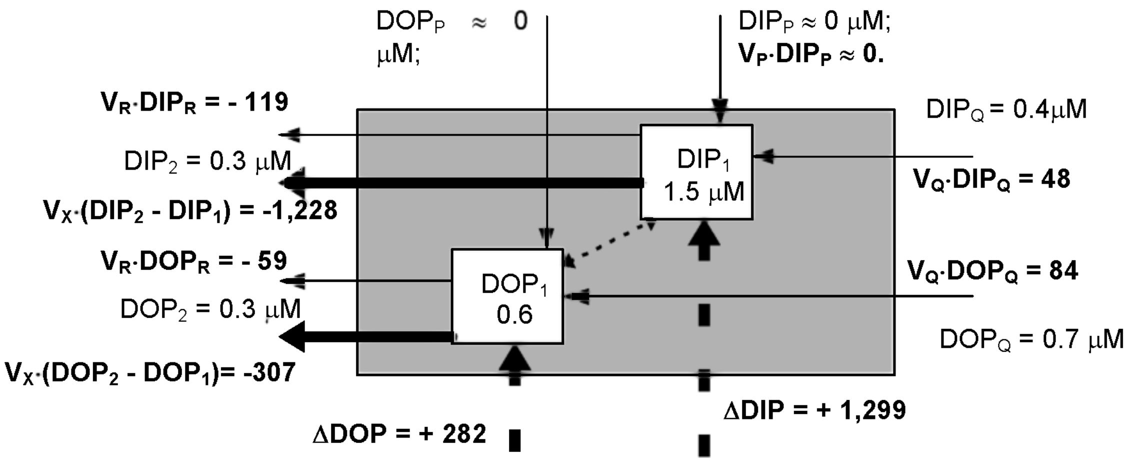
Land-Ocean Interactions in the Coastal Zone (LOICZ)

CORE PROJECT OF THE
INTERNATIONAL GEOSPHERE-BIOSPHERE PROGRAMME: A STUDY OF GLOBAL CHANGE (IGBP)
OF THE INTERNATIONAL COUNCIL OF SCIENTIFIC UNIONS



LOICZ BIOGEOCHEMICAL Modelling Guidelines

D.C. GORDON, JR., P.R. BOUDREAU, K.H. MANN, J.-E. ONG, W.L. SILVERT, S.V. SMITH, G. WATTAYAKORN,
F. WULFF AND T. YANAGI

LOICZ REPORTS & STUDIES NO. 5

LOICZ BIOGEOCHEMICAL Modelling Guidelines

D.C. GORDON, JR.
BEDFORD INSTITUTE OF OCEANOGRAPHY, DARTMOUTH, CANADA.

P.R. BOUDREAU
LOICZ CORE PROJECT OFFICE, TEXEL, THE NETHERLANDS.

K.H. MANN
BEDFORD INSTITUTE OF OCEANOGRAPHY, DARTMOUTH, CANADA.

J.-E. ONG
UNIVERSITI SAINS MALAYSIA, PENANG, MALAYSIA.

W.L. SILVERT
BEDFORD INSTITUTE OF OCEANOGRAPHY, DARTMOUTH, CANADA.

S.V. SMITH
UNIVERSITY OF HAWAII, HONOLULU, UNITED STATES.

G. WATTAYAKORN
CHULALONGKORN UNIVERSITY, BANGKOK, THAILAND.

F. WULFF
STOCKHOLM UNIVERSITY, STOCKHOLM, SWEDEN.

T. YANAGI
EHIME UNIVERSITY, MATSUYAMA, JAPAN.

LOICZ REPORTS & STUDIES No. 5

PUBLISHED IN THE NETHERLANDS, 1996 BY:
LOICZ CORE PROJECT
NETHERLANDS INSTITUTE FOR SEA RESEARCH
P.O. BOX 59
1790 AB DEN BURG - TEXEL
THE NETHERLANDS

THE LAND-OCEAN INTERACTIONS IN THE COASTAL ZONE PROJECT IS A CORE PROJECT OF THE "INTERNATIONAL GEOSPHERE-BIOSPHERE PROGRAMME: A STUDY OF GLOBAL CHANGE", OF THE INTERNATIONAL COUNCIL OF SCIENTIFIC UNIONS.

THE LOICZ CORE PROJECT IS FINANCIALLY SUPPORTED THROUGH THE NETHERLANDS ORGANISATION FOR SCIENTIFIC RESEARCH BY: THE MINISTRY OF EDUCATION, CULTURE AND SCIENCE; THE MINISTRY OF TRANSPORT, PUBLIC WORKS AND WATER MANAGEMENT; THE MINISTRY OF HOUSING, PLANNING AND ENVIRONMENT; AND THE MINISTRY OF AGRICULTURE, NATURE MANAGEMENT AND FISHERIES OF THE NETHERLANDS, AS WELL AS THE ROYAL NETHERLANDS ACADEMY OF SCIENCES, AND THE NETHERLANDS INSTITUTE FOR SEA RESEARCH.

CITATION: **D.C. GORDON, JR., P.R. BOUDREAU, K.H. MANN, J.-E. ONG, W.L. SILVERT, S.V. SMITH, G. WATTAYAKORN, F. WULFF AND T. YANAGI. 1996*. LOICZ BIOGEOCHEMICAL MODELLING GUIDELINES.* LOICZ/R&S/95-5, VI +96 PP. LOICZ, TEXEL, THE NETHERLANDS.**

ISSN: **1383-4304**

COVER: **PHOSPORUS BUDGET FOR KLONG LAD KHAO KHAO, THAILAND.**

THE LOICZ REPORTS AND STUDIES SERIES IS PUBLISHED AND DISTRIBUTED FREE OF CHARGE TO SCIENTISTS INVOLVED IN GLOBAL CHANGE RESEARCH IN COASTAL AREAS.

TABLE OF CONTENTS

PAGE

TEXT BOXES

TABLES

FIGURES

PREFACE

One of the central concerns of the "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.

To achieve such an understanding will require the compilation of the results from local and site-specific research, together with regional and wider scale approaches to understanding the flux of materials and energy in coastal systems. Modelling of carbon, nitrogen and phosphorus in such systems is therefore a necessary requirement for meeting the overall goals and objectives of LOICZ. To ensure comparability and compatibility of the results of local and national research and to allow the up-scaling required to develop regional and global scenarios of change in coastal areas will require the adoption of similar approaches to the collection of empirical data and to the estimation of budgets and fluxes in the world's coastal areas. As presented in the LOICZ Implementation Plan (Pernetta and Milliman, 1995), the framework activities of LOICZ, co-ordinated through the Core Project Office located in the Netherlands, include the development of a strong modelling component within the LOICZ research agenda and the provision of methods, standards and protocols for the conduct of LOICZ research.

The biogeochemical modelling guidelines presented in this document represent the consensus views of the LOICZ Scientific Steering Committee concerning the best available approaches which can be adopted to provide estimates of the role of coastal areas as sources and/or sinks of carbon, nitrogen and phosphorus. This document has been developed from an initial consideration of alternative modelling approaches conducted during a one day workshop held in conjunction with the "International Symposium on Global Fluxes of Carbon and its Related Substances in the Coastal Sea-Ocean-Atmosphere System" in Sapporo, Japan, during November 1994. This workshop (LOICZ, 1994) helped to identify the overall approach which could be used in the framework of LOICZ biogeochemical modelling. This framework was presented at the second LOICZ Open Science Meeting, held in Manila, The Philippines, during April 1995, for initial review and discussion (LOICZ, 1995a) and the proposal for developing guidelines for biogeochemical modelling within LOICZ was well supported.

Accordingly, during the summer of 1995 members of the LOICZ Scientific Steering Committee, assisted by other experts, contributed ideas and text which were compiled into an initial draft. This draft was presented to a small workshop convened by Dr. D. Gordon on behalf of LOICZ and hosted by the Bedford Institute of Oceanography in Dartmouth, Canada, in September 1995. During this workshop (LOICZ, 1995b), the draft document was reviewed and extensively rewritten. In October 1995, the revised document was despatched to selected experts for critical review and comments. At the same time, it was also sent to scientists participating in the SARCS/WOTRO/LOICZ Core Project being conducted in Southeast Asia. During early December 1995, the draft guidelines were thoroughly reviewed and tested at the SARCS/WOTRO/LOICZ Workshop on Biogeochemical Modelling which was held at the Centre for Marine and Coastal Studies, Universiti Sains Malaysia, Malaysia (LOICZ, 1995c). Participating scientists came from Australia, Brunei, Canada, Indonesia, Malaysia, The Netherlands, Philippines, Singapore, Sweden, Taiwan Thailand, Vietnam and United States.

