions involve transfers between these phases; there is no gas phase. In contrast, both N and C have prominent gas phases, and C and N fluxes involving the gas phases are known to be important in coastal systems. The working assumption is therefore made that the internal reaction flux of phosphorus is proportional to production and consumption of particulate material (generally dominated by organic matter). That is, phosphorus moves back and forth between dissolved and particulate material. N:P and C:P flux ratios are calculated from the budgetary analyses, and deviations of these flux ratios from proportionality with respect to the particle composition are attributed to gas-phase reactions for N and C.

For all practical purposes, it may be considered that the N_2 content of seawater is strictly controlled by gas solubility and equilibration of N_2 partial pressure between seawater and the overlying atmosphere. It will be seen in the case studies that the reactions involving nitrogen transfer to or from the gas phase generally must account for a large fraction of the net non-conservative fluxes of nitrogen in coastal systems. Therefore this stoichiometric procedure is a relatively robust way to estimate the difference between nitrogen fixation and denitrification.

Thus for the purposes of calculating water exchange in the coastal system, water and salt budgets are used. The departure of nutrient budgets from conservative flux behaviour provides the measure "system biogeochemical fluxes." The non-conservative DIP flux is assumed proportional to the difference between photosynthesis (p) and respiration (r). Thus by using the "Redfield Ratio", i.e. C:N:P = 106:16:1, the net ecosystem metabolism (primary production – respiration) can be calculated as (p-r) = - ΔDIP (C:P) using the Redfield ratio. Mismatch from "Redfield expectations" for DIP and DIN flux is assumed proportional to difference between nitrogen fixation and denitrification. The observed nitrogen flux (ΔDIN) represents the product of fixation whereas the denitrification product (expected DIN) is regarded as ΔDIP (N:P) using the Redfield ratio.

4.2.3 Results and Discussion

Biophysical description of the estuaries:

<u>*Mhlathuze Estuary*</u>

With the development of a deep-water harbour at Richards Bay in the 1970s the original Richards Bay estuary was divided into two distinct sections by means of a 4 km berm wall. This divided the original estuary into the new harbour area and a sanctuary area, which was designated to protect the estuarine character of the original system. The Mhlathuze River was canalized diverting the natural flow of the river into the "sanctuary" or estuary. During 1975 a new mouth was dredged approximately 5 km to the south of the original mouth. Based on Whitfield's classification for South African Estuaries (Whitfield 1992), the Mhlathuze estuary (28.80°S, 32.05°E) is situated in the subtropical coastal zone and could be regarded as a permanently open estuarine bay. The estuary covers an area of approximately 12 km^2 (Cooks and Bewsher 1993), has an axial length of 6 km, a width of 3 km, and a total shoreline length of 30 km (Begg 1978).

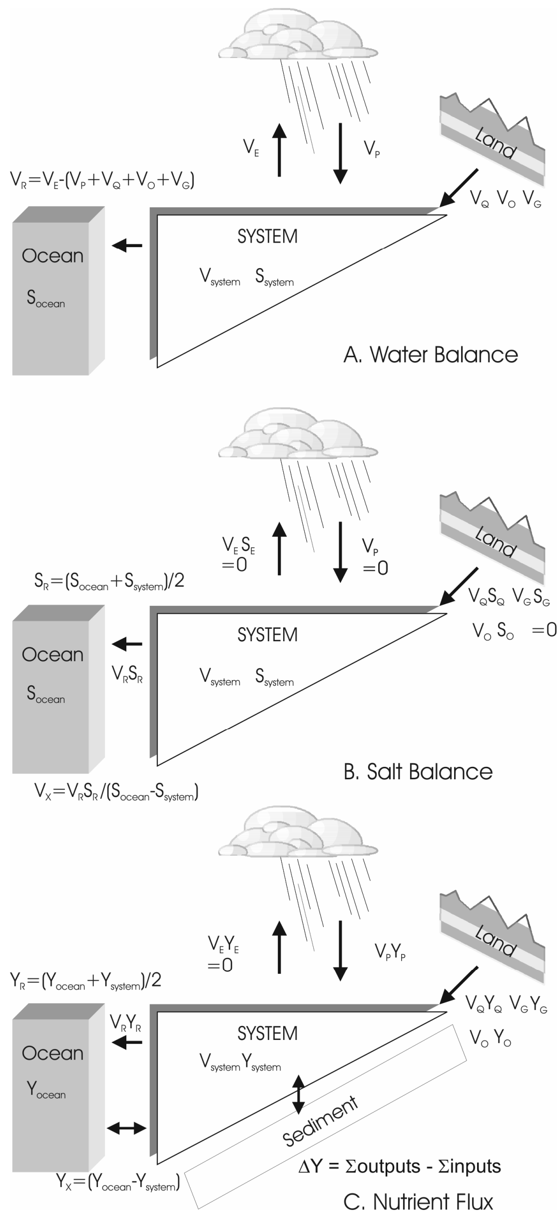

Figure 12. Generalised box diagrams illustrating the A) water budget, B) the salt budget and C) the budget for a nonconservative material, Y, in a coastal water bodies. (Adapted from Gordon et al. 1996).

The estuary can be divided into a "true estuarine area" that displays a salinity gradient and a marine dominated embayment. The "true estuarine area" is situated in the canalized lower reaches of the Mhlathuze River (Site 7 on Figure 13) through to the mouth. The large marine dominated embayment (the south-westerly part of the estuary represented by Sites 1 - 6 on Figure 13) receives very limited freshwater input from the Mtantatweni River, which drains Lake Cubhu. The ancient water-course of the Mhlathuze River forms a canal, which drains the sugar cane fields situated between the Mhlathuze and Mtantatweni Rivers. At the time of data collection the mouth was approximately 300 m in width. The new mouth has altered the tidal prism in the Mhlathuze estuary from 0.4 m before the development of the harbour to a current tidal range in the order of 1.8 m. Modeling of the physical dynamics of the mouth indicated that closure would not take place even if there were a total cessation of freshwater input into the estuary (Quinn 1999).

Sugar cane is cultivated extensively on the floodplain of the estuary. In recent years the number of informal settlements and subsistence farms on the eastern shore of the estuary has increased drastically. On the southern and western banks mangrove swamps occur, dominated by the white mangrove (*Avicennia marina*) and to a lesser extent by the black mangrove (*Bruguiera gymnorrhiza*). These mangrove stands represent 80% of the mangroves found in South African estuaries and bays. Other emergent and submerged macrophytes include *Phragmites australis* and eelgrass (*Zostera capensis*).

The substratum has been described as being a sequence of graded fluvial sand interspersed with silts and clay (Orne 1973). The alluvial deposits from the Mhlathuze River are currently extending the silt delta gradually into the estuary and this is accompanied by mangrove encroachment. This high degree of siltation has a pronounced effect on the volume of the estuary, resulting in a water exchange of about 90 % at each tidal cycle (Oliff 1977). There is a very limited salinity gradient in the greater part of the estuary. This is due to a number of factors including the mouth dynamics, the shallow nature of the estuary and the extent of water exchange. This results in the greater part of the estuary exhibiting marine salinities. The only salinity gradient is found along the canal of the Mhlathuze River. The Mhlathuze Estuary is therefore not an axial system.

Very little information is available on the water quality of the Mhlathuze Estuary. Hemens et al. (1971) analysed physico-chemical variables as part of a biological and sediment survey of the original Richards Bay during 1969. Follow-up studies, investigating pre- and post- harbour development conditions and conditions following the dredging of a new mouth for the estuary, were undertaken during 1974 (Hemens and Connell 1975), 1975, and 1976 (Hemens et al. 1976a; Hemens et al. 1976b). These data were collated and summarised by Begg (1978).

In 1996 the Coastal Research Unit of Zululand (CRUZ) initiated a study to investigate the effects of an intrabasin transfer scheme on the water quality and biology of the Mhlathuze Estuary (Cyrus et al. 2000). Quarterly sampling was undertaken from April 1996 to August 1998. No known water quality data (physico-chemical parameters) exists for the intervening period between the initial pre-harbour development study (1976) and the latter study (1996). Estuarine water quality data reported in this study are based on the results obtained from a CRUZ monitoring study between 1996 and 1998, whereas the water quality data for the Mhlathuze River were obtained from the water quality database of DWAF, Pretoria as well as data collected by CRUZ between 1996 and 1998 in the lower reaches of the river (Cyrus et al. 2000). Nutrient data for ground water were obtained from a database that forms part of a heavy mineral mining operation biomonitoring programme (Clean Stream 2000).

Mvoti Estuary

The abiotic and biotic characteristics of the Mvoti Estuary (29.40°S, 31.35°E; Figure 13) are not comparable with any other estuary in KwaZulu-Natal (Begg 1984). The system is best regarded as a river mouth with an extremely shallow mean depth (<0.5 m; Mackay *et al* 2000). The Mvoti catchment area is 2,730 km^2 (Chunnet et al. 1990) and the 2-km estuary occupies 0.2 km^2 of this space. The river length is 180 km to 215 km (Begg 1978), with flow to the estuary ranging from 7 $m^3 sec^{-1}$ to 15 $m^3 sec^{-1}$. Depth at high tide varies from 0 to 0.4 m (Porter 1990).

A one-km sandbar separating the estuarine area from the marine environment occupies approximately 20% of the total estuary area. Consequently, the river deflects 90° at the coast and opens to the south. The current opening is over a rocky ledge of Ecca shale to the south (Begg 1978). The mouth has remained stable since the mid 1990's and over the last decade has seldom closed, but if necessary has been breached by bulldozer to drain flooded sugarcane fields. Before this, records showed that the mouth is usually closed with an overflow channel only on the south side (Badenhorst 1990). Under flood conditions the river takes a straighter course to the ocean and breaks through the spit in a more northerly position.

Badenhorst (1990) calculated that due to a sedimented bed, the mouth area was –0.3 m above mean sea level (AMSL). However, 250 m in from the mouth the bed level was measured at 3.6 m (AMSL) and increased to 13.1 m (AMSL) in the mid reaches of the system. If it is assumed that tidal exchange through an open mouth is only possible to a bed level of +1 m (AMSL) then the Mvoti has limited potential for meaningful tidal exchange. The furthest penetration of seawater was 500 m upstream (Begg 1978). From a sedimentological point of view, the estuary is severely degraded. This condition deteriorates with time due to high sediment loads during floods (Badenhorst 1990).

The physico-chemical characteristics of the Mvoti have from as early as 1964 been described as 'grossly polluted' (Begg 1978). This pollution was almost entirely due to effluent input of treated sewage from Stanger via the Mbozambo swamp, and sugar and paper mill effluents from Gledhow Sugar Mill and Sappi Stanger. The lower Mvoti River is still used for treated effluent disposal, agricultural irrigation and various domestic uses by informal settlements. Abstraction from the river upstream of the estuary takes place for the sugar and paper mill operations. Although it has been for long recognised that there has been wide scale organic enrichment of the river and estuarine system from industrial and agricultural uses, dissolved oxygen levels have been described as favourable. However, in the most recent study, dissolved oxygen concentrations did not comply with DWAF standards set for the aquatic environment at 80% - 120% saturation or 6-12 mg/l (DWAF 1996). However, a slight gradient of increasing concentration existed from headwaters to the mouth. Generally, the poor water quality that was measured in the last 4 km of river was reflected along the length of the estuary with no improvement of conditions.

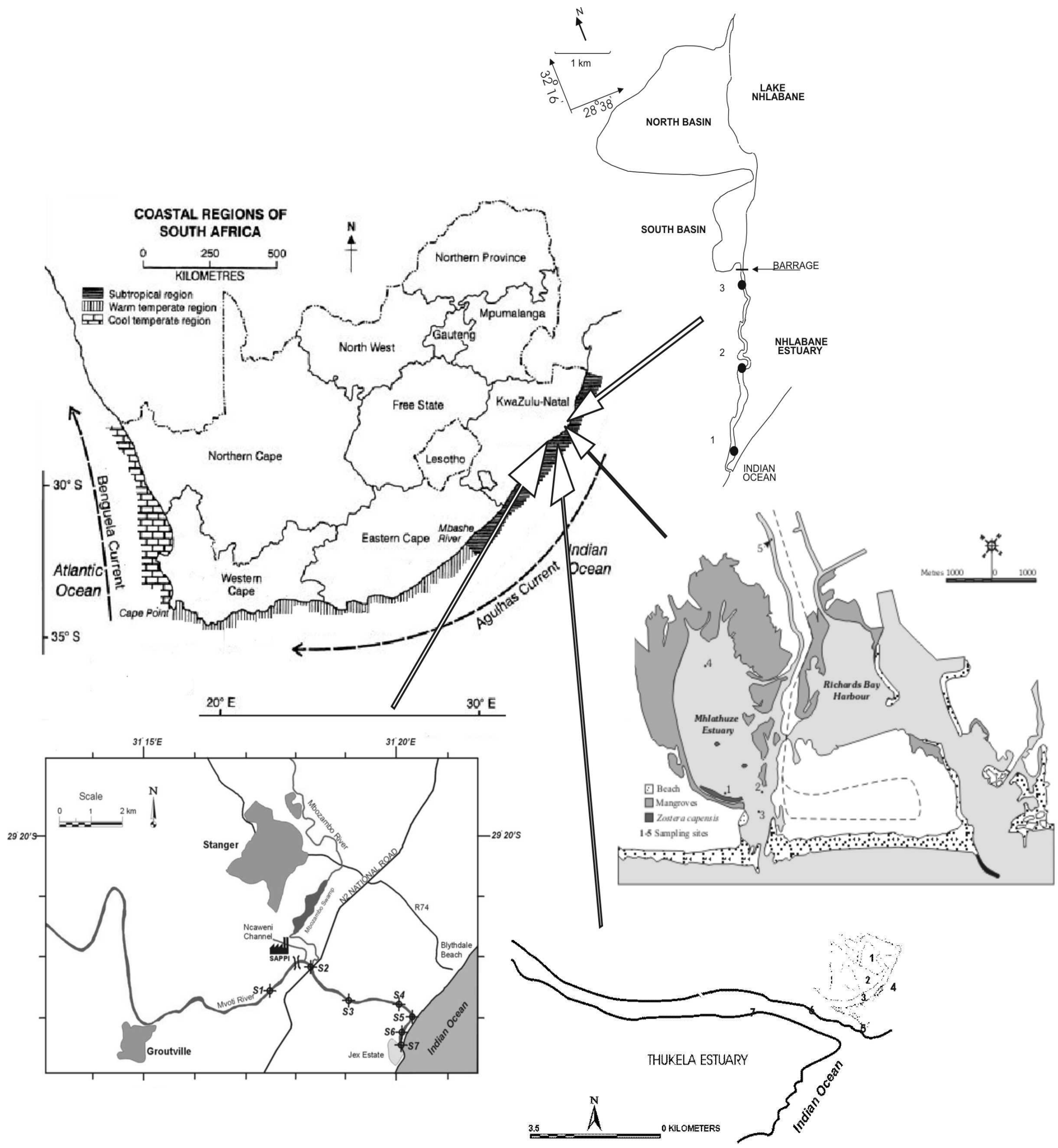

Figure 13. Diagram indicating the positions of the sampling sites in the selected estuaries for which nutrient budgets were calculated.

Data used for the budgeting purposes were obtained from a weekly sampling programme that was undertaken for six consecutive weeks during August 2000 in the Mvoti River and estuary. Sampling sites are indicated in Figure 13. All discharge and nutrient recordings representing the Mvoti River were sampled at Site 3, whereas all estuarine data were collected at sites 4 to 7. Note that the discharges from the paper mill and sewage treatment works at Site 2, would have been taken into account with the riverine samples being taken at Site 3 as was done for this study. The results from this study only allow a budget to be calculated for the low-flow dry season.

From a biological point of view, there are backwaters in the deeper areas that provide important refuge areas for fish. These backwaters occupy approximately 30% of the estuary (Porter 1990). Fringing the backwaters are reed beds and perennial weed species. The lower section on the Mvoti River is considered to have the poorest habitat integrity, both instream and along the riparian zone (Mackay *et al.* 2000). According to Tharme (1996) *'the riverine system has been modified completely, with an almost total loss of natural habitat and biota and the destruction of many basic ecosystem functions'*. The Mvoti Estuary also reflects the various impacts to which the river is subjected. Besides the combination of unacceptable levels of water quality variables and poor habitats, low volumes of outflow have a negative effect on this small estuary. The Mvoti Estuary is a degraded system with an ecosystem functioning far different from what it was in its pristine state (Mackay et al 2000).

From a conservation perspective, it has been stated that the Mvoti Estuary has some value in that it provides a nursery function for fish (seven species of obligate estuarine users; Porter 1990). It is the only estuary that has retained this function on 80 km of coastline and the bird life associated with the estuary includes Red Data species and a large variety of migrant species. The most important bird species present is the Redwinged Pratincole. This site hosts one of the few nesting sites of the bird in the country and has the only South African record of the Redthroated Pipit.

Nhlabane Estuary

Based on the classification by Whitfield (1992), the Nhlabane estuary (28.65° S; 32.25° E) is situated in the subtropical coastal zone on the east coast of South Africa and is regarded as a temporarily open/closed estuary. The estuary is small, 3 km in length and a maximum width of 55 m in the lower reaches (Figure 13). Although it has a relatively pronounced basin with steep banks and associated riparian vegetation, it does meander through a small floodplain area (Vivier et al. 1998). The marginal, and at times emergent vegetation, is dominated almost exclusively by *P. australis*.

