

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 databases (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 water 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, tributyl 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:

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

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 there 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, tributyl 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 (HC5,>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 HCp’s with associated hazard rank scores for the acute-based copper data example once again). Once categories 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 $\Delta_{\text{assemblage}}$ calculated from
$$\Delta_{\text{assemblage}} = \sum_i a_i |z_i - z_{\text{opt},i}|.$$
- 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.