All feedback on the draft guidelines received before the end of December 1995 was considered and used by the LOICZ Scientific Steering Committee and Core Project Office to prepare the final draft in early in 1996. It is hoped that through the application of the approaches outlined in this document to a wide enough spectrum of coastal sites and regions, our understanding of the role of the coastal system in global biogeochemical cycling will be improved.

EXECUTIVE SUMMARY

One of the long term objectives of LOICZ is to develop improved numerical models that describe the dynamics of biogeochemically important elements in the coastal zone at regional and global scales. To do so requires the development of common and consistent modelling approaches that can produce outputs at the local scale that can be integrated into larger-scale regional and global syntheses. These modelling guidelines have been developed by LOICZ for use by participating scientists in planning and conducting their research on a local scale in support of the broader regional and global syntheses.

This document presents recommended guidelines for initiating the development of carbon, nitrogen and phosphorus (CNP) models of the coastal zone. They have been developed as a LOICZ framework activity through a series of international workshops and represent the consensus of participating scientists. These guidelines can be used to develop models for specific coastal areas using either existing data, or data that will be collected as part of new field programmes. The guidelines are purposefully written so as to provide the information needed by scientists who wish to participate in LOICZ biogeochemical modelling but who have no or limited previous modelling experience. General background information is provided on the philosophy of modelling and different kinds of models are briefly reviewed. Numerous references provide an entry into the scientific literature on numerical modelling. In addition, the recommended procedures are described in considerable detail and illustrated by numerous case studies from representative coastal systems around the world.

From a LOICZ perspective, CNP models must consider both the current fluxes of these biogeochemically important elements in the world's coastal zone and how these fluxes might change in the future due to environmental change. In general, potential approaches for modelling the dynamics of carbon, nitrogen and phosphorus in the coastal zone range, from relatively simple budgets of boundary fluxes for specific elements, to detailed system simulation models which contain a large number of variables and processes. The data and resource requirements vary markedly along this gradient. Simple budgets require a relatively small amount of data and can be constructed in a short time period, while large systems models require several years to develop by large scientific teams.

The initial focus of LOICZ identified in these guidelines is on stoichimetrically linked CNP budget models. Even though they are very simple and require relatively little data, these kinds of budgets can provide a very good description and understanding of nutrient dynamics by identifying and quantifying the important fluxes, in and out of the coastal zone. Not only does it make sound scientific sense to start at the simplest end of the modelling spectrum, but this will allow for the potential development, in a short time, of local models of value to LOICZ for a large number of coastal areas around the world. The procedures and examples presented in this document cover a wide range of situations with varying amounts of available data. Although the methodology appears to be very robust, certain limitations in the application of these methods are identified and discussed in detail in the text. In general, the techniques presented here are most readily applied to marine systems which have a measurable salinity gradient.

While it is essential to generate budget models for the world's coastal zones, it is recognised that dynamic simulation models will also play a very valuable role in reaching the long-term objectives of LOICZ, especially in understanding how the dynamics of carbon, nitrogen and phosphorus in coastal systems may change under different environmental conditions. Once robust budget models of important CNP fluxes are developed, they can be used as the basis for developing dynamic simulation models, that can be used to explore the effects of changing environmental conditions on important biogeochemical fluxes in the coastal zone.

These recommended modelling approaches require site specific data. Therefore, modelling activities and field work should be conducted together, in an interdisciplinary manner, with the results from both activities being compared on a routine basis. The data requirements of linked carbon, nitrogen and phosphorus (CNP) budgets should be taken into account when designing new field programmes or modifying existing ones. The most important data requirements for linked biogeochemical budget modelling are water circulation and various forms of carbon, nitrogen and phosphorus. The simplest way to obtain information on water circulation is by way of water and salinity budgets; this information can also be extracted from physical oceanographic models where these are available.

If followed, these guidelines should lead to the development of models for a large number of coastal systems around the word. It is anticipated that the development of most of these models will be funded at the local or national level. By developing understanding of local physical oceanographic and biogeochemical processes, these models will be able to contribute to the management of local resources and understanding the socio-economic implications of global change. In addition, it is important that the local models produced using these guidelines in different coastal areas be compared and the results integrated to provide the regional and global syntheses required by LOICZ. Such a comparison and integration will be guided by the LOICZ coastal typology exercise.

2. INTRODUCTION

All countries with a coastline have an interest in the sound management of their coastal space and resources. The problems associated with coastal management are expected to become more difficult under the influence of global changes. The Land Ocean Interactions in the Coastal Zone (LOICZ) Core Project of the IGBP focuses on the role of the world's coastal zones in the functioning of the Earth system; the way in which global changes will influence that role; and the way in which such changes will affect the use of coastal space and resources by humanity.

The general goals of LOICZ, as stated in the Science Plan (Holligan and de Boois, 1993) and Implementation Plan (Pernetta and Milliman, 1995), are as follows:

- To determine at global and regional scales:
  - a) the fluxes of materials between land, sea and atmosphere through the coastal zone
  - b) the capacity of coastal systems to transform and store particulate and dissolved matter
  - c) the effects of changes in external forcing conditions on the structure and functioning of coastal ecosystems.
- To determine how changes in land use, climate, sea level and human activities alter the fluxes and retention of particulate matter in the coastal zone, and affect coastal morphodynamics.
- To determine how changes in coastal systems, including responses to varying terrestrial and oceanic inputs of organic matter and nutrients, will affect the global carbon cycle and the trace gas composition of the atmosphere.
- To assess how responses of coastal systems to global change will affect the habitation and usage by humans of coastal environments, and to develop further the scientific and socio-economic bases for the integrated management of the coastal environment.

Understanding the interactions between the coastal zone and global changes cannot be achieved by observational studies alone. Modelling of key environmental processes is a vital tool that must be used if LOICZ is to achieve its overall goals and objectives, particularly in view of the fact that many of the uncertainties in global carbon flow models may represent unquantified processes occurring within the coastal zone. This document is intended as a guide for those wishing to contribute to the objective of elucidating the dynamics of carbon, nitrogen and phosphorus in the coastal ocean within the framework of LOICZ.

2.1 The LOICZ Biogeochemical Modelling Strategy

The general LOICZ biogeochemical modelling strategy, as laid out in the LOICZ Implementation Plan, consists of six components (Text Box 1). The first three are framework activities and will be led by the LOICZ Core Project Office (LOICZ-CPO) with input from the proposed modelling nodes. These include the development of a coastal typology, the development of a modelling network and the development of improved upscaling methodology. The fourth and fifth components involve the development of new local and regional biogeochemical models as well as their evaluation and validation. It is anticipated that this work will be done primarily as part of national and regional programmes with LOICZ co-ordination. The sixth component involves the development of global biogeochemical models of the coastal zone which can provide data that can be used within models of the entire Earth system such as those being developed by the IGBP Framework Activity Global Analysis, Interpretation and Modelling (GAIM). This is seen as an integrative activity that would be led by the LOICZ-CPO but also requires strong input from the entire LOICZ community.

LOICZ BIOGEOCHEMICAL MODELLING

Carbon flow models of the world's coastal zone will be developed under LOICZ. These models will be aquatic models that will include water, sediment and nutrients as well as various forms of carbon. They will include internal dynamics as well as important exchanges across landward and seaward boundaries. The tasks (in parentheses) indicate where each activity is located in the LOICZ Implementation Plan.

Development of a system for formulating LOICZ global coastal typologies (Task F.2.1)

The typology will be used to determine regions for which models and model output are needed, and for developing global syntheses and models. This Task will be undertaken by the LOICZ-CPO.

Development of a strong, centralised framework for LOICZ modelling activities (Task F.5.1)

This Task will provide the overall framework for co-ordination and communication and provide guidelines for model development. This Task will be led by the LOICZ-CPO with strong inputs from the modelling nodes when established.