River hydrology does not play a role in natural variation within the estuary. The catchment of the estuary is very small (107 km^2) and is dominated by an impoundment, Lake Nhlabane. It is important to note that the lake has very small tributaries. Surface water runoff and groundwater recharge are responsible for water supply to the lake. The barrage effectively cut off all freshwater out flow into the estuary during the drought period from middle 1991 to

November 1995. This resulted in the closure of the estuary mouth for four years. The mouth was artificially breached in August 1995. The reasons for breaching are discussed in detail by Vivier et al. (1998). In the intervening period salt water entered the estuary through occasional overtopping during spring high tides. It is important to note that hypersaline conditions did not develop during mouth closure period. This is as a result of ground water recharge of the estuary due to seepage from the lake, surrounding catchment, and mine ponds in the adjacent dunes. Since the end of 1995 the mouth of the estuary has been opening and closing frequently with the result that a salinity gradient developed in the estuary.

The mouth of the Nhlabane Estuary is at an open coastline and directly exposed to wave action, without any protection (e.g. natural headland). The beaches at the mouth are very steep, which is typical for this area and this is caused by the interaction of the local wave climate and the coarse sand particles on these beaches. The breaker zone therefore normally consists of one offshore breaker line at about 100 m from the beach and the second breaker line being on the beach itself. The action of breaking waves at the beach places large quantities of sediments in suspension, which are flushed into the mouth during the incoming tide and thereby provide the main closing force at the mouth.

Due to the infrequent breaching of the mouth and the substantial freshwater inflow into the estuary there is limited salinity stratification. Under natural conditions, i.e. prior to the construction of the barrage in 1976 the mouth was normally open one to three times per year for periods of one to three weeks at a time (Quinn 1999). It is estimated that a total cumulative inflow of 10 million m^3 was required before a natural breaching would take place and based on experience from other estuaries it is estimated that the maximum flow rate after a breaching could well exceed 100 to 200 m^3 sec^{-1} for several hours. The outflow of freshwater would probably last for a few days after which the intrusion of saline marine water would then have occurred at high tides until mouth closure (Quinn 1999). Overtopping of the berm by high waves at high tides would later have caused additional inflow of marine water, especially in the period shortly after closure when the berm was still low. The influx of marine water under tidal flows would have resulted in some saline water reaching the southern basin of Lake Nhlabane as has been observed in the past (Begg 1978).

At present mouth normally closes within a few tidal cycles after a natural or artificial breaching (Quinn 1999). This is considerably shorter than the estimated open mouth periods of one to three weeks, which probably normally occurred under natural conditions. Under present conditions the flushing effects at mouth breachings are strongly reduced because of the much smaller storage volume of the estuary at present compared to that of the complete system under natural conditions. However, flushing of sediments during major floods will still take place (Quinn 1999). In the instances when artificial breaching was carried out salinities of up to 10 psu were recorded at the barrage. This clearly indicates that the artificial breachings were not only effective in keeping the water level in the estuary low, but also resulted in a meaningful influx of salt water into the estuary.

There is very little information available on the water quality of the Nhlabane Estuary. The only documented historical data for the estuary was recorded between February 1976 and January 1977 prior to the construction of the barrage (Begg 1978). Physico-chemical water quality data have been collected by the CRUZ since 1992 as part of a quarterly monitoring programme to study the effects of a dredger crossing on the fauna of the estuary. Due to a number of circumstances the programme is still ongoing with input by both CRUZ and the CSIR (Fowles et al. 1997; Vivier et al. 1998). During this period samples were collected and analyzed for selected chemical variables by the Environment Health and Safety department of Richards Bay Minerals (RBM). Data is presented through kind permission of RBM. Catchment derived nutrient data was based on limited nutrient surveys undertaken by RBM at eight sites in the northern and southern basins of Lake Nhlabane for the period 1993 to 1996. There was however no overtopping over the barrage for most of the study period and very limited (no quantitative data) towards the beginning of 1996.

Thukela Estuary

Based on the classification by Whitfield (1992), the Thukela Estuary is one of only two examples of an open river mouth estuarine system in South Africa. The estuary is situated approximately 100 km north of the city of Durban on the east coast of South Africa (29.22°S, 30.50°E; Figure 13). The Thukela system forms a very important component of water resource utilisation in South Africa with a number of large interbasin transfer schemes responsible for transferring water from the Thukela basin across the escarpment into the Vaal River system (Davies and Snaddon 2000). The total catchment area is approximately 29,100 km^2 and the Thukela River originates in the Drakekensberg mountains (Begg 1978). From the Drakensberg mountain range the river meanders for 520 km through the KwaZulu-Natal midlands before flowing into the Indian Ocean. The land-uses in the catchment are mainly rural subsistence farming and commercial forestry. It is only on the coastal plain that the river flows through urbanised areas. The only industries associated with the urban development are paper and sugar mills with large-scale commercial sugar cane farming along the banks of the lower reaches of the river.

Due to the high riverine runoff, the estuarine area of the Thukela is small. The surface area of the estuary during low flow periods is approximately 0.6 km^2. However changes in river flow cause considerable changes in the morphometry of the estuary, and during periods of high flows the estuary extends out to sea and becomes unconfined by banks (Begg 1978). The axial length is estimated to be 800 m during low flow, with a shoreline length of approximately 2 km. The maximum width during natural flow periods is approximately 350 m with a channel width of 50 m, which increases to over 1,000 m during floods (Begg 1978). Initial observations on the bathymetry of the estuary indicated that it was relatively deep (Begg 1978), but surveys undertaken by CRUZ from March 1997 to April 1998 (reported in Archibald 1998b) showed that the average depth of less than 1.5 m.

According to Begg (1978) the sandbar has a 700 m stable component on the floodplain (carrying a coastal dune forest) extending in a generally northern direction. There is also a 700 m unstable component without vegetation that forms across the mouth. This bar is periodically removed by flood discharges. During flood conditions an offshore bar is formed, directing floodwater into the sea in a southerly direction. It is unlikely that mouth closure occurred during virgin conditions. More frequent mouth closures recorded in recent times (for only a few days at a time) are probably due to the significant abstraction of water from the system via interbasin transfer schemes to the Gauteng province. However, under future transfer schemes and runoff scenarios it is predicted that a drastic increase in mouth closure conditions will occur, for prolonged periods of up to 4 or 5 months (Quinn 1997).

Although very little is known about the biological condition of the estuary, recent surveys have shown that it plays an important role as habitat for water birds along the Kwa Zulu-Natal coast (Quinn 1997) and that the fish and estuarine benthic invertebrates were found to be poorly represented. The same study found that very little natural vegetation remains, due to encroachment of sugar cane and forestry. However, there are still some stands of the brackwater mangrove (*Baringtonia racemosa*) and a small *Phragmites*-dominated wetland on the south bank close to the mouth. According to MacKay and Cyrus (1998) the paucity of benthic fauna points to the estuary being plankton-dominated.

A water quality survey of the estuary highlighted the paucity of data (Archibald 1998b). The only data available for the estuary were collected during a crab megalopa and benthic invertebrate survey undertaken by the CRUZ between 1997 and 1998. During this study, water quality was assessed at five sites in the estuary. Comprehensive data were obtained from the DWAF in Pretoria, South Africa. Biweekly water quality analyses were carried out at a number of stations in the Thukela catchment. However, for the purposes of this assessment, the data from Weir V5H002, the gauging weir closest to the estuary, were analyzed. Daily flow records were also available for this station. The dataset from 1994 to 1998 were analyzed to represent present day conditions of the runoff to the estuary. These data were taken during an extended wet period and therefore no dry period results are presented.

Water and salt balances:

The assumption required to apply the steady-state water balance equation to a system is that the water level is steady over time. All the estuaries in this study undergo marked water level changes due to a variety of factors. Thus the LOICZ modeling assumption is not valid over over short (i.e. daily) time frames and it is thus necessary to average the water balance equation over an extended period of time, which results in a constant estimation of water level.

The Mhlathuze Estuary undergoes marked water level changes due to tidal action through the permanently open mouth. For LOICZ biogeochemical modeling, it is important to estimate the mixing volume (V_X in m^3 d^{-1}) across the open boundary of the system. The basis for calculating the flux is the presence of a quantifiable salinity gradient. However, since there is a limited gradient in the Mhlathuze system, an alternative procedure to calculating the V_X is also included. That procedure (Yanagi 2000a) makes use of the dispersion process where the magnitude of the horizontal dispersion coefficient (D_h in m^2 d^{-1}) is estimated from the current shear and the diffusivity normal to current shear. For wide and shallow estuaries the following equation is used:

$D_h = W^{0.85} U^2 / 2180$ where: (Equation 5)

W denotes the width of the estuary mouth in m and U is the residual flow velocity at the surface layer of the open boundary in m d^{-1}. Since this value is not independently known, a numerical value of 8,640 m d^{-1} was applied (Yanagi 2000a). In order to express D_h in LOICZ notation, the following equation was used for calculating V_X (Yanagi 2000b):

$V_X = D_h (A/F)$ where: (Equation 6)

A denotes the cross section area of the open boundary of the system (m^2) and *F* is the distance (m) between the geographic center of the system and the observation point for oceanic salinity (typically near the mouth of the system).

The following results for D_h and V_X were calculated for the Mhlathuze Estuary using equations (5) and (6).

$D_h = (200^{0.85} (0.1*86{,}400)^2)/ 2180$
$D_h = 3{,}100\ 10^3\ m^2\ d^{-1}$
$V_X = D_h (A/F)$
$V_X = 3{,}100 \times 10^3\ m^2\ d^{-1}(5{,}000\ m^2/3{,}000\ m)$
$V_X = 5{,}200 \times 10^3\ m^3\ d^{-1}$

Figure 14A shows the water and salt balance for the Mhlathuze Estuary with annual averages using the two methods described above. V_X^a is volume mixing calculated using the LOICZ water and salt balance and V_X^b is calculated using the dispersion coefficient. For the purposes of this paper, the conservative estimate for total water exchange time (τ) calculated using V_X^b was used, i.e. four days. The relatively rapid exchange period is attributed to the large tidal prism of 1.8 m in this shallow estuary (average depth at high tide of 2 m). The system is therefore dominated by tidal mixing in the form of inflow of marine water in the greatest proportion of the estuary (i.e., the embayment area). Although there is significant freshwater outflow from the canalized area of the estuary, mixing of marine water and freshwater only occurs during high tide. During low tide the marine (estuarine brackish water) is replaced by freshwater flow from the river. The freshwater is mainly restricted to the canalized area, with the embayment remaining marine dominated.

The Mvoti Estuary has a permanently open mouth and levels therefore fluctuate markedly due to a combination of riverine inflow and to a lesser extent the effects of the incoming and outgoing tides. It is thus necessary to average the water balance equation over the entire study period (six weeks during August/September 2000), over which time the water level does remain essentially constant. Water fluxes, salinity and nutrient concentrations, and data sources for Mvoti Estuary used in this budgetary assessment are presented in Table 6. Figure 15A illustrates the water and salt balance for the Mvoti Estuary with six-weekly averages using the LOICZ methodology. Residual water flux (V_R in the notation of Gordon et al. 1996) from this system, to balance freshwater inflow, is approximately 236x10^3 m^3 day^{-1}, while exchange flux (V_X) is 121x10^3 m^3 day^{-1}. The system volume (125x10^3 m^3) divided by the sum of these water fluxes gives an estimate of water exchange time of less than a day. These results indicate an extremely rapid seawater exchange within the estuary, which is caused by the significant freshwater outflow through the mouth. The rapid water exchange is characteristic of the permanently open estuaries along the eastern seaboard of South Africa. The morphologies of most of these estuaries are relatively narrow riverine channels with little or no backwater areas that could contribute towards longer retention times.

Nhlabane Estuary also undergoes marked water level changes due to the opening and closing of the sand bar at the mouth. Water fluxes, salinity and nutrient concentrations, and data sources for Nhlabane Estuary used in this budgetary assessment are presented in Table 6. Figure 16A illustrates the water and salt balance for the Nhlabane Estuary with annual averages using the LOICZ methodology. Residual water flux (V_R) from this system, to balance freshwater inflow, is approximately 21x10^3 m^3 day^{-1}, while exchange flux (V_X) is 17x10^3 m^3 day^{-1}.

The system volume (200x10^3 m^3) divided by the sum of these water fluxes gives an estimate of water exchange time of approximately 5 days. During the study period the opening of the mouth was primarily driven by groundwater recharge from the surrounding dunes since no (or very little) freshwater input from the lake took place. Based on personal observations the estuary would drain very rapidly during low tide once the sandbar is breached. Normal tidal exchange would take place in the estuary for five to seven days before wave action closes the mouth of the estuary again. Continuous ground water recharge then fills the estuary over a period of approximately seven days resulting in the breaching of the sand bar again. It must be borne in mind that the data presented were recorded during an extreme drought period and it is probable that in the subsequent years additional freshwater input from the lake can be expected. However, there is no gauging facility on the barrage structure so no quantitative assessment of surface water input could be expected. Therefore this budget represents the conditions experienced during low flow periods in the Nhlabane Estuary.

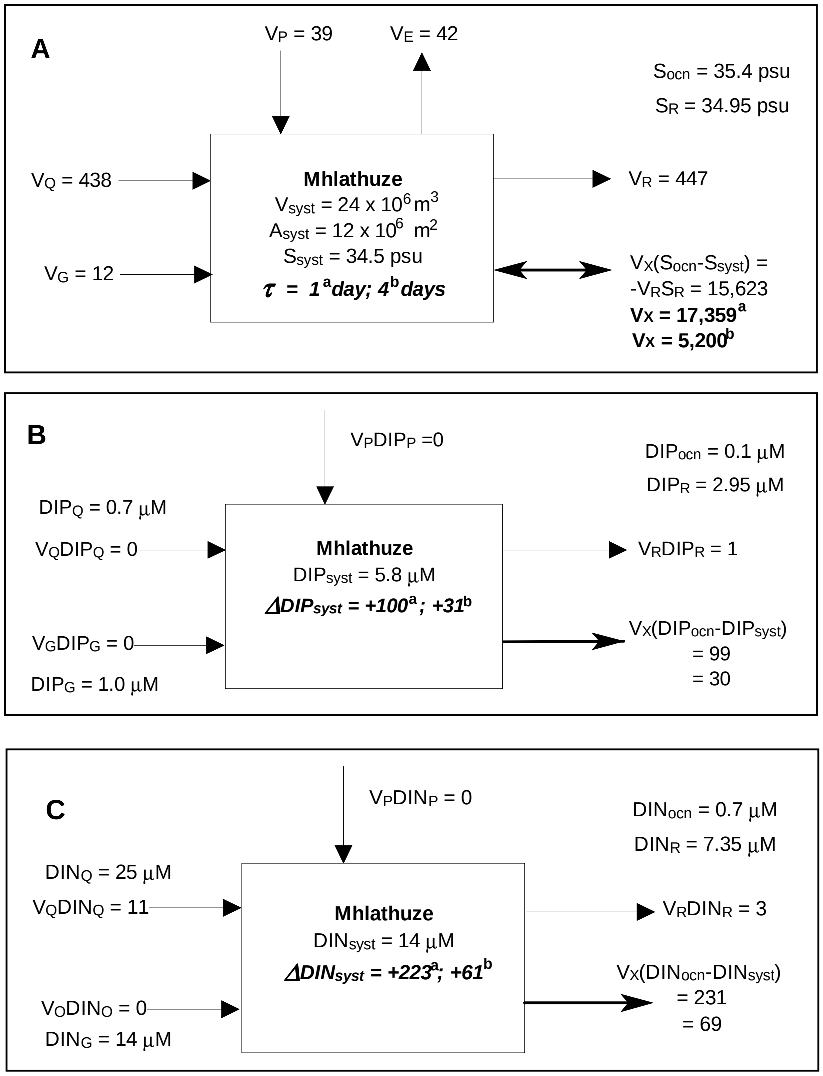

Figure 14. Water and salt budgets (A), dissolved inorganic phosphorous budget (B) and dissolved inorganic nitrogen budget (C) for the Mhlathuze Estuary. Water flux is presented in 10^6 m^3 d^{-1} and salt flux in 10^6 psu-m^3 d^{-1}, whereas nutrient fluxes are in 10^3 mol m^3 d^{-1}.