Develop improved methods for assimilating fine scale models into large scale models (Task F.5.2)

This Task links hydrodynamic models to biogeochemical models, and involves scaling up from local to regional models and from regional to global models. This Task will be led by the LOICZ-CPO with strong inputs from the modelling nodes when established.

The development of new local and regional ecosystems models (Task 1.4.1)

Building on existing data this Task involves constructing new budget and system models following recommended guidelines. Budget models will be developed first followed by system models for sites and regions identified through the typology exercise. An on-going activity that will continue as new data become available, this activity will primarily be undertaken as part of national and regional programmes with LOICZ co-ordination.

Evaluation and validation of budget and system models (Task 3.1.4)

Under this Task models of similar coastal units and contrasting coastal units will be compared and generic sub-models of key biogeochemical processes will be developed which have wider applicability. New models will be validated using new field data. Where possible models will be used to explore the effects of different scenarios on regional carbon flows. Undertaken primarily as part of national and regional programmes this will require strong LOICZ co-ordination.

The role of coastal Seas in the global carbon cycle (Integrative Activities - Core Research)

This activity is dependent upon all the above activities, especially the typology exercise and scaling up techniques. Using available regional models, develop carbon flow models for the world's entire coastal zone. Feed the results of coastal carbon flow models into Earth system models. Where possible, models will be used to explore the effects of different scenarios on global carbon flows. Led by the LOICZ-CPO this Task will require strong input from the modelling nodes and regional research networks when established.

TEXT BOX 1. ACTIVITIES RELATED TO THE DEVELOPMENT OF GLOBAL SYNTHESES AND MODELS OF CARBON, NITROGEN AND PHOSPHORUS IN THE COASTAL OCEAN ENVISAGED UNDER LOICZ. SEE LOICZ IMPLEMENTATION PLAN (PERNETTA AND MILLIMAN, 1995) FOR DETAILS.

The LOICZ approach is to encourage researchers around the world to develop models of the fluxes of carbon, nitrogen and phosphorus for their local geographic areas of interest. If constructed in a similar manner, these models would provide estimates which can be aggregated at regional and global scales. For any group of scientists wishing to investigate and model a particular local coastal system for subsequent up-scaling into larger models or wider regional estimates, there are two types of information required:

- estimations of biogeochemical fluxes in the system as it is now, for eventual incorporation into global estimates of flux through the coastal zone; and,
- dynamic simulations of processes in the coastal system which can be used to explore the consequences of environmental change, and produce forecasts of future fluxes.

The LOICZ Implementation Plan calls for the development of guidelines of recommended modelling techniques under Task F.5.1 and this document provides such guidelines for the LOICZ research community.

2.2 Spatial and Temporal Scope of LOICZ Modelling

Numerical modelling can be carried out at quite different spatial and temporal scales. Three spatial scales, defined in terms of linear coastline length, have been identified in the Implementation Plan as being of primary interest to LOICZ. They are:

- Local/Site (~1-100 km): These would address specific habitats such as saltmarshes, mangrove forests, deltas, coral reefs, estuaries, bays and fishing banks. Modelling on this scale would be generic in nature, for example, mangrove forests can be modelled in a way that allows application of the models to other sites with similar conditions.
- Regional (~100-10,000 km): These would incorporate a variety of near-shore and off-shore habitats, in some cases out to the 200 m isobath. Modelling on this scale would be geographic in nature and would be carried out for a particular region of the world such as the North Sea, South China Sea, etc.
- Global: These would incorporate several regional models representing either the entire world's coastal zone or a substantial proportion, based on representative regions, the results from which are up-scaled to the global scale.

Models can also have different temporal scales depending on their particular purpose, but the prognostic, global scale models ultimately required by LOICZ and the IGBP must have a temporal scale on the order of 10-100 years such that they can be used to resolve variability on inter-annual time scales such as El Nino Southern Oscillation (ENSO) events, or multi-year scales such as the effects of population growth, for example. They will also require relatively fine resolution to incorporate episodic events.

In order to study multi-year phenomena it will be necessary for LOICZ models to resolve seasonal cycles, annual cycles and directional changes over the next few decades.

2.3 Recommended Modelling Approach

The initial LOICZ priority is on the estimation of the present fluxes of carbon, nitrogen and phosphorus in particular coastal systems on the local scale. Following the initial identification and description of the system to be studied, possibly using simple budgets of water, nutrients and other materials, we recommend that the first approach to any system not previously studied should be to produce biogeochemical flux budgets of the system, integrating over annual or multi-annual scales. By comparing fluxes through systems that differ in certain environmental parameters, it should be possible to make tentative predictions of the consequences of environmental change. For example, Nixon *et al*. (in press) have shown that the rate of denitrification in North Atlantic estuaries is a function of residence time of the water. Changes in the amount of precipitation resulting from environmental change would interact with concurrent changes in population density and water use. The combined result might be a significant change in both runoff and denitrification.

LOICZ recognises that for more elaborate predictions it will be essential to identify key processes within representative coastal systems and produce dynamic simulation models based on coupled process models. At present there are limitations and difficulties with this approach but an important part of LOICZ is the working towards a solution of these problems. However, this is beyond the scope of the present document.

2.4 Integration of Biogeochemical and Socio-Economic Modelling within LOICZ

Economic and social impacts of global change in coastal systems are an integral part of LOICZ and the wide spectrum of proposed research activities is presented in the Implementation Plan. In a separate but parallel exercise, guidelines for the assessment of coastal zone resources have been developed (Turner and Adger, 1996). In order to meet the long term goals of LOICZ, it will be necessary to integrate the biogeochemical and socio-economic modelling approaches. This will be a difficult task because of limited collaboration between natural and social scientists in the past but a concrete start has already been made within the SARCS/WOTRO/LOICZ project in Southeast Asia. This collaborative project, which has been approved as a Core Research Project of LOICZ, involves initially natural and social scientists from Indonesia, Malaysia, Philippines and Vietnam. The research objectives are primarily focused on social and economic impacts of global change but also involve the quantification of land-ocean fluxes and the integration of socio-economic and biogeochemical modelling has a high priority.

2.5 Potential Benefits for Managers

While the primary aims of LOICZ and the IGBP are to carry out scientific research relevant to the study of environmental and socio-economic change in the coastal zone, the results of LOICZ research must also be applicable to management questions. The linkages between biogeochemical modelling and socio-economic and management issues can be seen in a wide variety of existing applied studies including fisheries management, eutrophication, effects of habitat alteration, and fate and effects of contaminants. The LOICZ biogeochemical modelling guidelines presented in this document will help scientists summarise existing and new data in consistent and rigorous formats that will be more useful to coastal zone managers. It is also hoped that they will assist in the development of more applied models that could be used by managers in the decision-making process.

There is now a consensus in the scientific community that cumulative changes, driven by direct human use of coastal space and resources, may result in changes to the Earth system which in turn will impact future human use of coastal space and resources. LOICZ is a project designed to improve our scientific understanding of this global feedback loop and hence provide a sound scientific basis for the management of the world’s coastal areas.

2.6 Objectives of the Guidelines

The objectives of these guidelines are to provide an introduction and overview of biogeochemical modelling methodologies that will:

- improve our quantitative evaluation of the role of the coastal zone in carbon, nitrogen and phosphorus cycling through provision of a common, widely usable analytical framework of modelling; and,
- lay out this framework in sufficient detail to be followed by coastal zone researchers world-wide.

The guidelines can be used to help analyse existing data sets where they exist as well as to assist in the design and conduct of new research programmes that will provide additional data for modelling. In this manner, LOICZ modelling activities will increase the number of sites within and between typologically similar units that can be compared and studied and so contribute to our overall understanding of the role of the coastal zone in global carbon, nitrogen and phosphorus cycling.

3. GENERAL CONSIDERATION IN CONSTRUCTING COASTAL MODELS

3.1 Why Build Models?

What is a model? By definition it is any simplified description or abstraction of a system or a process. In science, models are tools that help us to conceptualise, integrate and generalise scientific knowledge. Even in science the perception of models is vastly different depending on the scientific field, the problem studied or the tools commonly used in that particular field. For this document, a "model" may be considered to be any simplified representation of some aspect of the real world and a "mathematical model" presents this simplification in the form of a series of mathematical equations. In general, by simplifying reality, mathematical models allow system responses to perturbation, to be tested computationally. It is also important to note that modelling is an iterative process, with no fixed starting or end points and with varying goals, depending on the interests of the modellers.

There are two major benefits of modelling: the process and the product.

The **process** of building models is a valuable learning exercise for those involved. That is, it:

- forces interaction among participating scientists from different scientific disciplines;
- identifies critical information gaps; and,
- helps to identify research priorities.

The benefits gained by undertaking the process alone, often more than justify the effort expended in model development.

The **products** of modelling can be very diverse, ranging from a single estimate of a quantity of material or energy, to the temporal description of a single process, to the mathematical description of complex interactions among ecosystem components, such as internal dynamics. Assuming that the process produces a usable product that describes and/or predicts the behaviour of the system with sufficient accuracy, the models constructed can serve numerous purposes. For example:

- for the **scientist**, the model provides a tool for hypothesis testing and prediction and it can also be exchanged with other scientists and be used as the basis for developing better models;
- for the **manager**, models provide a quantitative tool that can be used for decision making; and,
- for the **general public** and **politicians**, models can serve as a means of visualising in graphical fashion, our understanding of the ways in which complex systems function.

3.2 Some Basic Modelling Principles

The most important consideration in modelling, is to determine at the outset, what kinds of questions are to be addressed. Most models can provide answers to only a limited range of questions, and asking the wrong questions of a model may lead to unsatisfactory answers. Building a model without a clear idea of what is expected from it, is like planning an experiment without a hypothesis to test, or designing a cargo vessel without knowing the nature of the cargo. This definition of the question is a critical first step in the development of any model.

Each type of model has advantages and disadvantages. Highly aggregated budget models of nutrient or material fluxes can provide good overviews of the inputs and outputs of a particular system. But these models cannot provide the kind of detailed process information required for many resource management decisions. In contrast, very detailed numerical simulation models are valuable tools for exploring the dynamic behaviour of systems on short time scales, but they seldom provide reliable estimates of long-term net fluxes. This is because small errors in the very detailed descriptions accumulate over time and often make the integrated results unreliable.

A second important consideration in modelling is the balance between the availability of suitable data and the understanding of the system to be modelled. Sufficient quantities of both are required to carry out successful modelling activities. Holling (1978) provides a useful classification that puts modelling into the overall context of in science (Figure 1). The horizontal axis in Figure 1 represents the degree of scientific understanding of the system, or process being studied, while the vertical axis describes the amount of data that are available for the system. The diagram is split into four domains.

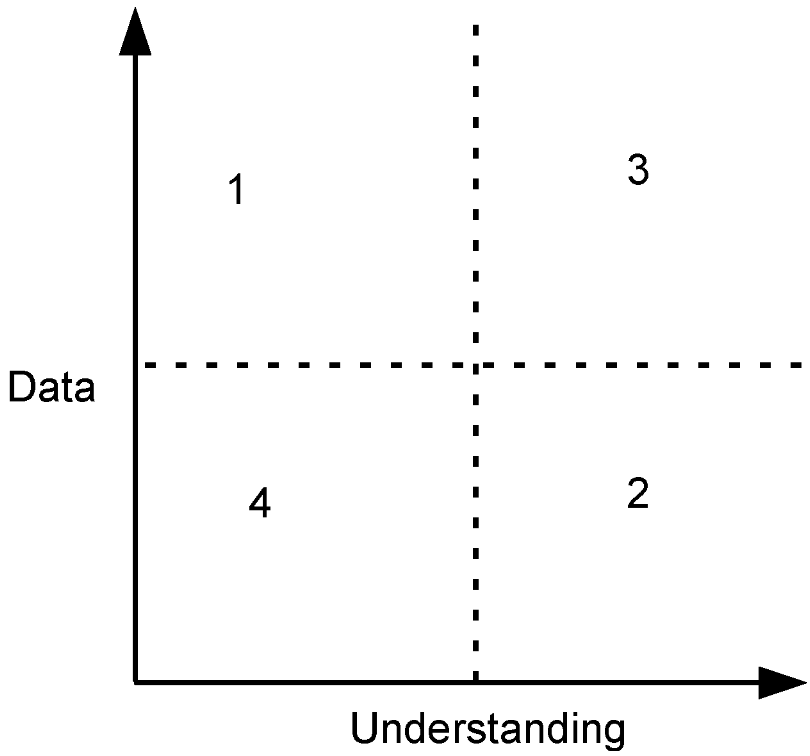


Figure 1. Data and understanding requirements for modelling, from Holling (1978).

Domain 3 is where we want to be; a good understanding supported by a wealth of good data. We are rarely in this domain in coastal and marine science. It is a more common situation however within the disciplines of engineering and physics where processes are limited and often well understood, and data are relatively easy to obtain. Here, highly accurate numerical models have been developed that are used routinely in everyday life. For instance, tides around the world can be predicted with a high degree of accuracy and speed. Models of the global water cycle are also reaching this domain.

Domain 1 includes those systems for which we have lots of data but little understanding. This is sometimes the case in marine science where there is a large amount of monitoring data, or data from various scientific cruises. These data are usually scattered among various government archives and department files, or if we are lucky in publications, and have been collected for many different purposes. For instance, fishery scientists often collect data on hydrography, chemistry, biology and economics in addition to data on fish. Hydrologists may provide data on fresh water and even nutrient inputs to the coastal region. Harbour authorities provide additional data on bathymetry, sea level variations and sediments. In such a case, compiling and structuring of the data may be sufficient to generate useful levels of understanding. There is a danger associated with collecting data without an identified purpose, although it may well be useful, it is generally inefficient. Nevertheless, putting available data into a common framework (for example a database) to describe the basic spatial and temporal characteristics of a system is a natural first step in any study of an ecosystem. Here statistical techniques are useful to find relationships and to develop hypothesis. Geographic information system (GIS) methods are becoming more useful for graphically describing the spatial patterns in observations.

Domain 4 is the usual domain of biogeochemical research in coastal environments, in that there are few data and little understanding. Sometimes we have a good conceptual idea of how a system operates, based upon studies done on similar systems elsewhere, but little data to support our hypotheses as in Domain 2. It is in these two domains, 2 and 4, where modelling is most useful.

In modelling, it is best to start simply and to gradually build more complicated models as needs dictate. How far to proceed along the modelling path depends very much upon the particular scientific objectives, as well as the availability of data and understanding. In some instances, quite simple models are sufficient for the task at hand. Since there are many possible paths to follow, it is important that objectives are clearly stated and defined at the outcome. A sound rule which should be followed in modelling, is to start with the simplest route possible and add complexity only when it is clearly justified. It should also be recognised that the field of environmental numerical modelling is evolving rapidly and that techniques in common practice today, will probably be superseded by better ones in just a few years.

The development of coastal zone biogeochemical models is not a simple procedure. There is no such thing as a standard approach that will work in all cases. Each coastal system must be evaluated from the viewpoint of both its inherent characteristics and in terms of the kind of information that the model will be expected to provide. It is also important to assess the data and conceptual understanding on which the model will be based, considering both the availability of existing data and the extent to which it is possible to collect new data. In all cases, modelling activities should be well integrated at the very beginning with field and experiment studies in an overall strategy to address the desired product.

The best overall modelling strategy is to begin by generating a basic description of the particular coastal system being studied and comparing it to similar systems that may already be well described and understood. This includes the critical step of defining system boundaries. Such an initial typological approach will identify the considerations that are most likely to be of importance for such a system, and help develop models that are most likely to provide the desired information. In many cases, the ultimate uses of the model may not be well-defined since several different parties, with varying interests, may be involved in model development. It is therefore necessary to proceed in an iterative fashion, alternating between the development of the models and evaluating their utility from different points of view. This of course means that the initial stages of modelling should focus on simple models which can be constructed rapidly and evaluated easily. In many cases the first step in the development of a model for a new area or system is simply to apply and refine an existing model, rather than to start designing a completely new one.