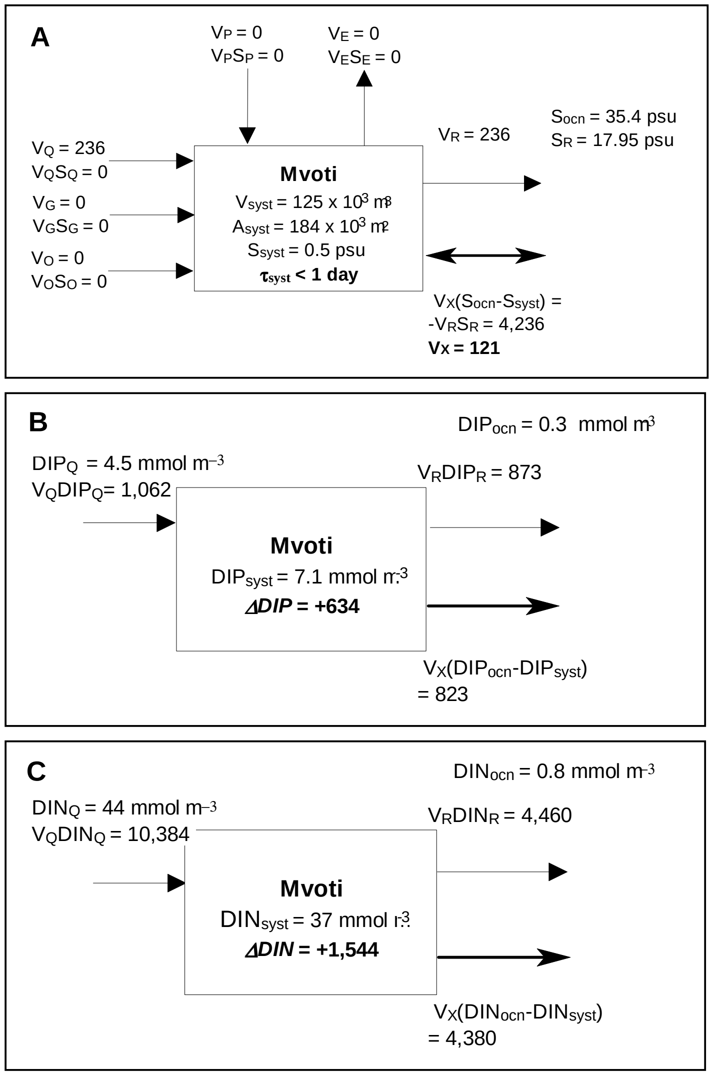

Figure 15. Water and salt budgets (A), dissolved inorganic phosphorous budget (B) and dissolved inorganic nitrogen budget (C) for the Mvoti Estuary. Water flux is presented in 10^6 m^3 d^{-1} and salt flux in 10^6 psu m^3 d^{-1}, whereas nutrient fluxes are in 10^3 mol m^3 d^{-1}.

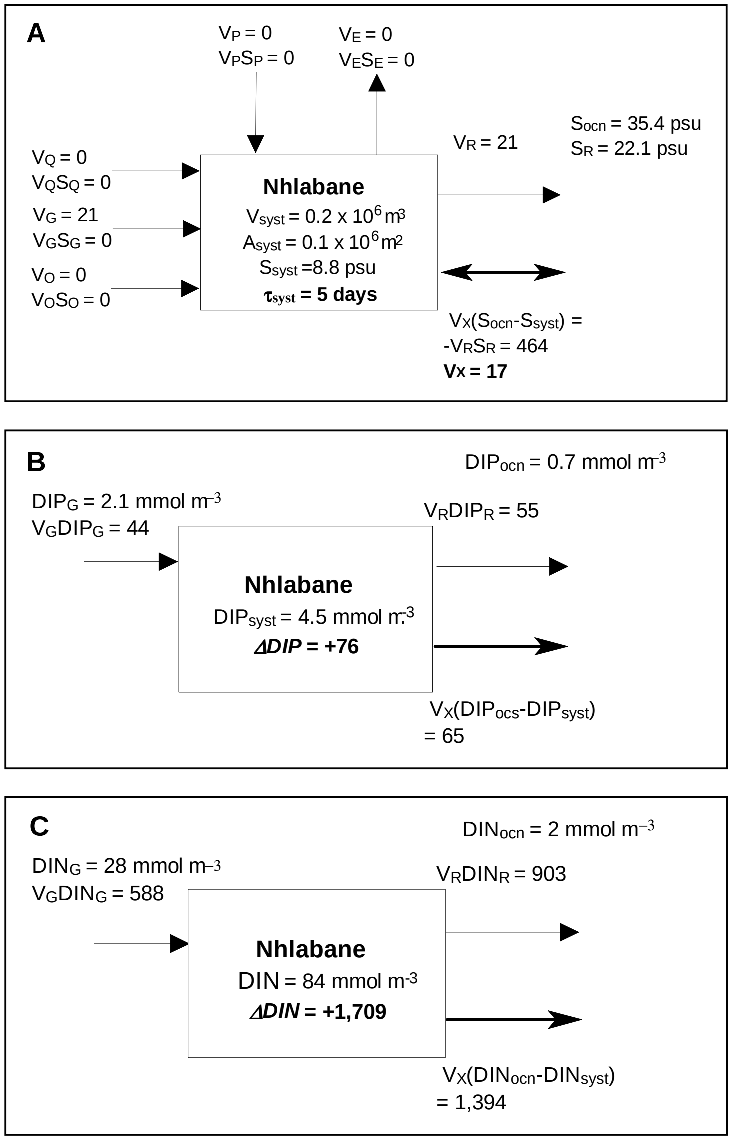

Figure 16. Water and salt budgets (A), dissolved inorganic phosphorous budget (B) and dissolved inorganic nitrogen budget (C) for the Nhlabane Estuary. Water flux is presented in 10^6 m^3 d^{-1} and salt flux in 10^6 psu-m^3 d^{-1}, whereas nutrient fluxes are in 10^3 mol m^3 d^{-1}.

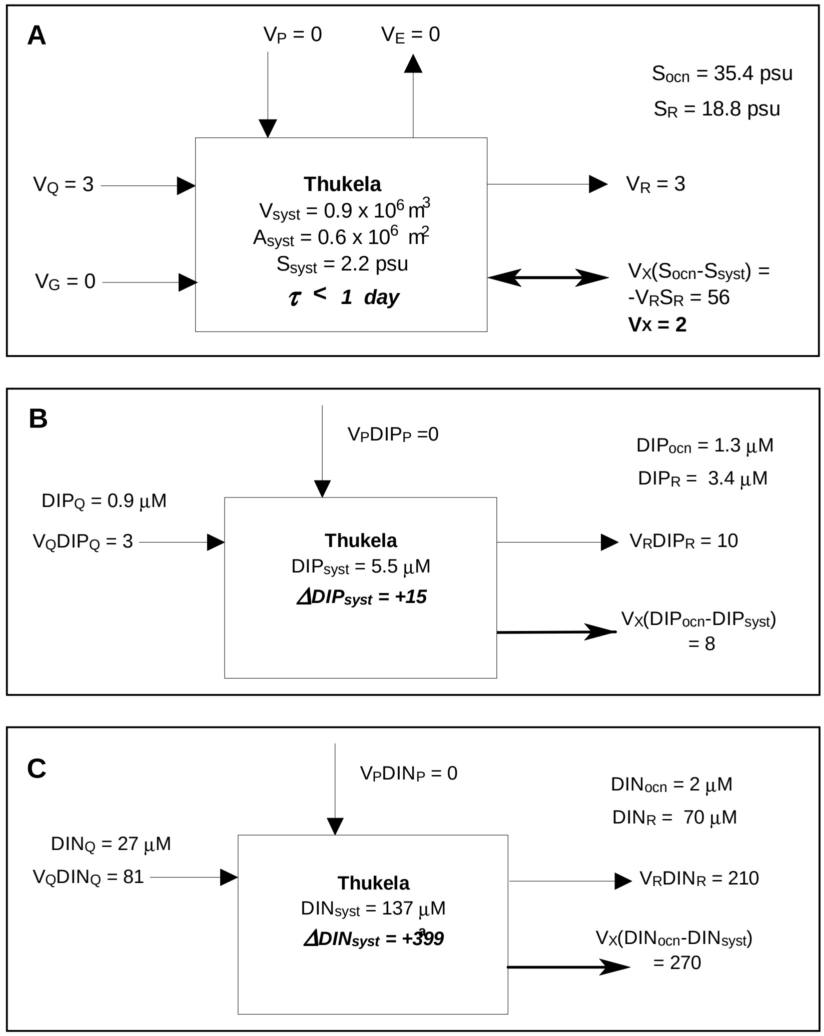

Figure 17. Water and salt budgets (A), dissolved inorganic phosphorous budget (B) and dissolved inorganic nitrogen budget (C) for the Thukela Estuary. Water flux is presented in 10^6 m^3 d^{-1} and salt flux in 10^6 psu m^3 d^{-1}, whereas nutrient fluxes are in 10^3 mol m^3 d^{-1}.

The water balance equation for the Thukela Estuary was also averaged over an entire year to obtain a measure of constant water levels since the estuary undergoes marked water level changes due the effects of the incoming and outgoing tides. Water fluxes, salinity and nutrient concentrations, and data sources for Thukela Estuary used in this budgetary assessment are presented in Table 7. Figure 17A illustrates the water and salt balance for the Thukela Estuary with annual averages using the LOICZ methodology. Residual water flux from this system, to balance freshwater inflow, is approximately $3x10^6$ m^3 d^{-1}, while exchange flux (V_X) is $2x10^6$ m^3 d^{-1}.

The system volume ($0.9x10^6$ m^3) divided by the sum of these water fluxes gives an estimate of water exchange time of less than a day. These results indicate an extremely rapid seawater exchange within the estuary, which is caused by the significant freshwater outflow. It is this abundant freshwater supply from the Thukela River, which has led to the large interbasin (Davies and Snaddon 2000) water transfer schemes currently in place and planned for the future.

Non-conservative DIN and DIP budgets:

Assuming a steady state for both dissolved inorganic nitrogen (DIN) and dissolved inorganic phosphorus (DIP) over the entire sampling period, and that the nutrient concentration in evaporated water and the nutrient contribution from groundwater and rainwater are negligible, the nutrient budget equation can be simplified to $\Delta Y = -V_R Y_R - V_G Y_G - V_Q Y_Q - V_X(Y_{ocn} - Y_{syst})$. It is known that the nearby coastal lakes in the Mhlathuze catchment are affected by significant aerial deposition of nutrients from surrounding industries (Archibald 1998a). However the prevailing wind conditions are such that the estuary should not be affected. Nutrient budgets are illustrated in Figure 14B and C. Non-conservative fluxes with superscript (^{a}) and (^{b}) were derived using $V_X{}^a$ *and* $V_X{}^b$, as indicated in the previous section respectively.

For the purposes of calculating nutrient balances and system metabolism the results based on the most conservative of the flux calculations were used (i.e., fluxes based on current shear). The Mhlathuze Estuary is a net source of nutrients and can be interpreted to indicate that heterotrophic processes prevail. The potential for aerial deposition could overestimate the heterotrophy. The differences in ΔDIP based on the derivation of V_X are shown in Figure 14C. The positive ΔDIN indicates that Mhlathuze Estuary seems a source for DIN. However this should be regarded with the same degree of caution as expressed for the DIP with regards to potential aerial deposition.

Due to extremely high flushing rate of the Mvoti and Thukela estuaries, nutrient budgets probably cannot be considered reliable. However assuming a steady state for both DIN and DIP over the sampling period, and that the nutrient contribution from groundwater is not known and rainwater is considered to be negligible, the nutrient budget equation can be simplified to $\Delta Y = -V_R Y_R - V_Q Y_Q - V_x(Y_{ocean} - Y_{out})$. The DIP and DIN concentrations used for calculating nutrient fluxes are shown in Tables 6 and 7.

In the case of the Mvoti Estuary the non-conservative flux of DIP (ΔDIP) is +634 mol d^{-1} or +3.4 mmol m^{-2} d^{-1} is probably indicative of removal of DIP from the system. Non-conservative DIN flux (ΔDIN) was positive (-1,544 mol d^{-1} or +8.4 mmol m^{-2} d^{-1}) indicating that the estuary is acting as sink for non-conservative DIN (Figure 15A and B). The source function of the estuary for both DIP and DIN from the system was expected since the input of primary treated sewage discharge into the Mvoti River is not reflected as concomitant increased DIP and DIN in the ocean adjacent to the estuarine mouth. The nutrient fluxes in the Thukela Estuary show a similar pattern and it should be borne in mind that nitrate in runoff is likely to be important since there are large sugar cane fields on the banks of the lower reaches of the river and the estuary. The ΔDIP and ΔDIN calculated for this one-box estuary model are positive, indicating that the estuary is a net source of nutrients (Figure 17A and B). The flux of non-conservative DIP is $+15 \times 10^3$ mol d^{-1} or 25 mmol m^{-2} d^{-1}; and non-conservative DIN is $+399 \times 10^3$ mol d^{-1} or 665 mmol m^{-2} d^{-1}.

Estuarine systems with very short water exchange time often appear to behave as high sinks or sources of DIP and DIN. This apparent behaviour reflects the dominance of hydrographic processes, along with uncertainty (even small uncertainty) in the nutrient loads or concentrations. In fact, these systems more properly should be considered to flush out all the nutrients (Dupra 2000a, 2000b). This conclusion does not, in any sense, suggest that there is no non-conservative flux of nutrients in such systems; rather, the non-conservative flux is small relative to the conservative flux and cannot be resolved.

The ΔDIP and ΔDIN calculated for the one-box model of the Nhlabane Estuary are positive, indicating that the estuary is a net source of nutrients (Figure 16A and B) The calculated flux of non-conservative DIP is +76 mol day^{-1} or +0.8 mmol m^{-2} day^{-1} and non-conservative DIN is +1,709 mol day^{-1} or +17 mmol m^{-2} day^{-1}. The system is a net source of DIP and DIN and can be interpreted to indicate that heterotrophic processes prevail. It is possible that the ground water input of DIN and DIP are an overestimation of input via this route since the data used were obtained from boreholes along the banks of Lake Nhlabane and not in the dunes surrounding the estuary.

Stoichiometric calculations of aspects of net system metabolism:

In the case of most of the permanently open river-driven estuarine systems along the east coast of South Africa, the water exchange is very rapid resulting in a time constraint for biological processes to take place. It is therefore not reliable to estimate system metabolism in systems with rapid water exchange such as the Mhlathuze, Mvoti and Thukela estuaries. However, assuming that the Mhlathuze Estuary behaves more as having V_X^b and a longer water exchange time, net system metabolisms were calculated. Since it is not completely obvious whether mangroves or phytoplankton are the dominating reactive organic matter, two N:P ratios are used. Assuming the bulk of the reacting organic matter is phytoplankton, the C:P ratio is 106:1, then for the Mhlathuze Estuary, net ecosystem metabolism: (*p-r*) = -300 mmol m^{-2} d^{-1}. Assuming the bulk of the reacting organic matter is mangroves, the C:P ratio is 1000:1 (Atkinson and Smith 1983) and for the Mhlathuze, the net ecosystem metabolism: (*p-r*) = -3,000 mmol m^{-2} d^{-1}. Both (*p-r*) values indicate that there is a net loss of organic matter from the Mhlathuze Estuary.

If the ΔDIP values in Mhlathuze Estuary are a measure of the net production of organic matter in the system, the expected ΔDIN (ΔDIN_{exp}) would be ΔDIP multiplied by the N:P ratio of the reacting organic matter. Large differences between ΔDIN_{obs} and ΔDIN_{exp} are indicators of processes other than organic metabolism, which alter fixed nitrogen. As nitrogen fixation and denitrification are important processes in coastal systems, the difference is taken as a measure of net nitrogen fixation minus denitrification. Again, because the major source of reacting matter is unclear, two N:P ratios are used. If phytoplankton is the principal form of organic matter in the Mhlathuze Estuary then, based on the Redfield ratio ΔDIN_{exp} =16 ΔDIP: [*nfix-denit*]$_{\text{phytoplankton}}$= -40 mmol m^{-2} d^{-1}. If the *Avicennia* mangroves are the principal form of organic matter then, based on a median ratio for mangroves of C:N:P 1000:11:1 (Atkinson and Smith 1983), ΔDIN_{exp} =11 ΔDIP, so that: [*nfix-denit*]$_{mangroves}$= -20 mmol m^{-2} d^{-1}. The negative values indicate that denitrification processes are responsible for smaller ΔDIN_{obs} than ΔDIN_{exp}.

The net ecosystem metabolism of the Nhlabane Estuary [primary production-respiration = (*p-r*)] was calculated as the negative of ΔDIP multiplied by the C:P ratio of the reacting organic matter. It was not completely obvious whether the expansive reed beds (*P.australis*) that filled the estuary during the drought period or phytoplankton are the dominating reactive organic matter, so two N:P ratios are used. Assuming the bulk of the reacting organic matter is phytoplankton, the C:P ratio is 106:1, then for the Nhlabane Estuary, net ecosystem metabolism (*p-r*) = -84 mmol m^{-2} d^{-1} and assuming the bulk of the reacting organic matter is reed beds, the C:P ratio is 300:1 (Smith *pers. comm.*[1]) and for the Nhlabane, the net ecosystem metabolism (*p-r*) = -240 mmol m^{-2} d^{-1}

The negative net ecosystem metabolism (*p-r*) values indicate that the system is net heterotrophic with a net loss of organic matter from the Nhlabane Estuary. If the ΔDIP values in Nhlabane estuary are a measure of the net production of organic matter in the system, the expected ΔDIN (ΔDIN_{exp}) would be ΔDIP multiplied by the N:P ratio of the reacting organic matter. Large differences between ΔDIN_{obs} and ΔDIN_{exp} are indicators of processes other than organic metabolism, which alter fixed nitrogen. As nitrogen fixation and denitrification are important processes in coastal systems, the difference is taken as a measure of net nitrogen fixation minus denitrification.

Again, because the major source of reacting matter is unclear, two N:P ratios are used. If phytoplankton is the principal form of organic matter in the Nhlabane estuary then, based on the Redfield ratio ΔDIN_{exp} = 16 ΔDIP: (*nfix-denit*) $_{\text{phytoplankton}}$= +4 mmol m^{-2} d^{-1}. If the *Phragmites* reedbeds are the principal form of organic matter then, based on a realistic ratio for these macrophytes of C:N:P 300:20:1, ΔDIN_{exp} = 20 ΔDIP, so that: (*nfix-denit*) $_{mangroves}$ = +1 mmol m^{-2} d^{-1} . The positive values obtained indicate apparent slight net nitrogen fixation in the estuary.