The initial description of a system can be useful to identify what modelling approach(es) should be taken to reach a desired goal. For example:

- in systems dominated by water transport, physical exchange processes are more important than internal cycling;
- in relatively homogeneous systems, or systems which can be highly aggregated, process-based nutrient budgets can answer many questions; and,
- in high-diversity systems with complex trophic interactions, network analysis may be useful after the trophic pathways and steady-state fluxes have been determined.

As understanding of a particular system increases, the models applied to the system frequently tend to evolve from simple, highly aggregated, to more complex models. In many cases this development proceeds by the progressive disaggregation of the existing model to add greater detail and descriptive power. This means starting with very general models that contain only a few components or levels, and subdividing these levels into finer levels with more detail only as it becomes necessary. There is however, a tendency to disaggregate unnecessarily, simply because the information to do so is available and often because specialists feel that the model cannot work unless all of their expertise is incorporated in it.

Therefore the following questions should always be asked before proceeding with disaggregating or refining any models:

- will this disaggregation improve the performance of the model in relation to the objectives of the study?
- will weaknesses in other parts of the model limit this improvement?
- do we have enough data to calibrate a more detailed submodel?

It is important to maintain a sense of balance in model development and starting from a highly aggregated model can help with this. If a flux consists of two components, and one of the components is highly variable, there may be little value to refining the modelling of the other component.

Another caution concerning the progression from simple aggregated models to more detailed complex modelling activities is the fact that, although the response of complex mathematical models may tend to mimic system response to some perturbations more closely than simple models, the observation that model response does mimic system response under controlled conditions does not guarantee that the model is actually an accurate description of real-world behaviour. One consequence is that complex mathematical models, which may be difficult in themselves to “understand,” may give very false views of how the real world works once they are run under uncontrolled, non-test conditions. Simple mathematical models which are robust with respect to specific aspects of a system may actually give more insight into those specific aspects of system function than more complex models.

In the short term, where data and understanding are limited, which is the usual situation for most of the world’s coastal zone (for example, Domain 4 in Figure 1) budgets and other empirical models are likely to provide greater predictive value for different management strategies than the development of detailed numerical models. Unfortunately, the predictive power of empirical models is restricted within the observed range of data. Therefore process oriented models have to be developed in parallel with empirical models in order to evaluate possible future management strategies. Prior experience shows that many mechanistic, reductionist modelling projects, particularly of entire ecosystems, have usually failed if they are based on a ‘bottom-up’ approach. Thus, a detailed understanding of various processes, used as sub-models and assembled into an ‘ecosystem’ model, do not describe total system properties (see for instance Platt *et al*., 1981). An holistic approach is necessary where the goals of the models and the critical scales are defined, prior to model formulation and simulation. The model is in itself a hypothesis, and the numerical simulation is a tool to test this hypothesis, not a goal in itself. It is likely that development of more detailed models, through a number of iterative steps where model evaluations interact with field measurements, will only be possible for coastal regions with highly developed databases and resident scientists with the necessary modelling skills. The development of typological relationships among coastal regions will play an important role in exporting such detailed models to other areas.

3.3 The LOICZ Classification of Modelling Approaches

The LOICZ Science and Implementation Plans (Holligan and de Boois, 1993; Pernetta and Milliman, 1995) have identified four general kinds of numerical modelling approaches that are of use to LOICZ research. They are budget models, process models, system models and prognostic models. It must be emphasised that these general categories of numerical models do not represent clearly defined divisions and that classifying a particular model can be difficult. Especially confusing at times is where to draw the line between budget and systems models. In reality, there is a wide spectrum of modelling techniques available ranging from simple budget models at one end, to the more complicated ecosystem process models at the other. In most, if not all cases, model construction begins with some basic information on the system in question such as spatial extent, topography, water volumes, dominant habitat types, number of trophic levels, etc. The easiest way to start modelling is to prepare a simple mass balance budget for the variable(s) of interest. One can then move along the spectrum from budget models to the more complicated systems modelling if required and if the necessary resources are available. If one cannot create a simple budget for an area, it is unlikely that one can develop a reasonable ecosystem model no matter how many resources are at hand.

3.4 Budget Models

Budget models are generally defined as mass balance calculations of specific variables (for example, water, sediment, carbon, nitrogen, phosphorus, etc.) for a defined geographic area and time period (for example, monthly, annual, or decadal). The geographic scope can range from a particular coastal habitat (for example, a mangrove system) to a semi-enclosed sea such as the Mediterranean or to the global ocean. The model should include all major sources and sinks, both external and internal, as well as the dominant internal transformation processes for the variable(s) in question. For example, a carbon budget for a coastal bay should include delivery by freshwater, exchange at the seaward boundary, production-respiration, sedimentation, etc. Focus is placed on resolving fluxes at the boundaries. The development of a budget usually requires a substantial amount of quantitative data for the geographic area in question. Although in some instances the lessons and experience of modelling can be transferred from one region to another with similar characteristics, most budgets usually consider only one variable for particular sites and this limits the ability to generalise model results between areas. 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. 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.

3.5 Process Models

Process models describe specific physical, chemical and biological processes which are important in understanding biogeochemical fluxes in the coastal zone and how they are influenced by major environmental forcing functions such as tide, wind, temperature and light. They are generally constructed on the basis of process studies done in the laboratory, mesocosms and the field. In most instances, they are developed in isolation from the total natural system and therefore tend to be reductionist in nature. Each contains a limited number of variables and parameters.

While developed using empirical data gathered at specific geographic locations, process models tend to be generic in nature and can often be applied with confidence to other geographic locations. For example, formulations developed to describe phytoplankton photosynthesis as a function of light, temperature and nutrient supply for the North Sea should also be applicable to other geographic areas with a similar environmental setting and forcing. In general, the best studied and described coastal processes are those operating in temperate regions. Process models of important environmental processes in tropical and polar regions are not as well developed and demand increased attention.

Also important to the long term success of LOICZ is the availability of process models dealing with the major exchanges of materials between the coastal zone and its boundaries. Probably the most important are inputs from the land which include river runoff, groundwater seepage and coastal erosion. Also important are the exchanges with the atmosphere and the seaward boundary that are controlled primarily by physical processes. Individual process models are important building blocks for building systems models as described below.

3.6 System Models

These models embrace aspects of physics and chemistry in addition to biological aspects and should not be confused with the purely biological models discussed in Section 3.4. They are models that attempt to describe the behaviour of whole ecosystems.

One type of system model is of a budgetary nature and summaries fluxes through the various pathways of the ecosystem. Others are coupled process models that describe internal dynamics. System models integrate information on what are considered to be the most important variables and processes for the total environmental system of particular interest. They have well defined spatial boundaries and temporal scales. Spatial scale can range from a particular coastal habitat, such as an individual coral reef, to an estuary, coastal bay or the entire continental shelf depending upon the objectives of the modelling project. Temporal scales usually range from tidal cycles to several decades. The behaviour of a system model depends very much upon the spatial and temporal scales selected. Systems models are commonly built using process models and often the first step is to construct a simple mass balance budget. Particular attention is given to describing the interaction among state variables. System models can be either descriptive (for example, flow or network analysis) or dynamic (for example, simulation models).

The most advanced systems models are those describing coastal circulation. The major physical forcing functions are limited in number and relatively well understood. Three dimensional circulation models with high spatial resolution have been developed for a large number of estuaries, bays and entire continental shelf regions (for example, Haidvogel and Beckmann, submitted). These coastal circulation models provide an essential foundation for the development of sediment transport, water quality, geochemical and ecosystem models.

The most complicated and least reliable systems models tend to be ecosystem models which of necessity contain a large number of physical, chemical and biological processes, variables and parameters many of which are poorly understood. Their development also requires a substantial investment of resources. However, very often submodels from existing models can be used in developing new models for similar geographic areas such as has been done with the ERSEM modelling activities in the North Sea described in Baretta *et al.* (1995).

The accuracy of mechanistic ecosystem simulation models (that is built from the bottom up from process models) has been questioned because they do not include the qualitative changes of state that commonly occur in the real world, the inherently greater variability in the parameters fed into biological models compared with engineering models, the hierarchical nature of ecosystems and the capacity for self-organisation that ecosystems possess (Platt *et al.*, 1981). Other more holistic approaches are needed for understanding important fluxes in marine ecosystems and some of these are reviewed by Ulanowicz and Platt (1985). One approach which has received considerable attention in recent years is network analysis (Wulff *et al.*, 1989).

Another different approach to systems modelling is top-down modelling (Silvert, 1981) which is the process of describing a set of models which generate output consistent with the empirical data and then analysing the structure of these models to arrive at smaller sets of acceptable models. This method facilitates the development of models having new and unexpected structural features, makes it possible to build new models which correctly describe emergent properties and assists in the diagnosis of errors in the interpretation of experimental data.

When correctly constructed, system models can be used to produce mass balance budgets. The comparison of such a budget with a budget from the raw data can be a very powerful way of validating process or system models. Nevertheless there is a real danger in using the output from system models as real data. Great care must be taken to ensure that the system models are operated within the data range of the process models that make them up and that the process models reasonably describe the observed conditions and processes in the system being studied. This again emphasises the importance of empirical data in the construction of all types of models.

3.7 Prognostic Models

Prognostic models are those that have the ability to predict how selected environmental variables may change if conditions are changed (for example rising sea level, increased temperature, reduced freshwater runoff, etc.). All three of the general model types described above have some degree of predictive ability. Although systems models offer great potential in generating an understanding on which to base predictions, it is most likely that within the relatively short time frame of LOICZ, the best predictive power will be found in empirical correlational models constructed for specific management objectives.

3.8 Historical Perspective

As has been stated, the main thrust of LOICZ is towards determining the biogeochemical fluxes of carbon, nitrogen and phosphorus through coastal ecosystems, and their interactions with parameters of global change. In the past, the majority of models developed for coastal ecosystems have been directed towards understanding the **biological** processes within those systems as an aid to management. These have usually been in the form of models of energy-flow or carbon-flow through the biological community. Occasionally, attempts have been made to determine fluxes across the boundaries of these systems, but the results have often been disappointing. For the needs of LOICZ, it is initially more important to get good estimates of the inputs and outputs of a coastal system than to capture the details of processes within the system. Hence the recommendation to begin with developing biogeochemical budgets which incorporate major, physical oceanographic exchange and mixing processes. Here, we review the differences between the biological energy/carbon flow models and the biogeochemical models required by LOICZ.

3.8.1 Energy flow/carbon flow models of biological communities.

In any given system the primary producers absorb solar energy and fix it into carbon compounds. Energy fixation during photosynthesis is often measured from the uptake of radioactive carbon isotopes. It is a matter of choice whether the investigator uses this information as the basis of an energy flow model or a carbon flow model, for the data may be expressed either way. Let us for convenience refer to them as carbon models.

By identifying the trophic pathways and the biomass and metabolic rates of the main consumers, we can budget the pathways in which carbon fixed is eventually converted back to carbon dioxide and energy is dissipated as heat. The detailed process has been codified in software known as ECOPATH (Christiansen and Pauly, 1993) by which attention is drawn to any gaps in the data that need to be filled with estimates from the literature, and by means of which different biological systems can be compared. A simpler alternative is to apply highly aggregated models such as the size-spectrum models of Platt and Denman (1978) and Silvert and Platt (1980).

Often, the data for such models are collected from a discrete geographic area, but in most cases the fluxes across the boundaries of that area are not of primary concern. While these models reveal the total amount of carbon dioxide fixed during photosynthesis and balance this against the amount released via respiration, there is seldom an accounting for the amount of carbon that is released to the atmosphere, the amount fixed in calcification or buried in the sediments, and the amount imported or exported in dissolved or particulate form across the boundaries with adjacent water masses. Yet data on these fluxes are the primary requirements of LOICZ.

There are examples of strenuous attempts to measure boundary fluxes in conjunction with biological carbon models. For example, Ong (1993) discusses the carbon fluxes within a mangrove system. As is discussed in Section 4, attempts to determine the time-varying fluxes in a water column at different seasons and at various states of the tide along a hydrodynamically complex boundary are extremely difficult, and estimates made in this way often fail to match the internal estimates of biological fluxes. For this reason, we recommend an entirely different approach which circumvents many of the difficulties encountered in the past.

3.8.2 Biogeochemical flux models.

The process of developing biogeochemical flux models begins with determining the spatial and temporal scales of the coastal system of interest, after which the physical, chemical and biological properties can be described and a water budget developed. It is essential to understand the basic physical mechanisms at work, including amongst other, estuarine circulation, upwelling, and tidal mixing, in order to have a qualitative grasp of the pattern of water movement and to delineate the boundaries of the system being studied. A useful guide to this stage is found in Mann and Lazier (1991). The terms in a water budget of a coastal system include river inflows, groundwater seepage, exchange at the seaward boundary, precipitation and evaporation, although in many circumstances river inflow overwhelms all of the other freshwater fluxes. On first approximation, one assumes that imports of water are balanced by loss across the boundary with adjacent water masses.

To get a better estimate of the exchanges with adjacent waters, that is water exchange by both flow and mixing of water masses, as well as the freshwater flow, it is often possible to construct a salt budget. If there are distinct salinity differences across the interface, salinity measurements will permit refining of the water budget.

One then moves on to construction of budgets for nonconservative materials, in particular carbon, nitrogen and phosphorus. As will be shown in Section 5, it is not necessary to investigate all of these materials. Phosphorus has the simplest biogeochemical pathways, and it is often sufficient to make a detailed study of the phosphorus budget and calculate other elements on the basis of stoichiometric relationships. The mathematics involved is relatively straightforward, and the method has been shown to give good results in a number of habitats (see case studies in Section 5). Although adoption of this method will involve a radical change in methodology for groups already involved in biological ecosystem modelling, we maintain **that this is the only way that flux data for use in global models can be obtained in a reasonably short time**.

At the same time it is also necessary to continue improving scientific knowledge of the internal dynamics of carbon, nitrogen and phosphorus in coastal systems, and how they influence overall biogeochemical fluxes, through the development of process-oriented system models as is being done for some regions of the world's coastal seas such as the North Sea (Baretta et al., 1995).

3.9 Modelling Requirements of LOICZ

The first step in achieving regional and global estimates of flux requires the development of a global coastal typology. A preliminary version on a regional scale has been prepared (LOICZ, 1995d) and was discussed at the Second LOICZ Open Science Meeting (LOICZ, 1995a). The intention is that such a system will subdivide the world's coastal zone into clusters of discrete, scientifically valid units based on both natural and socio-economic features and processes (see Table 1 for examples).

Such a system is necessary if the global syntheses which form a long-term goal of LOICZ are to adequately encompass the spatial and temporal heterogeneity of the world's coastal zone. Development of an appropriate typology will help determine the appropriate weighting to be applied to recognisable classes of coastline in preparing global syntheses, scenarios and models on the basis of spatially and temporally limited data.

The biogeochemical modelling requirements of LOICZ can be broken down into two general categories. The first is to develop an improved understanding of important biochemical fluxes in the coastal zone. The second is to develop prognostic models that can describe existing biogeochemical processes and predict how they will be altered due to environmental change.

The modelling procedures presented in this document will describe the integrated biogeochemical and ecological functioning of coastal marine ecosystems. The specific purpose of presenting such procedures is to guide the development of a global data base which characterises the role of the coastal zone as a source or sink for the biogeochemically reactive elements: carbon, nitrogen, and phosphorus.

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. 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 modelling 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.

Ecological simulation models, some with relatively sophisticated description of the physics of water flow and substantial details of biogeochemical processes, have been widely applied in ecosystem analysis and are of great use in the evaluation of the instantaneous function of systems. Simulation models are usually limited by: the limits of our theoretical and experimental knowledge of the performance of all components in the system; by mathematical chaos which exists within any ecosystem; and, by computational limitations (such as rounding errors). Despite the limitations, when applied correctly such models can provide useful insights into the internal processes of the system. The description of these processes can be used to attempt predictions of system behaviour with changes in the control functions, such as are envisaged with environmental change.

TABLE 1. FACTORS RELATING TO THE DEFINITION OF THE COASTAL ZONE AREAS FOR THE DEVELOPMENT OF COASTAL BUDGET MODELS.