4.2.4 General conclusions relating to the use of the LOICZ budget procedure on the data from the four estuaries

Due to the paucity of estuarine water quality data single box LOICZ budgets were developed for all four estuaries in this study. During the period for the Mhlathuze study (1996-1997), the inflow from the Mhlathuze River was very constant and did not display any seasonal fluctuation (i.e. wet/dry seasonal flow patterns). This is because the Mhlathuze River is highly regulated and during wet cycles the winter and summer flows is similar. Since the monitoring of

[1] S. Smith, LOICZ workshop-2002, Simons Town, South Africa

the Mhlathuze Estuary is an ongoing project it is anticipated that seasonal models will be developed once nutrient data from dry cycles are available. The data for the Mvoti study period (August 2000) is representative of dry seasonal flow patterns. In future, it would be possible to construct models for wet seasons since an ongoing monitoring programme has been initiated for the estuary. During the study period for the Nhlabane (1993-1996), the estuary was subjected to extreme drought conditions and water input was limited to ground water recharge through the dune cordon. It must therefore be borne in mind that the data presented were recorded during an extreme drought period and it is probable that in the subsequent years additional freshwater input from the lake can be expected. However, there is no gauging facility on the barrage structure so no quantitative assessment of surface water input could be expected. Therefore this budget represents the conditions experienced during low flow periods in the Nhlabane Estuary. Very little seasonal fluctuation (i.e. wet/dry season flow patterns) was recorded during the study period for the Thukela Estuary (1997-1998). An extensive study of the Thukela River and its estuary was undertaken as part of the Estuarine Freshwater Requirements (EFR) of the ecological Reserve determination for this system. Future studies should allow for extensive nutrient surveys on the mudflats, off the mouth of the estuary and on the offshore Thukela banks. This would allow for the development of a three-box budget, which would be a better representation of the nutrient fluxes taking place.

4.2.5 Interpretation of LOICZ budget results in terms of RDM classification

Since ecosystems are able to function at various levels of integrity, classification procedures recognizes a range of functioning conditions from excellent (pristine or unmodified conditions) to impacted but still sustainable. A water quality reference condition is used to describe the natural unimpacted characteristics of a particular section of system (i.e. in a particular ecoregion prior to the influence of humans). Ideally, the reference condition should remain stable and not vary over time. However, due to seasonal variation it should be recognised that variations in the reference will occur. It is against this reference condition that changes within a system are benchmarked.

With the LOICZ modeling approach the assumption required to apply the steady-state water balance equation to a system is that the water level is steady over time, and it is this steady state that is required to construct a reference condition. However, most water quantity and quality data for South African river systems only go back to the end of the 1970s and it is therefore extremely unlikely that data representing unimpacted conditions are available. The situation for estuaries is even worse. According to Whitfield (2000) the status of information on 68% of South Africa's estuaries is poor to nil. In many instances the data lacking most is on the physico-chemical properties of the water. The results from the LOICZ modeling procedure could therefore be regarded as steady state conditions for an estuary and as such it satisfies the data requirements for a reference condition, in the case of an unimpacted system, or the present ecological status, in a system that is impacted. The LOICZ model could therefore provide a reference (or best attainable reference condition) for nutrient fluxes in a particular estuary. Any changes, be it changes in freshwater inflow, nutrient input, salinity change, etc. will be reflected as a deviation from the benchmark fluxes. Since the changes in fluxes would affect the estuarine functioning, it would inevitably also affect the general integrity of the estuary. The degree to which the flux deviates from the benchmark can be represented as a change in the integrity of the system, which in turn may be represented as an assessment category.

No reference conditions can be specified without data being available. In such a case it is essential that a monitoring program is designed and implemented to generate data for use in the model. It is recommended that a MINIMUM of weekly sampling is carried out over a 60 day period (DWAF 1999). The data required and potential sources of these data are presented in Table 8. Once the data have been sourced and/or collected (following a monitoring programme) the fluxes can be calculated using the LOICZ modelling approach. The fluxes can be calculated manually or using the *Cabaret* software package (See Section 5).

Table 6. Water fluxes, salinity and nutrient concentrations for the Mvoti and Nhlabane estuaries.

Quantity	*Mvoti Estuary*		*Nhlabane Estuary*	
	Value	**Data source**	*Value*	**Data source**
V_Q ($10^3\ m^3 d^{-1}$)	236	Runoff measured at gauging weir in the Mvoti River at Site 3 (Figure 1) during August 2000 (Mackay et al. 2000)	192	Average annual runoff in Nhlabane catchment (Quinn, 1999) but was not used in the budget calculation due to no water entering the estuary from the lake during the study period.
V_P ($10^3\ m^3 d^{-1}$)	0.5	Mean annual precipitation in Mvoti catchment (Chunnet et al. 1990; Mvoti IFR Starter Document 1996)	0.5	Average yearly rainfall in the Nhlabane catchment – Source R. Hattingh (Environmental Scientist, RBM).
V_E ($10^3\ m^3 d^{-1}$)	-0.8	Mean annual evaporation in Mvoti catchment (Mvoti IFR Starter Document 1996)	-0.4	Average yearly evaporation rates from the South African Weather Bureau as supplied by the Computing Center for Water Research (CCWR) for the Richards Bay coastal plain area.
V_G ($10^3\ m^3 d^{-1}$)	0.05	Ground water recharge for the Mvoti estuary subcatcment calculated as 30% of MAR in estuarine catchment. (Prof. B. Kelbe *pers. com*., Department of Hydrology, University of Zululand)	21	Ground water recharge calculated for the Nhlabane system (Quinn, 1999).
S_{ocn} (psu)	35.4	CSIR off-shore sampling – KwaZulu Natal coast	35.4	CSIR off-shore sampling
S_{syst} (psu)	0.5	The average salinity of four sites measured in the Mvoti estuary during August 2000 (Mackay et al. 2000).	8.8	This represents the average salinity of the outflowing surface layer measured at three sites between 1993 and 1996 (Vivier *et al.*, 1998).
DIP_Q, DIN_Q (ΔM)	4.5, 44	Six-week average of nutrients measured at Site 3 in the Mvoti river during August 2000 (Mackay et al. 2000).	2.1, 28	Nutrient concentrations measured in borehole samples from Lake Nhlabane catchment – Source R. Hattingh (Environmental Scientist, RBM).
DIP_{syst}, DIN_{syst} (ΔM)	7.1, 37	Six-week average of nutrients measured at Sites 4-7 in the Mvoti estuary during August 2000 (Mackay et al. 2000).	4.5, 84	Average of three sites in Nhlabane estuary monitored during 1993-1996 (Kemper, 1999).
DIP_{ocn}, DIN_{ocn} (ΔM)	0.3, 0.8	Since the mouth of the estuary was never completely flushed with fresh seawater it was necessary to use average nutrient data for the east coast of South Africa as contained in the Levitus 94 dataset of the Lanman-Doherty Environmental Observatory.	0.7, 2	Readings at Site 1 when completely flushed with fresh seawater.

Tabl e 7. Water fluxes, salinity and nutrient concentrations, and data sources for the Thukela and Mhlathuze estuaries.

Quantity	Thukela Estuary		Mhlathuze Estuary	
	Value	**Data source**	*Value*	**Data source**
V_Q ($10^3\ m^3d^{-1}$)	3,014	Average annual flow as measured at DWAF weir V5H002 for the period 1970-1996 presented by Roussouw and Claasen (1998) as reported by Archibald (1998b).	438	Average annual flow as measured at DWAF weir W1H032 for the period 1995-1998 (Cyrus et al. 2000).
V_P ($10^3\ m^3d^{-1}$)	1.64	Average yearly rainfall from the South African Weather Bureau as supplied by the Computing Center for Water Research (CCWR) for the Thukela catchment.	39	Average yearly rainfall from the South African Weather Bureau as supplied by the Computing Center for Water Research (CCWR) for the Mhlathuze catchment.
V_E ($10^3\ m^3d^{-1}$)	-2.14	Average yearly evaporation rates from the South African Weather Bureau as supplied by the Computing Center for Water Research (CCWR) for the Thukela catchment.	-42	Average yearly evaporation rates from the South African Weather Bureau as supplied by the Computing Center for Water Research (CCWR) for the Mhlathuze catchment.
V_G ($10^3\ m^3d^{-1}$)	0.08	Ground water recharge calculated for the Thukela catchment as approximately 5% of the mean annual precipitation.	12	Ground water recharge calculated for the Mhlathuze coastal plain as approximately 30% of the mean annual precipitation (Louw 1998).
S_{ocn} (psu)	35.4	CSIR off-shore sampling.	35.4	CSIR off-shore sampling.
S_{syst} (psu)	2.2	Average salinity of site 1 in surface when the mouth is open is opened. Monthly data from April 1997 to March 1998. This represents the average salinity of the outflowing surface layer.	34.5	Average salinity at all sites sampled at the surface when the mouth is open. Quarterly data from March 1996 to April 1998. This represents the average salinity of the outflowing surface layer (Cyrus et al. 2000).
DIP_Q, DIN_Q (ΔM)	0.9, 27	Average biweekly water quality data (1994-1998) from DWAF sampling site Weir V5H002 (Archibald, 1998)	0.7, 25	Monthly averages of six sites sampled in the lower reaches of the Mhlathuze River from 1996-1998 (Cyrus et al. 2000).
DIP_G, DIN_G (ΔM)		No data	1.0, 14	Bore-hole monitoring results from the Mhlathuze floodplain for the period 1986-2000 (Clean Stream, 2000).
DIP_{syst}, DIN_{syst} (ΔM)	5.5, 137	CRUZ monthly data from April 1997-March 1998 collected from 7 sites in the estuary and reported by Archibald (1998)	5.8, 14	Averages of five sites sampled in the Mhlathuze Estuary (Cyrus et al. 2000).
DIP_{ocn}, DIN_{ocn} (ΔM)	1.3, 2	Readings at Site 5 when completely flushed with fresh seawater.	0.1, 0.7	Readings at Site 3 when completely flushed with fresh seawater (Wepener and Vermeulen 1999).

Table 8. Data requirements and potential sources of data for calculating water, salinity and nutrient fluxes using the LOICZ mass balance model.

Quantity	Data source
System catchment area (m^2)	Available literature (Colloty, 2000) or computed using Cabaret software
System volume (m^3)	Available data or computed using Cabaret software
V_Q ($10^3\ m^3 d^{-1}$)	Average flow as measured at the most downstream DWAF weir for the particular river (DWAF Hydrological database)
V_P ($10^3\ m^3 d^{-1}$)	Average yearly rainfall from the South African Weather Bureau as supplied by the Computing Center for Water Research (CCWR) for the particular river catchment.
V_E ($10^3\ m^3 d^{-1}$)	Average yearly evaporation rates from the South African Weather Bureau as supplied by the Computing Center for Water Research (CCWR) for the particular catchment.
V_G ($10^3\ m^3 d^{-1}$)	Ground water recharge calculated for a particular geographical region (WR90 hydrological data base)
S_{ocn} (psu)	Average measured marine salinity.
S_{syst} (psu)	Average salinity measured in the estuary.
DIP_Q, DIN_Q (mM)	Averaged nutrients recorded by DWAF in the lower reaches of a particular rivers system (DWAF water quality database) or average measured nutrients.
DIP_{syst}, DIN_{syst} (mM)	Available data or in the case of no available data the weekly averages of nutrients recorded for at least eight consecutive weeks from a site in the particular estuary.
DIP_{ocn}, DIN_{ocn} (mM)	Available data or use the Levitus 94 dataset of the Lanman-Doherty Environmental Observatory.

Future changes in fluxes can be evaluated once a reference condition or present nutrient status condition has been calculated. Table 9 presents the proposed nutrient flux categories with corresponding conditions for nutrient fluxes. At present there is no scientific basis for the selection of the allowable deviation within each assessment class. This aspect needs to be considered in future.

To demonstrate the application of the technique described above, the data from the Mhlathuze Estuary (Table 7) were used as an example. The fluxes calculated in Section 4.2.3 were taken as the RC for the estuary and the hypothetical effect of a 20% reduction in riverine runoff was assessed on the water, salt and nutrient budgets. In this example the nutrient concentrations from all the sources (river, system and ocean) remained constant. A further hypothetical 100% increase in riverine input of DIN, without any changes in volume, was also assessed. These results are presented in Table 10.

Table 9. Assessment of nutrient status based on deviations of fluxes from the reference condition.

EWQII Nutrient flux category	**The median flux (water, salinity, DIN, DIP) should not differ from the Reference Condition (RC) by greater than:**
Natural	15%
Good	20%
Fair	30%
Poor	>40%

It must be borne in mind that this is a very crude example with only one input parameter changing. In a real-time situation the altered freshwater inflow would have an effect on the salinity of the system, the salt budget, mixing flux and nutrient load into the system. These changes can only be quantified with actual measurements of these parameters. The calculated flux values, based on the changed volume and concentration data are related to the RC in terms of a percentage deviation from the benchmark using the classification system given in Table 9. It becomes evident that changes in flow result in drastic changes in both the mixing flux (Δ21.8%) and the ΔDIN (Δ24%). This would place the Estuary in a **Fair** category with respect to mixing and nutrient fluxes. In contrast the doubling of the DIN from freshwater input only changes the DIN flux by 7.4%, resulting in the estuary remaining in the **Natural** category. It must once again be emphasized that in this example only one parameter was changed and the fluxes would be considerably different if all the other LOICZ modeling parameters were measured. However, this example does show that it is possible to use this relatively simple budget model to set benchmark flux conditions, and then assess any deviation from the RC in terms of awarding a EWQII category.

Table 10. The effect of changed water volumes and nutrient concentrations on the water, salt and nutrient budgets of the Mhlathuze Estuary.

Variable	Value	New flux values	New flux values
	RC	20% lower flow	Increased DIN
V_Q (10^3 m^3d^{-1})	438	350	438
V_P (10^3 m^3d^{-1})	39	39	39
V_E (10^3 m^3d^{-1})	-42	-42	-42
V_G (10^3 m^3d^{-1})	12	12	12
S_{ocn} (psu)	35.4	35.4	35.4
S_{syst} (psu)	34.5	34.5	34.5
DIP_Q, DIN_Q (µM)	0.7, 25	0.7, 25	0.7, 50
DIP_G, DIN_G (µM)	1.0, 14	1.0, 14	1.0, 14
DIP_{syst}, DIN_{syst} (µM)	5.8, 14	5.8, 14	5.8, 14
DIP_{ocn}, DIN_{ocn} (µM)	0.1, 0.7	0.1, 0.7	0.1, 0.7
V_X (10^6 psu-m^3d^{-1})	17,359	13,572	17,359
ΔDIP (10^3 M m^3d^{-1})	100	100	100
ΔDIN (10^3 M m^3d^{-1})	223	168.8	206

4.3 SPECIES SENSITIVITY DISTRIBUTIONS: AN APPRAISAL OF THE CONCEPTS, METHODS INCORPORATED AND THE APPLICATION OF THE TECHNIQUE.

4.3.1 General Introduction:

The possible threat of toxic compounds to ecosystems has elicited a request by society to science, to derive “safe” ambient concentrations of these compounds for the protection of ecosystems, and methods to assess ecological risks. Although this societal request is difficult to answer for many reasons, one major difficulty is the estimation of effects on diverse species and ecosystems (Posthuma et al. 2002). This is an appraisal of the development, concept, models implemented and the application of Species Sensitivity Distributions (SSDs) in ecotoxicology.

Different ecologists and ecotoxicologists independently designed ecotoxicological assessment systems based on the variance in response among species (Klapow and Lewis 1979, Mount 1982, Blanck 1984, McLaughlin and Taylor 1985, USEPA 1985, and Kooijman 1987). Interspecies variation in sensitivity to environmental pollutants is apparently not only a core problem, but also a basis for finding solutions (Posthuma et al. 2002).

4.3.2 Introduction to Species Sensitivity Distributions:

A SSD is a statistical distribution describing the variation among a set of species in toxicity of a certain compound or mixture. The species set may be composed of a species from a specific taxon, a selected species assemblage, or a natural community. Since we do not know the true distribution of toxicity endpoints, the SSD is estimated from a sample of toxicity data and visualised as a cumulative distribution function (Posthuma et al. 2002). The basic assumption of the SSD concept is that the sensitivities of a set of species can be described by a parametric or more rarely a nonparametric distribution function (Posthuma et al. 2002).

Because of clear deficiencies in the setting of environmental standards, SSD’s are increasingly recommended either to complement or replace the use of arbitrary assessment factors in the risk assessment of chemicals (OECD 1992 and Posthuma et al. 2002). The SSD approach, proposed in both North America by Stephan et al. (1985) and by Kooijman (1987) in Europe, involve fitting a statistical distribution to data obtained from many toxicity tests for a particular substance. At lower risk assessment tiers, this may involve selecting a threshold level that represents a safe concentration of the substance, which thereby protects most organisms (usually 95%) in an assemblage of species (Aldenberg and Slob 1993; Van Straalen and Denneman 1989, and Wagner and Lokke 1991). Most commonly, this safe level is specified in terms of a percentage p (usually 5%) of the assemblage that remains unprotected and is denoted by the abbreviation HCp (hazardous concentration percentile) (Grist et al. 2002). The SSD concept is now being incorporated into ecological risk assessment frameworks, particularly in North America and Europe (Posthuma et al. 2002), South Africa (e.g. O’Brien et al. 2004), Australia and New Zealand (ANZECC 2000a and b).

Origin and first use of SSD's

The first use of SSD's was in the National Water Quality Criteria by the U.S. Environmental Protection Agency. The use of expert judgement was replaced in 1978 with a formal method based on protection of a percentage of species (Mount 1982). The method for calculating criteria based on the 5^{th} percentile of SSD's (HC_5) was repeatedly revised until the establishment of the current U.S. EPA (1985) protection method, which is still in use (Posthuma et al. 2002).

Independently, Klapow and Lewis (1979) proposed a method for deriving marine water quality standards in California using the 10th percentile of empirical SSD's of LC_{50} values. However, California, like other state regulatory agencies in the United States, now follows the 1985 EPA method (Posthuma et al. 2002).

The use of statistical methods to support risk assessment of chemicals and the derivation of environmental quality criteria in Europe followed a course that, in hindsight, was quite independent from the developments in North America. This was because the earlier publications in North America were reports of the Environmental Protection Agency, which at that time were not widely distributed in Europe (U.S. EPA 1984; U.S. EPA 1985). Conversely, the first papers published by European authors were in journals that were not well known by North American scientists involved in environmental policy. In those days, the protection of the aquatic environment was a clear common goal of people working in the two fields. In the early 1990s the attention shifted toward other environmental compartments such as aquatic sediments and soils.

One of the earliest scientists systematically reporting on interspecies variability in sensitivity to toxicants was in Europe by Slooff (Slooff and Canton 1983; Slooff et al. 1983). The aim of Slooff's investigations was not so much to construct SSD's, but to compare the relative sensitivity of species considered as indicators of water quality (Posthuma et al. 2002).

In the Netherlands, the science-policy question about how to assess the risk of toxic chemicals for ecosystems was addressed by the Minister of Housing, Physical Planning and Environment to the Health Council. A scientific advisory body was established and in 1988 the Health Council published its advice, followed by an English translation in 1989 and this was implemented in a policy paper on risk management (VROM, 1989) and discussed in Parliament. Similar science-policy discussions and methodological developments took place in Denmark, Germany, and Spain. Several informal meetings were held in Europe, one of which was a meeting organized by the Commission of the European Communities in October 1990 (CEC 1990).

The period of independent development of SSD models and criteria ended in 1990 with an Organisation for Economic Cooperation and Development (OECD) workshop on extrapolation of laboratory aquatic toxicity data to the field (OECD 1992). The workshop brought North American assessors together with their counterparts from Europe and Australia. It originated the term *species sensitivity distribution* and recognized for the first time that SSD's are a class of ecological models and not simply a set of regulatory techniques. The workshop endorsed the EPA log-triangular method along with the log-logistic and lognormal methods of the Netherlands and Denmark, respectively. This result served to reinforce the confidence of the U.S. EPA in its method. The workshop also raised issues for research and consensus development concerning SSD's, which are still being considered (Posthuma et al. 2002).

After this workshop the methodology was implemented on a wider scale. In particular, risk assessment of the compound 'DTDMAC', a cationic surfactant used as fabric softener, contributed intensely to further discussion about the strength and weaknesses of the statistical extrapolation tools then implemented (Van Leeuwen et al. 1992). This stressed the need for further validation of the extrapolation methodology (Emans et al. 1993, Okkerman et al. 1993, and Van Leeuwen et al. 1994), which at the time was already applied in risk assessment and the derivation of environmental quality guidelines in the Netherlands (Posthuma et al. 2002).

Introduction to the concept of sensitive species

The use of species sensitivity distributions is based on the recognition that not all species are equally susceptible to toxicants. This trivial observation must have been commonplace knowledge to even the earliest toxicologists; however, a statistical treatment of toxicological data became possible only after systematic investigations were made with a large-scale comparison of species (Posthuma et al. 2002). Living organisms constitute a vast diversity of taxonomy, life history, physiology, morphology, behaviour and geographical distribution. In terms of ecotoxicology, these biological differences mean that different species respond differently to a compound at a given concentration (Posthuma et al. 2002). In retrospect, it is remarkable that little attention was paid to the reasons species would differ in their sensitivity to toxicants. Interspecies variability can be broken down into a series of factors namely (Slooff and Canton 1983, Slooff et al. 1983):

- Differences in uptake—elimination kinetics
- Differences in internal sequestering mechanisms
- Differences in biotransformation rates
- Differences in the nature or presence of the biochemical receptor
- Differences in the rate of receptor regeneration
- Differences in the efficiency of repair mechanisms

4.3.3 Species Sensitivity Distribution Models:

A SSD is a probabilistic model for the variation of the sensitivity of biological species for one particular toxicant or a set of toxicants. The toxicity endpoint considered may be acute or chronic in nature. The models are probabilistic in that in its basic form the species sensitivity data are only analysed with regard to their statistical variability. One way of applying SSDs is to protect laboratory or field species assemblages by estimating reasonable toxicant concentrations that are safe, and to assess the risk in situations where these concentrations do not conform to these objectives (Posthuma et al. 2002). This area of quantitative risk analysis is currently an active area of research, but mainly methods from classical statistics, such as bootstrap (Davidson and Hinkley 1997, Frey and Rhodes 1998) or maximum likelihood approach (Burnmaster and Wilson 1998) have been applied so far, with an emphasis on parametric analyses. Parametric bootstrapping and maximum likelihood methods were found to produce similar results (for sample sizes 5, 10 and 20) (Frey and Rhodes 1998). Jagoe and Newman (1997) compared the non-parametric bootstrapping (re-sampling) with the maximum likelihood method (assuming log-normal distributed data). The parametric method was found to be superior to the re-sampling, only in the case of log-normally distributed data. Newman et al. (2000) proposed non-parametric bootstrapping as the best technique (for sample sizes larger than 20) because no assumptions have to be made on underlying distributions. But, so far all these techniques together have not been compared for small data sets (e.g. sample size = 20 or less) (Verdonck *et al.* 2001).

Initially we address the question: What (statistical) population or data of a population is considered a sample? We want to protect communities, and the - on many occasions - implicit assumption is that the sample is *representative* for some target community, e.g., freshwater species, or freshwater species in some type of aquatic habitat. One may develop SSDs for species, genera, or other levels of taxonomic, target, or chemical-specific organization. This section investigates the statistical methods, which can be brought to bear on a set of single-species toxicity data, when that is the only information available (Posthuma et al. 2001).

The SSD model may be used in a forward or inverse sense, as previously stated. The focus in forward usage is the estimation of the proportion or fraction of species (potentially) affected at given concentration(s). Mathematically, forward usage employs some estimate of the cumulative distribution function (CDF) describing the toxicity data set. The fraction of species (potentially) affected (FA or PAF), or “risk,” is defined as the (estimated) proportion of species for which their sensitivity is exceeded. Inverse usage of the model amounts to the inverse application of the CDF to estimate quantiles (percentiles) of species sensitivities for some (usually low) given fraction of species not protected, e.g., 5%. In applications, these percentiles may be used to set ecological quality criteria, such as the hazardous concentration for 5% of the species (HC*5*) (Posthuma et al. 2002).

Toxicity data sets are usually quite small, however, especially for new chemicals. Samples below ten are not exceptional at all. Only for well-known substances, there may be tens of data points, but almost never more than, say, 120 sensitivity measures (Posthuma et al. 2002). For relatively large data sets, one may work with empirically determined quantiles and proportions, neglecting the error of the individual measurements. In the unusual case that the data set covers all species of the target community that is all there is to it. Almost always, however, the data set has to be regarded as a (representative) sample from a (hypothetical) larger set of species. If the data set is relatively large, statistical resampling techniques, e.g., bootstrapping yield a picture of the uncertainty of quantile and proportion estimates (Posthuma et al. 2002).

If the data set is small (fewer than 20), we have to resort to parametric techniques, and must assume that the selection of species is unbiased. If the species selection is biased, then parameters estimated from the sample species will also be biased. The usual parametric approach is to assume the underlying SSD model to be continuous, that is, the target community is considered as basically “infinite.” The ubiquitous line of attack is to assume some continuous statistical probability density function (PDF) over log concentration, e.g., the normal (Gaussian) PDF, in order to yield a mathematical description of the variation in sensitivity for the target community. These statistical distributions are on many occasions unimodal, i.e., has one peak. Then, the usual number of parameters to specify the distribution is not more than two or three. Data sets may not be homogeneous for various reasons, in which case the data may be subdivided into different (target) groups. Separate SSDs could be developed for each subgroup. One may also apply bi- or multimodal statistical distributions, called mixtures, to model heterogeneity in data sets (Aldenberg and Jaworska 1999). A mixture of two normal distributions employs five parameters (Posthuma et al. 2002).

The single-fit SSD estimation allows reconciliation of parameter estimation with the assessment of the fit through probability plotting and goodness-of-fit testing. There are several ways to estimate parameters of an assumed distribution. Moreover, the estimation of the parameters of the probabilistic model may not be the same thing as assessing the fit. We will use the ordinary sample statistics (mean and standard deviation) to estimate the parameters (Posthuma et al. 2001).

Graphical assessment of the fit may involve probability plotting. There are two major kinds of probability plots: CDF plots and quantile-quantile (Q-Q) plots (D'Agostino and Stephens 1986). The CDF plot is the most straightforward, intuitively, with the data on the horizontal axis and an estimate of the CDF on the vertical axis (the ECDF, empirical CDF, is the familiar staircase-shaped function). It turns out that the sensitive, and easily calculable Anderson-Darling goodness-of-fit test is consistent with ordinary CDF plots. In Q-Q plots, the data are placed on the *vertical* axis. One may employ plotting positions, now on the horizontal axis, that are tailored to a particular probability distribution, e.g., the normal distribution. The relationships between Q-Q plots and goodness-of-fit tests are quite complicated. Some well-known goodness-of-fit tests are used based on regression or correlation in a Q-Q plot (Posthuma et al. 2002).

In environmental toxicology, risk characterization employs plots of exposure concentration exceeding probability against fraction of species affected for a number of exposure concentrations. These so-called joint probability curves (JPCs) graphically depict the risk of a substance to the species in the SSD (Posthuma et al. 2001).

Aldenberg and Jaworska (2000) compared Bayesian and the maximum likelihood estimation method (MLE) approaches for the Gaussian (normal) model (for several sample sizes). Despite vastly different numerical schemes both approaches lead to identical answers. In practice, data sets on toxicity tests are scarce and if available often only at small sample sizes. As a consequence, Verdonck et al. (2001) raised the question: “Given a small sample size which technique/s is most suitable and which parametric or non-parametric distribution should be used?” This leads us to examine each parametric and non-parametric technique available (Verdonck et al. 2001):

Bootstrapping

A detailed description of the bootstrapping method can be found in literature (Efron and Tibshirani 1993, Davison and Hinkley 1997, and Cullen and Frey 1999). Given a data set of sample size *n,* the general approach in bootstrap simulation is to assume a non-parametric or parametric (e.g. lognormal, triangular, etc.) distribution which describes the quantity of interest, to perform *r* replications (e.g. *r* = 5000) of the original data set by randomly drawing, with replacement, *n* values, and then calculate *r* values of the statistic of interest. (Verdonck et al. 2001).

Different types of bootstrapping are available and have been assessed. Verdonck et al. (2001) assessed two non-parametric techniques, each with two different plotting systems for constructing an empirical cumulative distribution function, and one parametric technique (assuming the lognormal distribution). They included non-parametric and parametric techniques:

Non-parametric bootstrapping

One approach is to use the actual data set itself and to randomly select, with replacement, the actual values of the data set. This is sometimes referred to as re-sampling. The data can be represented via an empirical distribution function (EDF). A second approach is to fit an interpolated empirical cumulative distribution function to the data. Such a distribution has minimum and maximum values, which can be constrained by the minimum, and maximum values in the data set, or has to be determined explicitly. In the application of standard setting, zero can be considered as a minimum. (Verdonck et al. 2001).

Parametric bootstrapping

A third approach is to assume a parametric distribution rather than an empirical distribution. This approach is called parametric bootstrapping. Efron and Tibshirani (1993) discussed this method in detail. Each approach will lead to a different estimate of the confidence interval. Non-parametric or distribution-free approaches do not require assumptions regarding the probability model for the underlying population distribution. However, they also tend to yield wider confidence intervals than parametric methods do (Verdonck et al. 2001).

Maximum likelihood estimation method (MLE)

The general idea of MLE is to choose an estimator for the parameter(s) in a distribution (e.g. mean, 5th-percentile, etc.) so as to maximise the likelihood of the sample data. An ML-estimator can be thought of as an estimate for which the observed data are most ‘likely’. From a statistical point of view, the method of maximum likelihood is considered to be more robust (with some exceptions) and yields estimators with good statistical properties. In addition, they provide efficient methods for quantifying uncertainty through confidence bounds. Although the methodology for maximum likelihood estimation is simple, the implementation is mathematically intense. More information on the strengths of the MLE can be found in (Cullen and Frey 1999, and Verdonck et al. 2001).

Bayesian approaches

The Bayesian statistical method reverses the role of sample and model, the sample is fixed and unique, and the model itself is uncertain. This statistical viewpoint corresponds better to the practical situation the individual researcher is facing; there is only one sample and there are doubts what model to use, or, if the model is chosen, what values the parameters will take (Aldenberg and Jaworska 2000). If one assumes parameter values to be distributed, one has to presuppose a so-called (in this case a non-informative) prior distribution for the parameters, to specify the initial state of knowledge about them, before the data are used. The prior distribution is transformed into the so-called posterior distribution by multiplication with the classical likelihood function, by which the information in the data is introduced. This is essentially Bayes' theorem. The posterior distribution summarises our increase in knowledge about the parameters due to observing the data. A Bayesian simulation focuses on the evaluation of the joint posterior distribution of the parameters. For further technical details the reader is referred to (Box and Tiao 1973, Verdonck et al. 2001).

4.3.4 Application of SSD's in practice

The aim of a SSD analysis is to determine a chemical concentration protective of most species in the environment. Usually a point estimate known as the HC_5 (hazardous concentration for 5% of species), or the 95% protection level (Van Straalen and Van Rijn 1998) is calculated. This is a concentration that will exceed no more than 5% of species effects levels, usually based on chronic NOECs. It has been proposed that the lower confidence interval of the HC_5, possibly with an additional safety factor of up to 10, be used to derive predicted no effect concentrations (PNECs) for risk assessment (Feibicke and Ahlers 2001). SSDs are constructed using a cumulative plot of logarithmically transformed toxicity endpoints (e.g. NOECs or LC_{50}s) against rank assigned percentiles for each value to which a statistical distribution is fitted. In Europe and the United States this is typically a log-normal (Wagner and Lokke 1991) or log-logistic (Aldenberg and Slob 1993) model, whilst in Australia and New Zealand the Burr Type III method is used (Shao, 2000). From each of these models the HC_5 endpoint is extrapolated (Wheeler *et al.* 2002). Species sensitivity distributions are increasingly used in for example ecological risk assessment procedures (e.g. Solomon et al. 1996, Steen et al. 1999 and O'Brien et al. 2004) and formulation of water quality guidelines (ANZECC 2000a and b). This is because, when used correctly, they can introduce greater statistical confidence into risk assessent processes when compared to traditional quotient and assessment factor approaches. In Europe, risk assessment methods for new and existing chemicals are described in the technical guidance document (TGD) developed by the European Commission, the European Union member states and the European Chemical Industries (Crane et al. 2001). The TGD is currently under revision, and the inclusion of statistical extrapolation methods using SSD's is likely to be adopted (Posthuma et al. 2001).

To date most published ecological risk assessments using SSDs have centred on freshwater environments for which there is an abundance of good quality data, predominantly for pesticides (Solomon et al. 1996, Giesy et al. 1999, Campbell et al. 2000). There is generally less data available for saltwater species than for freshwater species, especially for organic compounds (e.g. Solbe et al. 1993), which presents fundamental problems when attempting to apply the SSD approach to ecological risk assessments for substances in marine environments (Leung et al. 2001).

Intensive discussions have taken place on principles, statistics, assumptions, data limitations and applications (e.g. Hopkin 1993, Forbes and Forbes 1993, Smith and Cairns 1993, Chapman et al. 1998, and Forbes and Calow 2002). Having originated in North America and Europe the use of SSDs has spread to for example South Africa (e.g., Roux et al. 1996 and O'Brien et al. 2004), Australia and New Zealand (ANZECC 2000a and b), and elsewhere. The concepts of SSDs are expanding both conceptually and technically (Posthuma et al. 2002).