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

3.9.1 Understanding biogeochemical fluxes for global models

The most important biochemical fluxes from the LOICZ perspective are those across the major boundaries of the coastal zone (that is, land-ocean inputs, air-sea interaction, and exchanges with the open ocean) as well as those associated with benthic/pelagic coupling and exchanges. These must first be determined at the local/regional scale but in time the results must be integrated into regional and global models of the coastal zone. It is argued that biogeochemical fluxes are best estimated in the first instance by the construction of budgets. This simple class of mathematical model provides the most robust estimates of integrated ecosystem performance. Budget models are little more than an ordered, objective description of what is known about the system in question. In many instances, collection of data which can be used in a budget may have occurred incidentally in other studies. Conservation of mass is, of course, a fundamental principle of nature. Therefore a comprehensive budget of the inputs of materials into the system of interest, outputs from that system and amount in the system is an objective description that goes beyond, simple tabulation of such data. While such budgets provide neither direct experimental nor direct theoretical information about how the system works, the budgets can describe the system at space and time scales which may not be amenable to experimentation or detailed simulation modelling. One result is that the descriptive output from budgets can be used in a statistical sense to evaluate and compare how systems work and how the parts of the Earth system are linked together.

In Section 5, detailed procedures for developing a class of mass balance budgets that we define as “stoichiometrically linked water-salt-nutrient budgets” are presented. The elements of specific interest here are carbon, nitrogen, and phosphorus, all of which are essential to life. As will be seen, these budgets can be used in comparative studies to generalise coastal biogeochemical processes in two ways:

- time-series analysis of budgets within systems; and,
- comparison of “static” (or average) budgets between systems.

Both of these types of studies will be used to achieve the goals of LOICZ.

3.9.2 Use of prognostic models for predicting consequences of global change

While budget models provide robust overviews of the flow of nutrients and material across boundaries, they are very limited in their ability to identify the actual processes that are taking place within the coastal zone. They are also very limited in their ability to extrapolate beyond the conditions for which they are created and thus allow prediction of the system functioning under new conditions. The coastal zone is subjected to various kinds of environmental change, due to both natural variability and human activity. These include changing sea level, habitat alteration and release of contaminants. For LOICZ to achieve its objectives of understanding the processes, predicting response and investigating alternative management and response scenarios to climate change, it is necessary to develop prognostic models which can be used as management tools. The best method to achieve these goals is to develop numerical simulation models which focus on the internal dynamics of coastal systems and describe how critical biogeochemical processes are influenced by environmental variables. This class of models can be used to explore numerically the potential impacts of different environmental scenarios. In LOICZ they should be developed in conjunction with budget models and will be constrained by the boundary conditions and overall fluxes identified by the budget models. These will have to be developed at different spatial and temporal scales depending upon the particular issue(s) of concern.

3.10 Importance of Scaling in Modelling

In concluding this section on general considerations in developing coastal biogeochemical models for LOICZ, we wish to emphasise again the importance of scaling. At the very outset of a coastal modelling project, it is absolutely essential to clearly defined the spatial boundaries of the system, as well as the temporal scale of the model. Decisions will depend upon the properties of the system and on the overall objectives of the model. They should be made in full consultation with the entire project team, both natural and social scientists. Whenever possible, model boundaries should reflect the natural boundaries of the particular coastal system being studied (for example Table 1).

4. THE MERBOK MANGROVE EXPERIENCE

While modelling techniques as outlined in the previous section are very powerful tools to investigate the functioning of a system, the successful use of these techniques in many cases requires a number of iterative steps that involve careful thought, data collection and analysis and the selection of alternative approaches. In an effort to illustrate such steps in the evolution of a real modelling exercise, this section presents a case study of a long-term programme to determine the fluxes of water, carbon, nitrogen and phosphorus from a tropical, mangrove ecosystem.

Mangrove forests constitute a dominant ecosystem of the low energy tropical coastlines of the world. In these areas the forests not only occupy, but in many ways determine, the nature of the interface between land and sea and the fluxes across this interface. They play many roles in the coastal zone including protection from coastal erosion, the provision of direct products, such as wood, and indirect products, such as nursery areas for coastal fisheries, and tourism. The impact of environmental change on these ecosystems is clearly identified as an important LOICZ research question in the Implementation Plan and details of an overall economic assessment of the importance of their diverse roles is treated in more detail in LOICZ. Mangrove forests are currently subjected to considerable human-induced change including: clear-cutting for timber; changes of use to mariculture and rice production, and use for human habitation. These changes in regions such as Southeast Asia and Central America are affecting, to an unknown degree, the flux of nutrients and organic carbon to coastal and near-shore waters.

There are numerous physical, chemical and biological processes that occur between the head and the mouth of an estuary. As water flows from rivers into estuaries, mixing with seawater causes numerous chemical transformations to occur. Changes in both chemical (such as redox) states and physical processes (such as electrical charges) result in some of the chemical settling out (for example, through flocculation). Some of these chemical species are also taken up or transformed by living organisms. The important processes occurring between the inputs from the riverine end and outputs at the marine end of the estuary must be identified and quantified. Biogeochemical modelling can play an important role in quantifying these processes sufficiently to produce a balanced budget.

The primary site for this study is the Sungai Merbok mangrove estuary in Malaysia $5^{\circ}40'$N, $100^{\circ}25'$E). The physical characteristic of the site have been described by Ong *et al.* (1991). The estuary is 30 km long and its depth varies from 3 - 15 m. Mangroves, dominated by *Rhizophora apiculata* and *Bruguiera parviflora* that grow to about 30 m, cover an area of about 50 km^2. The estuary is characterised by a 1.7 m semidiurnal tide, with peak currents of 1.3 m s^{-1}, and mean freshwater discharge of 20 m^3 s^{-1}. The estuary displays a pronounced neap-spring stratification-destratification cycle, and the effective longitudinal dispersion is approximately 10^7 m^3/d.

The main aim of the programme which started in the mid 1970's is to determine the fluxes of carbon and nutrient from the mangrove estuary. Initially this was linked to the question of the extent to which mangroves can be put to alternative uses without affecting the mangrove ecosystem and adjacent capture fisheries. Some 10 to 15 years later the question remains: are mangroves a source or a sink of atmospheric carbon? (Ong, 1993).

4.1 Single Cross-section Hydrodynamic Budgeting

The initial information required to model a system such as the Merbok Mangroves is an understanding of the underlying physical transport system. Initially the Kjerfve method (Kjerfve *et al.*, 1981) using measurements of current speed and direction across the width of the estuary was used. It involved using these data to obtain the covariance with the concentration of the scalar, at the mouth of the mangrove estuary. Despite data from 45 tidal cycles (4 to 9 stations, 3-5 depths at lunar hourly intervals), including a set with 31 continuous tidal cycles that covered a full spring/neap tidal cycle, estimates of water flux remained about an order of magnitude higher than those based on calculations from rainfall, evapotranspiration and catchment area. The difficulty with this application was that a salt balance could not obtained (Dyer *et al.*, 1992). The reason for this failure is not clear but it may have resulted from inaccuracies in the current measurements made with simple current vanes.

Although this method appears to be successfully applied in the salt marsh estuary of North Inlet, South Carolina, there appear to be problems when applied to mangrove estuaries, not only in the Merbok Mangrove estuary but also in the Ranong Mangroves in Thailand (Wattayakorn *et al.*, 1990). Fortunately in the Thai study it was possible to apply the modelling method of Wolanski and Ridd (1986) with better success. Unfortunately this method is applicable only during the dry season when there is no freshwater flow and thus cannot be applied to mangroves situated in areas where there is no dry season such as the Merbok.

In the Merbok case, trying to resolve a small residual from a huge tidal variation would require much more accurate current measurements as well as possibly more complete temporal and spatial sampling. Ten years down the hydrodynamics road from these first attempts to measure water flux through the system, there is still no solution, although much has been learned about the estuary (Uncles *et al.* 1990; Ong *et al.*, 1991; Uncles *et al.*, 1992; Ong *et al.,* 1993). A recent assessment of the data (Simpson *et al.,* in press) suggests that it may be possible to arrive at a solution with more accurate measurements.