Past Assessments of SSD's

An assessment of the use of SSDs in practice was undertaken by Forbes and Calow (2002), they reviewed the Hazard/Risk Assessment section of *Environmental Toxicology and Chemistry* Journal from volume 15 (1996) through to volume 20(3) (2001). This involved slightly more than 100 articles of which 14 employed a SSD approach. The aim of their study was not to carry out a comprehensive review of the use of SSD, but to draw attention to specific aspects implemented in the studies reviewed. For each of the 14 articles that they analysed the source of the data implemented in the study, the endpoints used, the chosen protection levels and related confidence limits, the sample size used, and the distribution that was assumed. Taking that into account they made the following generalisations:

- Data implemented in the studies were mainly taken from the Literature and not from the target community/ecosystem of interest. In other words, none of the distributions were based on the communities assessed, despite the fact that a number of studies had site-specific communities as targets of the risk assessment. We also noted that the species were generally selected to represent major trophic or taxonomic groups but that these were not represented in proportion to their abundance in actual systems. In some cases species from very different ecosystems (e.g. freshwater and marine) were combined into a single distribution. This means that all studies assessed did not take into account that the species used to construct the SSD should according to Forbes and Calow (2002) be an unbiased sample of the target group of species about which conclusions are to be drawn. In one case the relative risks for very different regions and habitat types were compared on the basis of the same SSD, despite the fact that the local species compositions would have differed greatly among sites (Cardwell *et al.* 1993). The SSD approach presumes that the sensitivity of a community depends on the sensitivity of the individual species of which it is composed.
- The effects represented in a single distribution were often based upon a variety of endpoints for different species going into the distribution, These are not all of the same

ecological relevance given differences in the life cycles of the species used (Forbes et al. 2001). This causes problems with regard to the assumption in SSD that the endpoint is ecologically relevant (Forbes and Calow 2002).

- A variety of distributions were employed and not always with rigorous justification, so as to raising questions with regard to the shape of the distribution being appropriate.
- The percentage of species chosen for protection was often 5 to 10%, although in some studies no 'acceptable' percentage was defined, but rather centiles were used to compare relative risks. In one case effects on up to 20% of species were considered as 'negligible risk' (Jones et al. 1999). Solomon et al. (2001) stated that any centile could in principle be used, 'provided that this measure can be validated against a knowledge and understanding of ecosystem structure and function or calibrated in tests conducted in microcosms or in the field'. Because the species going into the SSD mostly have been taken from the literature and not from an intact ecosystem, the relation between any distribution-derived protection level and ecosystem structure/function is arbitrary, and this raises questions under assumption of SSD (Forbes and Calow 2002) which states that the chosen level of protection is appropriate. We recognize that the risk quotients are based on the same data set of test species, but here the lack of precision in interpretation of the risk quotient is more obvious. Using an SSD to generate a precise probability statement that a certain fraction of species is likely to be affected by a chemical is only helpful to the risk assessment process to the extent that it is also accurate.
- Confidence limits around the effects threshold either could not be defined, were not defined, or if defined were specified somewhat arbitrarily. So this raises doubts about whether the assumption that chosen confidence limits around the protection level were appropriate, and even if it was, given the importance of this assumption on the outcome, it was rarely justified clearly enough.
- The a number of species used was generally greater than five and sometimes more than 50, but data were usually taken from databases and this, raises questions of relevance as already discussed above.
- In addition, in at least one instance, application factors were used to convert acute effects endpoints to chronic values for input into the distribution, which introduces the sources of uncertainty associated with the risk quotient approach into the SSD.

Improving the use of SSD's

Forbes and Calow (2002) offered some practical suggestions for improving implementation of the SSD approach to enhance transparency and reduce uncertainty in risk assessment. A summary these suggestions are presented below:

- The simplest and most transparent way to address the issue of appropriate sampling is to ensure that the risk assessment targets are defined such that they more accurately reflect the data on which they are based. Since an important use of SSD's is in comparative risk assessment (e.g., comparing risks of the same chemical among different sites, or comparing the relative risks among different chemicals for the same kinds of communities) an important priority for research should be an in-depth analysis of the consequences of species input selection on the resulting SSD.

- Endpoints for input into SSD's should be more rigorously chosen. When the assessment endpoint is the persistence of species populations, individual-level endpoints measured in ecotoxicological tests should be translated to likely population-level impacts and the resulting values used as input into the SSD (Calow et al. 1997, Akcakaya et al. 1999, Caswell 2001).
- Decisions about the fraction of species to protect should be based on considerations of the total number of species per taxonomic and/or functional group in the target system. The identity of the most sensitive species in the SSD should also be considered, and if there are indications that the left tail is biased toward certain taxa or functional groups, the 'acceptable' effects level could be adjusted downwards if necessary. In any case justification for the chosen protection level should be stated clearly and the uncertainty associated with the decision articulated.
- Although confidence limits can provide a useful measure of the statistical uncertainty in a sample parameter, there remain substantial biological uncertainties that may influence the distribution of species sensitivities, but not be reflected in the calculated parameters of an SSD. Therefore interpreting confidence limits for SSD's requires great care.
- As a general rule, data should not be assumed to follow a particular distribution without explicit justification, for example, provided by a goodness-of-fit test. However, recognising that the number of data points used to generate SSD's may be too small to place much confidence in lack-of-fit statistics, empirical distribution curves may be a more transparent alternative, provided that the original data points (and not just the fitted curve) are presented.
- Debate as to the minimum number of data points necessary to generate reasonable SSD's is ongoing (Newman et al. 2000). It seems that the issue of quantity has taken precedence over the issue of quality (i.e., appropriate endpoints measured in an appropriate sample of species), which is equally if not more important to reducing the uncertainty in effects assessment. The effect of adding more species to an SSD may depend on whether the added species represent a new taxonomic or functional group. If the species selected for input into an SSD are truly an unbiased random sample of the distribution of target species, then as the sample size increases the spread of the resulting SSD should decrease. However, if the additional species are intentionally chosen to represent new taxonomic or functional groups, then it is likely that the spread of the SSD will increase as more species are added. This is an important consideration given that the application of SSD's is meant to reduce uncertainty in the risk assessment process.

4.3.5 Conclusion

In conclusion it is evident that SSDs have been widely used in the ecotoxicological field, and more specifically SSDs have been adopted as a assessment technique in Ecological Risk Assessment. Species Sensitivity Distributions have been widely used in the establishment of water quality criteria and guidelines in industrialised democracies in North America and Europe primarily. The SSD approach has additionally been actively implemented in South Africa, Australia and New Zealand. Methods and approaches of SSD's are currently still being optimised and developed. The SSD approach is one of the leading approaches to facilitate Ecotoxicological, environmental management in the world.

4.4 INTERPRETATION OF ESTUARINE WATER QUALITY MODIFICATION BY INORGANIC AND ORGANIC TOXICANTS

The following variables were selected to form part of the EWQII: organic toxicants (Alachlor, Benzene, Chlordane, Chlorpyrifos, DDT, Dieldrin, Endosulfan, Lindane, Malathion, Phenol, Thiobencarb, Toluene and Total petroleum hydrocarbons.), neutral toxicants (ammonia, chlorine) and metallic toxicants (arsenic, cadmium, chromium, copper, cyanide, lead, mercury, tributhyl tin and zinc).

4.4.1 Requirements for quality of toxicity data

At the start of the revision process, the USEPA ECOTOX databases were accessed to obtain a consistent level of data quality (which included measured concentrations of chemicals, all conditions documented, water quality reported, species used, etc.). Forbes and Calow (2002) specifically caution against the indiscriminate use of toxicological data. These authors advise users of SSD techniques to screen the databases using predetermined criteria. Table 11 describes the characteristics of the criteria that were selected to delimit the laboratory ecotoxicological tests reported in the ECOTOX database. These were used as criteria to select the effect concentrations for each index variable. Because of clear deficiencies in the setting of environmental standards, SSDs are increasingly recommended either to complement or replace the use of arbitrary assessment factors in the risk assessment of chemicals. The data obtained from the USEPA databases were used as the basis for determining the SSDs of the selected toxicants. For the purposes of this report a single example, i.e. copper is used throughout. The following procedures were applied to all the variables listed in the previous paragraph.

Both LC_{50} and EC_{50} data were obtained using the criteria presented in Table 11. Chapman (1995) commented on the conceptual dichotomy that exists in the use of mortality-based toxicity test results as the basis for environmental standards. He does concede that acute-based toxicity results still provide the most reliable and reproducible results, and until a new innovative test is designed acute toxicity tests using standard test organisms will remain the "white laboratory rat" of aquatic toxicity assessment. It is for the aforementioned reasons that both chronic and acute toxicity data were selected to develop the SSD's. The data obtained for copper LC_{50} concentrations using this screening process are presented as an example (Figure 18). A total of 25 taxa were included for copper SSD assessment, which comprised of 12 invertebrate taxa and 13 fish families. It is important to note that only one endpoint value per taxon was used. In the cases where a number of studies have been conducted on the same species, the median of all the LC_{50} values was calculated and this single value was used in the development of the SSD.

4.4.2 Estimating protection concentrations using the SSD-approach

In recent years, statistical distribution methods for deriving guideline values have been developed that are based on calculations of a probability distribution of effects based on laboratory toxicity data and they attempt to calculate a pre-determined level of protection for a particular chemical, usually 95% of species (refer to section 4.3.3). There is a level of uncertainty associated with this derived figure, and some of the methods compute a figure with a given confidence level (e.g. again 95%), resulting in a guideline which in fact protects more than 95% of species. Such risk-based approaches allow for a degree of flexibility in both derivation and use of the guidelines and are consistent with principles of ecologically sustainable development.

The SSD's, proposed in both North America and Europe, involve fitting a statistical distribution to data obtained from many toxicity tests for a particular substance. At lower risk assessment tiers, this may involve selecting a threshold level that represents a safe concentration of the substance, which protects most organisms (usually 95%) in an assemblage of species. Most commonly, this safe level is specified in terms of a percentage (usually 5%) of the assemblage that remains unprotected and is denoted by the abbreviation HC*p* (hazardous concentration percentile). The SSD concept is now being incorporated formally into ecological risk assessment frameworks, particularly in North America (http://www.epa.gov/oppefed1/ecorisk).

Table 11. Criteria used to delimit the toxicological data in the USEPA ECOTOX database.

Data criteria	Criterion descriptor
Organism characteristics (primarily invertebrate and vertebrate data)	Only families or genera that also occur in the warm temperate and subtropical estuaries of South Africa were considered. In the case of fish taxa, particular emphasis was placed on selecting families with known estuarine dependence (Whitfield 1998).
Exposure duration	The exposure duration was similar for all the taxa for a given variable. For fish species a 96 hr exposure period was selected. If no 96 hr LC_{50} data were available for invertebrate taxa, the most prevalent exposure duration was selected (e.g. 24 and/or 48 hr exposure).
Exposure type	Static or static renewal bioassays.
Exposure medium	Estuarine and marine salinities 10 to 34 ‰.
Exposure chemical	In the case of metals, the same salt solution (e.g. copper chloride salts) and concentration reported as dissolved metal concentration.
Exposure conditions	Physical conditions (at least temperature and dissolved oxygen) must have been monitored and remained constant during the bioassay.
Endpoint	Acute lethal endpoints (i.e. 24-96 hr LC_{50}-concentrations) and chronic growth inhibition or reproductive impairment endpoints (i.e. 24-96 hr EC_{50}-concentrations) were selected. It was important to ensure that the exposure duration was similar for all the taxa for a given variable.

The SSD methodology offers a clear advantage over the traditional calculation of a PNEC. The PNEC is usually calculated by applying a safety factor to the statistical summary of a single toxicity test (e.g., 50%-effect concentration [EC_{50}] or no-observed-effect concentration [NOEC]). This toxicity test is selected by reviewing available toxicity data and discarding all but the most sensitive result. A safety factor may then be applied to produce a single value that is assumed to be highly conservative but that does not include any expression of uncertainty. In direct contrast, an SSD incorporates available toxicity effects data for a range of different species (albeit through standardization of collected data) and permits assemblage-level uncertainties to be estimated and expressed quantitatively based on the proportion of species impacted, to identify those taxa that are most at risk, and to estimate the costs and benefits to the environment of particular environmental standards and levels of protection.

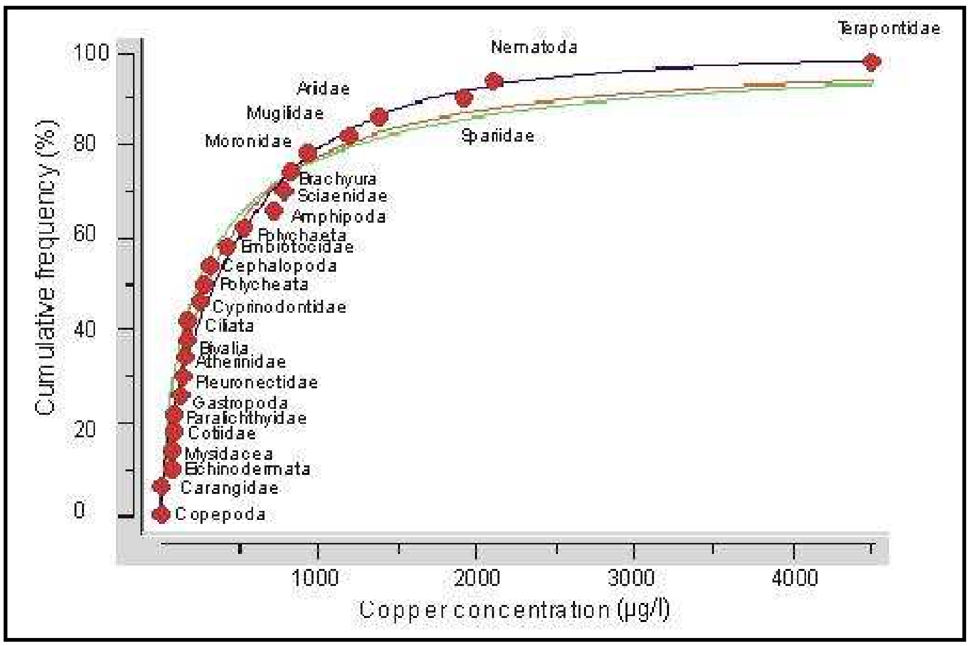

Figure 18. A plot of the SSD following acute exposure to copper.

The protecting concentrations for copper, HC*p*, were estimated by fitting the Burr Type III distribution to the LC_{50} and EC_{50} data. This was carried out by using BurrliOz software (CSIRO v I.0.14: Perth, Australia) (Campbell et al. 2000). A number of other distributions are fitted to the data, including the log-normal and log-logistic as these are familiar to environmental managers. However, in the software they are provided only as a reference and are not used for the estimation of protection concentrations.

The Burr III distribution is a very flexible three-parameter distribution, which can provide good approximations to many commonly used distributions such as the log-normal, log-triangular and Weibull (Shoa 2000). The cumulative distribution function for the Burr III distribution is:

$$F(x) = \frac{1}{\left[1+\left(\frac{b}{x}\right)^{c}\right]^{k}}$$

(Equation 7)

The three-parameters of the Burr III distribution, *b*, *c*, and *k* are estimated by maximum likelihood using the Nelder-Mead simplex algorithm, a derivative free optimisation technique. A feature of the Burr Type III distribution is that as some of the parameters tend to limiting values. The Burr Type III distribution tends to one of a set of limiting distribution (Shao 2000). For example, as $k \to \infty$ the Burr III distribution tends to the reciprocal Weibull distribution. As $c \to \infty$ the Burr III distribution tends to the reciprocal Pareto distribution. In practice, if *k* is estimated to be greater than 100 in a fit of the Burr distribution, then the parameter estimation is repeated, a reciprocal Weibull is fitted. Similarly if *c* is estimated to be greater than 80 then the reciprocal Pareto distribution is fitted. The user requires the concentration corresponding to the statement that "p% of the species should be protected if the concentration of the chemical is less than the estimated protecting concentration". Thus, for a given value for q, the protecting concentration is estimated from the Burr III distribution fit as:

$$\text{HC}p = \frac{b}{\left[\left(\frac{1}{1-q}\right)^{\frac{1}{k}}-1\right]^{\frac{1}{c}}}$$

(Equation 8)

Typical values for *p* are 80, 85, 90 or 95.

4.4.3 Estimating a confidence interval for the protection concentration

Unlike the estimation of the protection concentration, there is no theoretically derived equation for estimating the lower bound of a confidence interval (CI) about the protecting concentration estimate, though Shao (1998) showed that a delta method approximation works sometimes, particularly for large samples. Instead, a technique known as bootstrapping is used to estimate the lower bound of the CI. Bootstrapping is a standard statistical approach in situations where theoretical results are difficult to obtain, or require unrealistic assumptions (Efron and Tibshirani 1993). To perform the bootstrapping, a new dataset of the same size as the original dataset is created by selecting values from the original set at random, but with replacement. The HC*p* is estimated from this new dataset as above. This process is repeated many times. This gives a large set of estimates for the HC*p,* which, in essence, is a representation of the distribution of the HC*p*. The lower bound of a 90% confidence interval (for example) for the HC*p* can then be estimated by ordering all the HC*p* values and selecting the value that is ranked at 5%. It should be noted that the estimated lower bound to the CI is based on a random sampling method and will not be exactly the same if the bootstrap procedure is repeated. The copper data were subjected to curve-fitting techniques and Figure 19 indicates the data-fitting using standard log-normal and log-logistic distributions vs. Burr-type distribution. From Figure 19 it is clear that the Burr-type distribution provides the best fit of the data.

4.4.4 Sensitivity of the bootstrap estimation method

A set of data representing effects of salinity on freshwater species was submitted to the Burrlioz software and the resultant SSD curve is presented in Figure 20. Inspection of Figure 20 reveals a possible significant outlier data point at the tail of the distribution, at a very low concentration. Often, effects observed at low concentration of chemical stressor may be difficult to observe. In addition, it may be difficult to determine with sufficient accuracy what the analytical concentration of the stressor is at low values. It is considered a rule of thumb to place greater uncertainty on data obtained at low concentration values. It might thus be seen to be reasonable to remove this data point from the calculations.

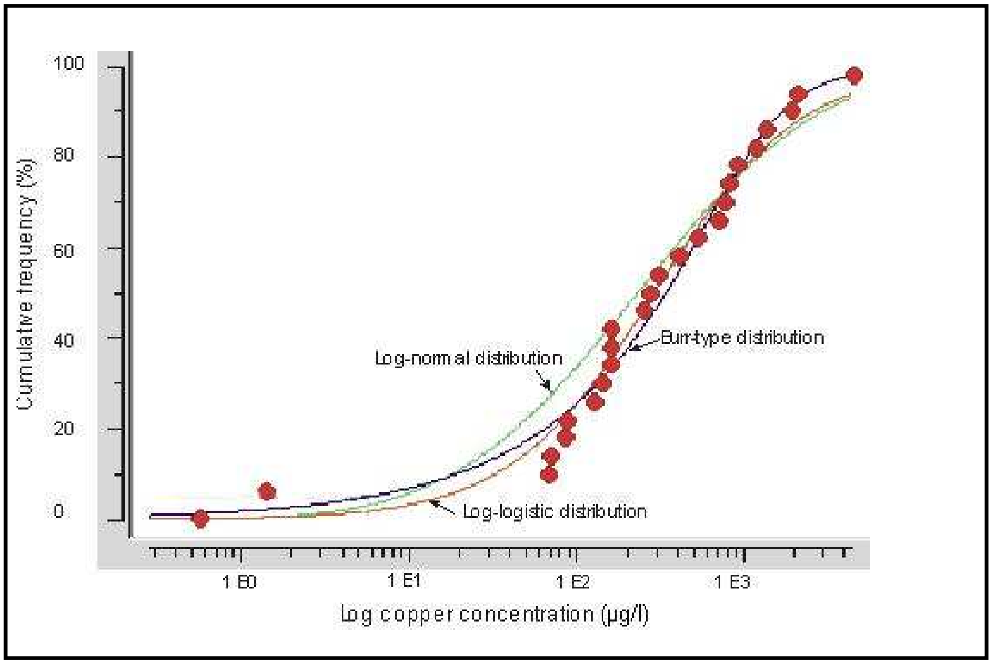

Figure 19. Cumulative distribution functions for the copper datasets (filled circles) based on log-normal, log-logistic and Burr-type distribution fitting using the Australian EPA software, BurrliOz. Data are for seawater acute toxicity 50% effect concentration (LC_{50}) endpoints for copper, n=25, extracted from the aquatic toxicity information retrieval (ECOTOX) database.

However, removal of the data point influences the calculations greatly (Figure 21). The HC5(50) changes from 1701 mg/l in the case of the full dataset, to 2466 mg/l NaCl in the case where the data is trimmed by one point – the possible outlier. This sensitivity to inclusion or deletion of "tail outliers" may be seen to be a potentially serious limitation of the application of this computational technique for estimating protecting concentrations.

The “bootstrap” technique used in Burrlioz is initially a simplex routine. The simplex routine is robust to numerical failure, but is not “intelligent” when faced with optimising a function when the response surface is highly wrinkled. It might be better to perform the Burr III optimization with a neural network (S Jooste, *pers. com*[2].).

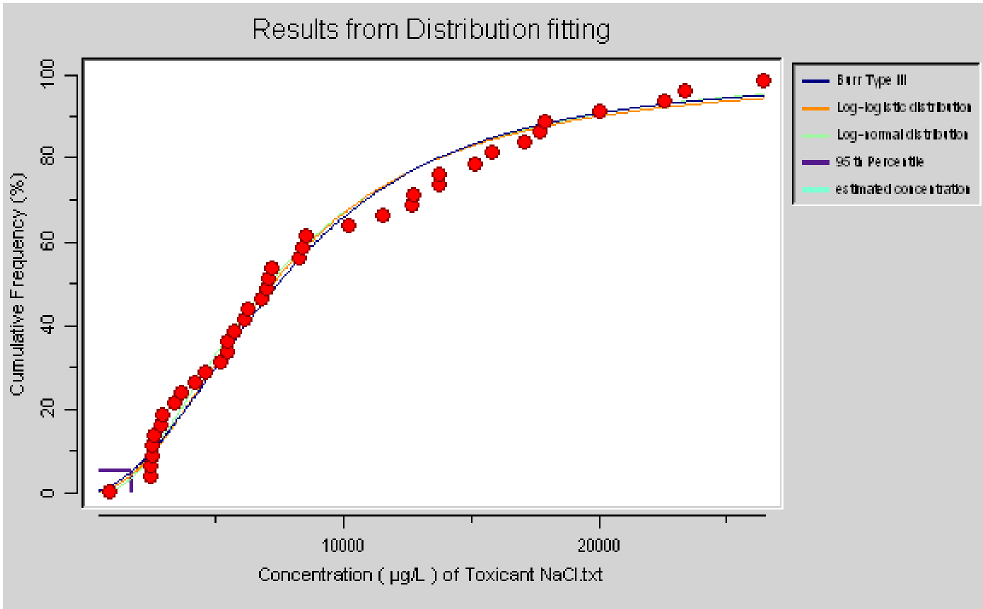

Figure 20. Bootstrap regression (501 replicates) applied to a sample SSD and HC*5*,50 was calculated through bootstrap regression with data superimposed (closed circles). Data are acute toxicity 50% effect concentration (LC_{50}) endpoints for Sodium Chloride, n=40, extracted from the aquatic toxicity information retrieval (ECOTOX) database. HC*5*(50) = 1701 mg/l.

4.4.5 Interpreting protection concentration in terms of an index or risk value

SSD models aim to account for unknown species sensitivities so will only be enhanced by larger datasets. In addition, risk assessments can combine a SSD with chemical exposure data or predicted exposures from simulation models. Therefore, the probability of exceeding an exposure estimate with an unacceptable adverse biological effect can be estimated. These probabilistic estimates of risk are a major strength of the SSD approach over the simpler assessment factor method. There are a number of issues that still need to be resolved before SSD methodologies can be fully integrated into current risk assessment frameworks. For regulatory purposes it is necessary to estimate a safe threshold that must account for the fact that the range of species for which toxicity data are available represents only a small proportion of those that may become exposed to the chemical. Threshold (the PNEC) is usually derived by applying assessment factors to the lowest effects concentrations from studies. But now that SSD

[2] Dr. Sebastian Jooste, Department of Water Affairs and Forestry.

models are used by some regulatory authorities, a new definition of PNEC, incorporating these probabilistic methods, needs to be developed. Should an HC*5* based on a minimum number of sensitive long-term toxicity tests be used as a PNEC or should the lower confidence limit of such an HC*5* be the PNEC? Another alternative is to apply a modest safety factor still to a HC*5* or its lower confidence limit to account for outstanding uncertainty. Ultimately, the answers to these questions will not be answered on theoretical grounds and it is therefore likely that political decisions about acceptable levels of precaution, combined with practical experiences in the use of SSD's, will decide the issue. In essence this decision has already been made for South Africa since the method followed in setting the water quality guidelines for the aquatic environment is based on protecting 95% of the species (Roux et al. 1996)

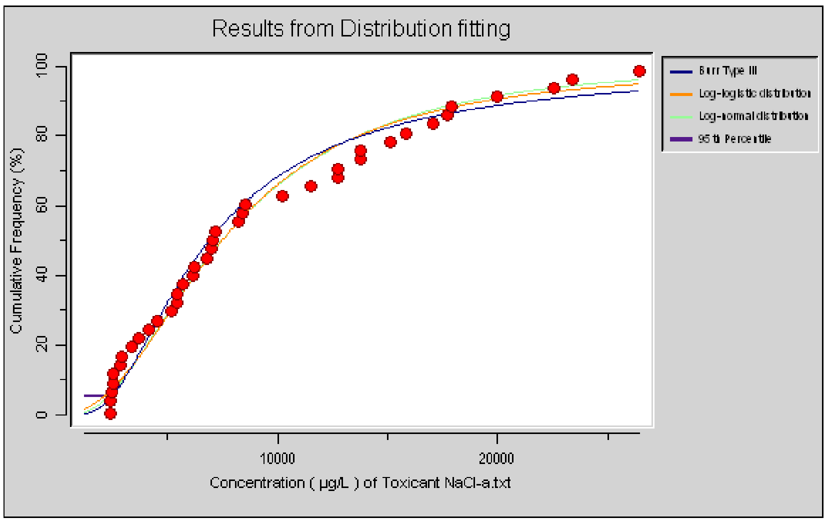

Figure 21: Bootstrap regression (501 replicates) applied to a sample SSD and HC*5*,50 was calculated through bootstrap regression with data superimposed (closed circles). Data are acute toxicity 50% effect concentration (LC50) endpoints for Sodium Chloride, n=39, extracted from the aquatic toxicity information retrieval (ECOTOX) database. HC*5*(50) = 2466 mg/l.

It is desirable that the level of protection is known at the start, before risk class values are derived or refined. The level of protection chosen for deriving the guideline trigger levels for the Australian and New Zealand water quality guidelines, was protection of 95% of species with a 95% level of certainty, at least where there were sufficient data to satisfy the requirements of the method. The Dutch use a 95% level of protection with 50% certainty (95,50), whereas the Danish suggests a 95,95 approach. There will always be the criticism that 95% level of protection may not protect normal ecosystem functions and also may not protect important or *keystone* species (ANZECC 2000a). This type of criticism can be leveled at any approach. It can be overcome by increasing the level of protection to 99% but this would markedly increase the level of uncertainty in the tail of the distribution.

For the development of the EWQII, HC*1* and HC*5* with varying levels of certainty were calculated for all the variables, using both the acute (LC_{50}) and chronic (EC_{50}) data sets. For the purposes of this project the EWQII categories (Table 1) were allocated percentile hazard concentrations (HC*p*'s), or conversely protection concentrations with different levels of certainty for each category. A brief summary of the selection of the different HC*p*'s and corresponding categories is given below:

- The 99% level with 50% certainty (HC*1,* 50) was selected to represent conditions in a **"Natural"** system.
- The 95% level of protection and between 75 and 95% certainty (HC*5* ,5-25) were chosen to represent a slightly modified system – **"Good"** system. A 95% level of protection, should be sufficient to protect the ecosystem provided keystone species are considered (it should be emphasised that increasing the certainty level from 50% to 95%, i.e. 95,95 results in a guideline value which, in practice, would actually protect considerably more than 95% of species in most cases and frequently over 99%).
- The 95% level of protection and between 50 and 75% certainty (HC*5*, 25-50) were chosen to represent a moderately modified system – **"Fair"** system.
- The 95% level of protection with less than 50% certainty (HC*5*,>50) was chosen to represent an unacceptably modified system – **"Poor"** system.

Once again the SSD based on the acute copper dataset is used to demonstrate the concepts outlined above (Figure22). These SSDs were developed for all of the toxicants listed under Section 3.6. The SSDs and their calculated hazard concentrations and levels of certainty associated with each category are presented in Table 12. From Table 12 it is evident that the number of data points used for the calculation of chronic-based toxicity data is much less than the data availability for acute-based data. As mentioned in Section 4.3.2 a non-parametric bootstrapping technique such as the Burr type III distribution is not suitable for datasets with n<20. Therefore the level of confidence in the chronic-based calculations (with the exception of cadmium and chromium) is low. This is a constraint that Leung et al. (2001) were also faced with. These authors then reverted to using the acute-based toxicity data and went even further by attempting to determine the relationship between saltwater toxicity and freshwater toxicity since the freshwater database is considerably larger than the saltwater database. Indeed according to Van den Brink et al. (2002) and Maltby et al. (2003) there is no theoretical reason why SSDs cannot be based on acute-effect data. For the purpose of the EWQII the SSD-derived concentrations with the largest sample size were used to allocate a category for each toxicant. In almost all cases the chronic-based HC*p*'s were based on less than 10 data points and therefore the acute-based HC*p*'s were used to derive the categories. It is only the categories for cadmium and chromium that were based on chronic HC*p*'s.

4.4.6 Calculation of Estuarine Water Quality Integrity Index and associated category

Based on the HC*p*'s derived from the individual SDDs, each water quality variable is assigned to a category. However, in order to calculate and derive a composite EWQII score, the individual category needs to be aggregated. This is achieved through the assignment of a rank value to each category (see Table 13 for HC*p*'s with associated hazard rank scores for the acute-based copper data example once again). Once categories have assigned to all 28 variables (25 toxicants and 3 nutrient budget fluxes), the hazard rank scores of the individual variables are used to calculate the composite EWQII score and associated category. The aggregation method, which is proposed, is the most commonly used aggregation formula in water quality indices, i.e. Solway's unweighted modified mean. The Solway weighted and unweighted sums have been suggested to be sensitive and without bias to changes in water quality variables throughout their range and is said to provide the "best" results for general water quality indexing (Richardson 1997).

$$I = \frac{1}{100}\left(\frac{1}{n}\sum_{i=1}^{n} q_i\right)^2$$

The resultant hazard rank value obtained is then reinterpreted in terms of an associated EWQII category as demonstrated in Table 14.

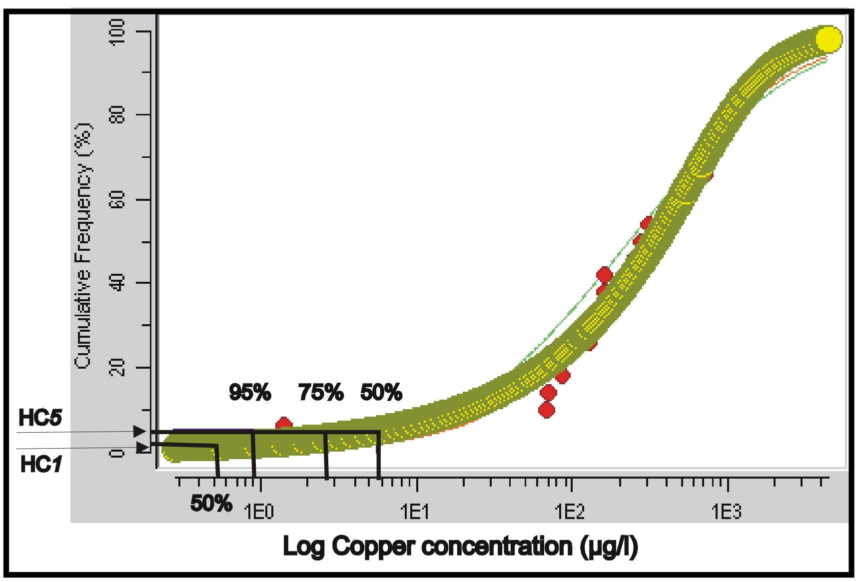

Figure 22. Bootstrap regression (501 replicates) applied to a sample SSD and 95% certainty for HC*1* and 5, 25 and 50% point-wise percentiles for HC*5* were calculated through bootstrap regression with data superimposed (closed circles). Data are seawater acute toxicity effect concentration (LC_{50}) endpoints for copper, n=25, extracted from the aquatic toxicity information retrieval (ECOTOX) database.

Table 12. Categories for the selected toxicants based on HC*p*'s at different levels of certainty, which were derived from SSD curves. The highlighted data for cadmium and chromium were the only chronic-based data used. All concentrations are in µg/l.

Assessment Class Hazard concentrations		Natural <HC*1* (50)	Good HC*5* (5-25)	Fair HC*5* (25-50)	Poor >HC*5* (50)	n
Ammonia	Acute	<682	683- 1009	1010 - 2097	> 2097	17
	Chronic	Not enough data available				
Arsenic	Acute	<37.6	37.7 – 76.8	76.9- 159.7	>159.7	8
	Chronic	Not enough data available				
Cadmium	Acute	<14.8	14.9 - 71.7	71.8 - 141.3	>141.3	56
	Chronic	<12.5	12.6 – 17.8	17.9 – 31.8	>31.8	33
Chlorine	Acute	< 6	6.1 - 12.4	12.5 - 19	>19	11
	Chronic	Not enough data available				
Chromium	Acute	< 3157	3158- 4543	4544- 6668	>6668	33
	Chronic	< 101.2	101.3 - 139.9	140 - 289.2	>289.2	13
Copper	Acute	< 39.6	39.7 - 56.3	56.4 – 64.7	>64.7	38
	Chronic	< 1.9	2 - 3.5	3.6 - 8.4	>8.4	12
Cyanide	Acute	<15.9	16 - 22.2	22.3 – 34.2	>34.2	5
	Chronic	Not enough data available				
Lead	Acute	< 287.6	287.7 - 419.1	419.2 - 498.3	>498.3	21
	Chronic	Not enough data available				
Mercury	Acute	<11.1	11.2 - 16	16.1 - 19	>19	44
	Chronic	<1.2	1.3 - 2.3	2.4 - 3.5	>3.5	7
Tributhyl tin	Acute	< 0.79	0.8 - 0.91	0.92 – 1.2	>1.2	16
	Chronic	< 0.02	0.021 - 0.03	0.031 – 0.11	>0.11	9
Zinc	Acute	<5	5.1 - 20.1	20.2 – 43.5	>43.5	37
	Chronic	<19.7	19.8 - 22.5	22.6 - 47	>47	5
Alaclor	Acute	<7.2	7.3 - 10	10.1 – 14.4	>14.4	6
	Chronic	Not enough data available				
Benzene	Acute	< 0.6	0.7 - 1.5	1.6 - 1.9	>1.9	42
	Chronic	< 0.06	0.07 - 0.17	0.18 - 0.3	> 0.3	5
Chlordane	Acute	< 0.4	0.41 - 0.7	0.71 - 1.9	>1.9	7
	Chronic	Not enough data available				
Chlorpyrifos	Acute	< 0.23	0.23 - 0.32	0.33 - 0.47	>0.47	14
	Chronic	< 0.01	0.01 - 0.03	0.03 - 0.01	0.01 - 0.03	7
DDT	Acute	< 0.3	0.03 - 0.37	0.37 - 0.52	0.52 - 0.63	29
	Chronic	Not enough data available				
Dieldrin	Acute	< 0.69	0.69 - 0.83	0.83 - 1.18	1.18 - 1.46	21
	Chronic	Not enough data available				
Endosulfan	Acute	< 0.04	0.041 - 0.07	0.071 – 0.1	>0.1	26
	Chronic	< 0.08	0.081 - 0.15	0.15 - 0.17	>0.17	6
Lindane	Acute	< 2.17	2.18 - 2.68	2.69 - 3.56	>3.56	29
	Chronic	Not enough data available				
Malathion	Acute	< 0.17	0.18 - 0.28	0.29 - 0.96	>0.96	26
	Chronic	< 0.53	0.54 - 0.81	0.82 - 1.2	>1.2	9
Phenol	Acute	< 22.79	22.8 - 41.1	41.2 - 137.3	>137.3	27
	Chronic	< 7.87	7.88 - 3.84	3.85 – 10.3	>10.3	6
Thiobencarb	Acute	< 217.4	218 - 270	271- 327	>327	7
	Chronic	Not enough data available				
Toluene	Acute	< 241	242 - 385	386 - 1320	>1320	9
	Chronic	Not enough data available				
Tph	Acute	< 14	14.1 – 34.6	34.7 – 51.8	>51.8	14
	Chronic	< 115	116 - 147	148 - 136	>136	6

Table 13. Description of HC*p*'s, Hazard Rank Score (HRS), catagories, hazard concentrations and perceived conditions for each Assessment Class. Hazard concentrations (in µg/l) for copper (HC) are presented as percentile species affected (p) with a certain percentage of certainty (e.g. HC5(50) represents 5% of species affected with a 50% degree of certainty). All concentrations are presented in µg/l.

HC*p*	**HRS**	**Category**	***Hazard concentrations associated with each category***	***Description of Perceived Conditions***
<HC*1* (50)	100	Natural	[Cu]<39.6	Unmodified, or approximates natural condition.
HC*5* (5-25)	75	Good	39.7<[Cu]<56.3	Largely natural with few modifications. Although the risk to the well-being and survival of especially intolerant biota, depending on the nature of the disturbance, at a very limited number of localities may be slightly higher than expected under natural conditions, the resilience and adaptability of biota has not been compromised
HC*5* (25-50)	50	Fair	56.4<[Cu]<64.7	Moderately modified. Risks to the well being and survival of intolerant biota depending on the nature of the disturbance may increase substantially with resulting low abundances and frequency of occurrence, and a reduction of resilience and adaptability at a large number of localities.
>HC*5* (50)	25	Poor	64.7<[Cu]	Largely modified. Risks to the well being and survival of intolerant biota depending on the nature of the disturbance increase substantially with resulting low abundances and frequency of occurrence, and a reduction of resilience and adaptability at a large number of localities.

Table 14. Description of hazard ranks and perceived conditions for each EWQII category. Final hazard rank is based on the aggregation of individual variable ranks using Solway's unweighted modified mean.

Hazard Rank	**Estaurine Water Quality Integrity Index Class**	***Description of Perceived Conditions***
76-100	Natural	Unmodified, or approximates natural condition.
51-75	Good	Largely natural with few modifications. Although the risk to the well-being and survival of especially intolerant biota, depending on the nature of the disturbance, at a very limited number of localities may be slightly higher than expected under natural conditions, the resilience and adaptability of biota has not been compromised
26-50	Fair	Moderately modified. Risks to the well-being and survival of intolerant biota depending on the nature of the disturbance may increase substantially with resulting low abundances and frequency of occurrence, and a reduction of resilience and adaptability at a large number of localities.
<25	Poor	Largely modified. Risks to the well-being and survival of intolerant biota depending on the nature of the disturbance increase substantially with resulting low abundances and frequency of occurrence, and a reduction of resilience and adaptability at a large number of localities.

4.4.6 Calculation of a EWQII score: Mhlathuze Estuary example

By way of an example the available metal concentration data for the Mhlathuze Estuary (Mzimela et al. 2003) were subjected to the SSD-HC*p* derived categories and EWQII categories were calculated for the metal toxicants (Table 15). The example used to demonstrate the use of the mass balance approach for nutrients was also subjected to this calculation. Individual EWQII scores were generated for each individual variable. The Solway unweighted arithmetic mean was calculated to derive a single EWQII category for the Mhlathuze Estuary. Based on the available water quality data the estuary can be classified as Fair to Good.

Table 15. An example of calculating the EWQII based on data from *Mzimela et al.* 2003[1] and the altered freshwater input volume in Section 4.2.5. All discrete toxicant concentrations are in µg/l, mixing flow (V_x) is in 10^6 psu-m^3 d^{-1} and nutrient fluxes are in 10^3 Mol m^3 d^{-1}.

Variable	Concentration	EWQII Class	HRS
Ammonia			
Arsenic			
Cadmium			
Chlorine			
Chromium	14[1]	Natural	100
Copper	58[1]	Fair	50
Cyanide			
Lead	236[1]	Natural	50
Mercury			
Tributhyl tin			
Zinc	68[1]	Poor	25
Alaclor			
Benzene			
Chlordane			
Chlorpyrifos			
DDT			
Dieldrin			
Endosulfan			
Lindane			
Malathion			
Phenol			
Thiobencarb			
Toluene			
Tph			
V_x –mixing flow	13,572 – Δ21% of RC	Fair	50
ΔDIN	168.8 - Δ24% of RC	Fair	50
ΔDIP	95.8 – 4.2% of RC	Natural	100
Final EWQII score and category		Fair-Good	46.1

5.0 DEVELOPMENT OF A DECISION SUPPORT SYSTEM (DSS)

5.1 SELECTION OF A SUITABLE DSS FORMAT

Many databases are available in an electronic format but are mostly incomplete for effective decision-making since they are not supported by tools that are able to create information from the available data. The use of the numerical tools to assist in management decision support is considered the principle method of providing the relevant information (Kelbe et al. 2001). However, all these tools (models) require data to drive their exogenous variables and to derive estimates of their endogenous variables (parameters). The Mhlathuze DSS developed by Kelbe et al. (2001) was developed to store, create and disseminate the information to general users through a suitable Graphical User Interface (GUI). The ICIS system developed by the CCWR (**http://www.ccwr.aqua.ac.za/icis/pamphlet.html**) has adopted a commercial GIS (ArcView) as the most suitable interface. The format of this DSS is user-friendly when accessed but setting it up and maintaining it requires high skills and is extremely labour intensive. Web-based and web-enabled DSS became feasible in about 1995 (Power, 2003). The Internet and Web have speeded-up developments in decision support and have provided a new means of capturing and documenting the development of knowledge in this area.

Many web-based models are developed using Hypertext Markup Language (HTML), which is used in the development of Internet web pages. HTML, click-able diagrams, Java, and JavaScripts may be used to develop an interlinked/cross-linked hierarchy of text and figures (Kidder and Harris 1997). According to Graz (2003) there are many advantages to developing and HTML-based DSS:

- Stepwise refinement may be implemented almost boundlessly, while retaining simple diagrammatic presentation.
- The model may be accessed using standard Internet web browsers, making it a useful teaching tool. Students, managers, and community leaders may browse through different components and levels of complexity on their own, backtracking to previous screens as desired.
- The various components of the model may be revised and updated individually at a central point. The various sections of the model are stored in separate HTML documents that are linked to a parent document using uniform resource locators (URL). Each of the sub-documents, in turn, may act as parent document for further refinement. Similar to the implementation of hyperlinks on the Internet, many documents may point to one parent; conversely, a single document may point to many parent or child documents. The various child documents may also cross-reference one another.
- The structure of the HTML documents makes the model more widely and consistently accessible.

- Access to the knowledge base is facilitated through a web browser rather than through sophisticated software and this is of particular importance in a society where people are computer literate, but have only limited numerical skills.
- It does not need to remain simple since where communication technology and browser software permit HTML, JavaScript, Java, and XML may provide additional tools in structuring knowledge and making it readily accessible to a wide variety of users.
-

5.2 INCLUSION AND INTEGRATION OF EXISTING ESTUARINE INDICES AND MODELS IN THE DSS

Consequently, there is a need to determine a suite of methods and models which are required in the EWQII to provide the information needs for the classification of estuaries based on water quality integrity. This is an ongoing process in, which some of the information requirements described above have been identified. An assessment of available published estuarine indices developed in South Africa revealed that only one water quality index (eWQI - Harrison et al. 2000) exists. This index only uses three water quality variables (i.e. oxygen adsorbed, ammonia and chl a) against, which the health of estuarine organisms are measured while the rest of the variables represent an indication of aesthetic quality. Since one of the variables used by Harrison *et al.* (2000) is incorporated into the EWQII (i.e. unionized ammonia), it was felt that it was not necessary to include the calculation of eWQI scores in the DSS. However, the available eWQI scores for all estuaries are included in the DSS. Other tools such as the Cabaret and BurliOz Software that are used to develop the nutrient mass balance model and SSD's, respectively is also accessible through the DSS.

All the other available estuarine indices relate to physical aspects (i.e. Whitfield's physical classification - Whitfield 1992; Zonal-type rarity score – Turpie et al. 2002), habitat (Habitat rarity score – Turpie et al. 2002), biodiversity (Biodiversity importance index – Turpie et al. 2002 taking into account the following indices: Botanical importance rating - Colloty et al. 2000; Fish – Maree et al. 2000 and Harrison et al. 2000; Bird abundance – Turpie 1995). These indices, together with the weighted size, were used to calculate an Estuarine Importance Score (EIS) for each estuary. Based on the EIS, each estuary was allocated an Estuarine Reserve Class (ERC) as part of the RDM process in estuaries. The ERC is allocated on the basis of the estuary's importance score, using the present ecological status as a starting point (Turpie *et al.* 2002). Since, the calculation of the ERC does not take water quality into account the development of the current EWQII Assessment Class will enhance the reserve class set by the ecological status-derived ERC. For the purposes of the SSD development, the individual index scores (physical, habitat and biodiversity indices) as well as the derived EIS and ERC will be included. It is important to note that it is not intended that the software will calculate the above mentioned scores – they will merely be listed in a window in order to contribute towards and enhance the decision support function of the EWQII. A function will be provided to allow for changing of these indices in the event of the scores being revised.

6.0 GENERAL CONCLUSIONS AND RECOMMENDATIONS

6.1 CONCLUSIONS

The recognition of the importance of including a rating scheme for estuarine water quality requirements, that may be used in decision making and setting of management objectives has been recognised. Since estuaries are also subjected to the requirements of the NWA, methods need to be developed to determine the Ecological Reserve. A number of methods in the form of estuarine indices have been developed over the past decade to address the Ecological Reserve requirements. However all these estuarine assessment indices have concentrated mainly on physical and biological characteristics only.

A major objective of this project was therefore to develop an estuarine water quality classification system that assesses the integrity of the system based on the measured water quality parameters (*viz*. Estuarine Water Quality Integrity Index - EWQII). The regulatory endpoint is the the maintenance of ecological integrity in the face of adversity, with the conditions for each category in the Ecological Reserve Assessment process expressed in terms of the "risk to the well-being of biota". It is the formulation of these categories in terms of "likelihood" that allows for the application of a risk-based approach to classifying estuaries into categories based on water quality. However there is still some confusion as to what uniform classification system is to be applied to data. The classification system of water resource management in South Africa currently in use varies from resources that are extremely impacted (class E or F) to those that are largely natural (class A). However, for the purposes of this report, the classification system for the variables contained in the EWQII was expressed in the form of categories ranging from Natural to Poor, similar to the RHP classification system.

Selection of water quality variables for inclusion in the EWQII

An extensive survey of available literature on water quality classification systems was undertaken to determine, which classification system would be the most suitable for the EWQII and, which water quality variables would be most suitable for inclusion in the EWQII. There was a distinct difference in the ranking of water quality variables based on their importance between estuaries and freshwater systems. Emphasis in most WQIs appears to be on organic loading, with very little attention paid to other forms of pollution. Indeed the eWQI used by Harrison et al. (2000) contained only three variables that reflected biotic responses to water quality (in the form of a stressor-response relationship), i.e. ammonia, DO and AO.

The lack of information on the stressor-response relationships between estuarine organisms and water quality variables is most probably related to the unique physicochemical environment, primarily because of their variable salinity but also because of their strong gradients in other parameters, such as temperature, pH, dissolved oxygen, redox potential, and amount and composition of particles. Since the main aim of the project was to interpret estuarine integrity in terms of water quality, implying chemical constituents, the following variables were selected for inclusion in the EWQII:

- Salinity
- Organic loading (nitrogenous compounds and phosphate)
- Toxicants (trace metals, ammonium, chlorine and organics)

Transformation of water quality variables

The purpose of variable transformation is to eliminate concentration units to produce a dimensionless scale with two end-points, defined by acceptable and unacceptable limits within a range on an ordinate scale. There are a number of different methods of variable transformation. The most common of these is rating curves, which may be based on either empirical information or environmental standards.

Salinity

The conclusion of the literature survey and the mathematical analysis is that at this stage it is extremely difficult to predict the impact on an estuarine ecosystem, based on hypothesised modifications of salinity regimes, and using the current tools of ecotoxicology. There is simply not enough currently known about the structure of estuarine communities, and the relationship between this structure and macro-variables such as temperature, pH, dissolved oxygen, redox potential, amount and composition of particles, and specific chemical impacts. It is hypothesised that a promising classification system in terms of salinity may be based directly on the distribution of estuarine fauna or functional groups ("optimal assemblage") that one expects in an unmodified estuary of a particular type.

Nutrient status

No rating curves based on international standards for nutrients such as the Australian guidelines were adopted in the index since virtually all of South Africa's estuaries would be classified as eutrophic. A more suitable approach to assessing nutrients in relation to ecosystem integrity is through compiling a nutrient mass balance for an ecosystem, which can often help to identify major sources and sinks of nutrients. A mass balance represents all of the nutrients already present (i.e. water, sediments and biota) plus inputs, less the outputs (i.e. outflows & harvested biota like fish); what is left equals the internal load. Once the internal load is quantified, the external and internal processes which influence the load (e.g. biogeochemical cycling, primary production, etc.) can be identified. A relatively simple budget model developed by LOICZ Programme of the United Nations provides both robust estimates of the flux across the coastal zone boundaries and long-term, integrated biogeochemical performance of the entire system.
Formulation and computation of the index score

Interpretation of estuarine water quality modification by discrete chemical discharges

For the development of the EWQII, SSD curves provided HC*1* and HC*5* values with varying levels of certainty. These plots were calculated for all the variables, using both the acute (LC_{50}) and chronic (EC_{50}) data sets. For the purposes of this project the categories presented in

Table 1 were allocated percentile hazard concentrations (HC*p*'s), or conversely protection concentrations with different levels of certainty for each class.

Formulation and computation of the index score

Many authors regard this process as the most important step in WQI design, due to the potential for loss of information. The Solway unweighted aggregation formula was selected as aggregation formula in this study. The composite EWQII score is derived by aggregating the individual categories obtained for each variable. This is achieved through the assignment of a rank value to each class. Once Assessment Classes have assigned to all 28 variables (25 toxicants and 3 nutrient budget fluxes), the hazard rank scores of the individual variables are used to calculate the composite EWQII score and then reinterpreted in terms of an associated EWQII category.

Incorporation of the EWQII into a DSS

The use of the numerical tools to assist in management decision support is considered the principle method of providing the relevant information. However, all these tools (models) require data to drive their exogenous variables and to derive estimates of their endogenous variables (parameters). A DSS can assist in storing, developing, creating and disseminating the information to general users through a suitable Graphical User Interface. The platform selected for the EWQII DSS is a web-based shell in HTML and Java-Script. The major advantage of this GUI is that it is readily accessible to a wide range of users. The DSS contains links to the software programmes used to calculate the EWQII, nutrient mass balance model and SSD. In addition information on a number of estuarine indices for each estuary is provided.

6.2 RECOMMENDATIONS FOR FUTURE RESEARCH

- The implementation of the concept of "optimum" assemblages that represent particular types of estuaries particularly in relation to responses to natural variable parameters such as salinity. Implementation of this function in a management context will entail: a) Classification of morphologically distinct estuaries (which is already available); b) determination of assemblage status (in terms of proportions of species or functional groups) in these estuaries; c) determining the "keystoneness" of the species or functional groups; and d) Assigning classes based on $\Delta_{\text{assemblage}}$ calculated from $\Delta_{assemblage} = \sum_i a_i \left| z_i - z_{opt,i} \right|$.
- The EWQII Assessment Class classification system for nutrients is not based on any scientific basis. The relevance and applicability of the different Assessment classes need to be verified.

- A major stumbling block in the application of the LOICZ mass balance model is the paucity of water quality data for estuaries in South Africa. A National Estuarine Water Quality Monitoring Programme should be initiated.
- The “bootstrap” technique used in Burrlioz is initially a simplex routine. The simplex routine is robust to numerical failure, but is not “intelligent” when faced with optimising a function when the response surface is highly wrinkled. Research should be undertaken to study the Burr III optimization with a neural network.

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