4.2 3-D Numerical Hydrodynamic Flow Modelling

The more numerical fluid modelling approach has also been explored for the Sungai Merbok Estuary (see Haidvogel and Beckmann (submitted) for a review of available methods). Three-dimensional hydrodynamic models are designed to mimic the flow of water in an estuary based on mathematical description of bathymetry, tides, currents, and other physical parameters. An attempt was made by Phang (1994) to apply a small data set for the Sungai Merbok mangrove estuary to the TRIM 3D numerical model (Cassuli and Cheng, 1992; Cassuli and Cattani, 1993). Although this application of the TRIM model indicated that the results are often too complicated for use in understanding the biology of an ecosystem, they also suggested that this approach may be worth following up if better bathymetric and hydrographic data were available. Application of the TRIM model may be more appropriate if Acoustic Doppler Current Profilers (ADCP) can be used to more accurately measure current speeds in future research efforts.

4.3 Modelling The Mangrove-Atmosphere Interface

As with the measurement and modelling of the water movement in a system, a significant effort is often required to quantify a single important biogeochemical process. A second example of this from the Merbok study is the atmospheric inputs to the system. Budgets cannot be complete if the atmospheric interface is not considered, so another aspect of this study, though more related to GCTE and IGAC than to LOICZ, is on fluxes from mangrove tree canopies. A number of photosynthesis and related environmental and ecophysiological parameters in the mangrove canopy have been measured (Ong *et al.*, in press). This study has reached a stage where there is a need to carry out detailed modelling, such as the MAESTRO model of Jarvis *et al.* (1990), that will allow a certain amount of prediction of this one particular aspect of the ecosystem.

A project is also being initiated on measuring carbon dioxide fluxes from mangrove canopies using the eddy covariance method. This is essentially based on the same principle as the Kjerfve method that is used for measuring fluxes in the water but converted from hydrodynamics to aerodynamics. This again is a pure single point budgeting procedure with no predictive capacity; nevertheless it is hoped that it will be useful in quantifying fluxes in the mangrove forest.

4.4 A Mass Balance Carbon And Nutrient Budget In A Mangrove Ecosystem

In the absence of raw data for the system being studied, it is often possible to use substitute information from other sites or known relationships between easily measured variables and those that cannot be measured to estimate required information. For mangrove forests the standing biomass of trees and or parts of trees like leaves, branches, trunk and roots can be estimated using allometric relationships between easily measured parameters such as circumference of the tree trunk. Standard equations are now available for a number of mangrove species from a few different sites so it is not absolutely necessary to go through the rather tedious process of deriving your own equations.

Net primary production of a mangrove forest consists of a number of components: fine litter production, fine root turnover, herbivory, dead trees and tree growth. In mature or steady state systems the biomass that goes into dead trees is about equal to tree growth so that the standing crop or biomass remains constant. The other components detach from the trees and are either, buried, as in the case of the fine roots, leaf litter and some dead trees, eaten by detritivores such as sesarmid crabs that feed on leaf litter, or are removed from the system by tides. These components are thus released and part or all may be exported from the system. Using established relationships it is possible to estimate the standing crop and fluxes of nutrients in a mangrove swamp. When using a combination of measured and estimated values a budget can often be compiled to obtain at least an order of magnitude estimate of plant biomass (= carbon) and nutrient flux. Gong and Ong (1990) have attempted this for the Matang Mangrove Forest. They showed that annual export of N and P from the Matang Mangrove system was approximately 0.3 tonne ha^{-1} in both cases.

4.5 Mangrove Modelling with STELLA

In a mangrove ecosystem the mangrove trees are both the major primary producers and the major constituent of the standing crop or biomass. These plants take up nutrients like nitrogen and phosphorus from the estuarine waters, and return them to the water via decomposition of litterfall, dead trees and fine root turnover. If the litter, parts of dead trees and fine root get buried, then the estuary becomes a sink for carbon and mineral nutrients. This has to be taken into account in the input-output budget (often termed "storage"). In many places the plants are harvested, and so this amount has to be accounted for in the estimates of output.

A considerable amount of data, along with a few assumptions, are required to carry out budgeting that can accurately account for all of the sources, sinks and exports from such a system. Nevertheless the "storage" and harvest terms can be calculated (Gong and Ong, 1990). Unfortunately, as stated above in the last section, this empirical approach does not have a predictive capacity beyond the range of the empirical observations. As an alternative, this process may be modelled by using system modelling techniques and software. For this example the modelling tool STELLA is used (see Section 6 and Annex 1 for details).

One particularly useful aspect of STELLA as a tool for modelling is that one can use it to conceptualise how a particular system works. It is possible to build conceptual models that are either very simple or very complex. If the relevant data are available it is possible to turn the conceptual model into a quantitative model that can be used in a “predictive” mode. Two examples using STELLA are given here.

The first is a simple example of what happens to the mangrove biomass under different management strategies. In this case the modelling software is used to investigate how the amount of harvest changes with changes in the thinning and rotation periods. In Malaysia, many of the mangrove forests are managed for the production of timber. The management system used varies from state to state. In the Merbok Mangroves the forest is harvested in patches of a few hectares over a 30-year rotation. If there are 3,000 hectares of productive forest then the coupes, that is the size of area cut at a single harvest, can only be around 100 hectares, that is 100 hectares of forest are harvested each year. The Matang Mangroves located in another State are reputedly the world's best managed mangroves. A 30-year rotation is also used but here, instead of harvesting in coupes or patches, the trees are thinned at 15 years and at 20 years. About half the trees are removed at each thinning.

Since the forests are managed and the forestry departments keep records of the coupes, it is possible to estimate the age of trees in particular stands to within a year or two. Allometric equations of the girth of the tree against the total biomass of the tree are used to estimate the above- and below-ground biomass of the different aged stands. Ltterfall data for the different age stands are also available. From these it is possible to make very reliable estimates of the above-ground net productivity of these forests. One unknown in the biomass and productivity estimates is rate of turnover in the fine roots of the trees which could be almost as high as total litterfall.

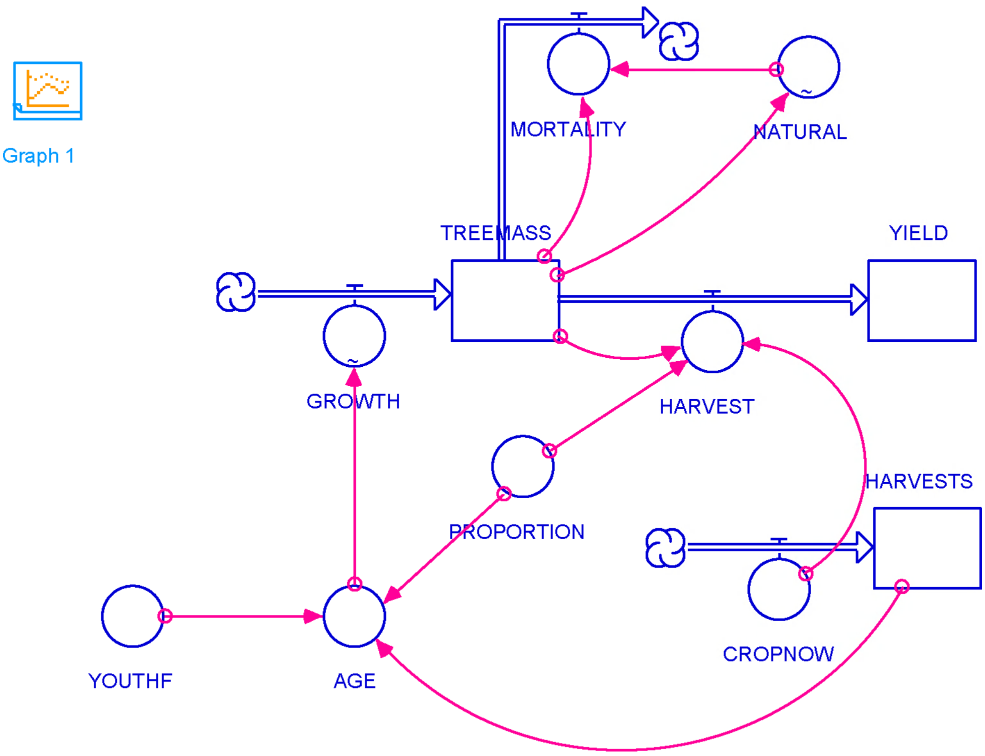


Figure 2. Detailed model for Merbok mangrove developed using STELLA software.

HARVESTS(t) = HARVESTS(t - dt) + (CROPNOW) * dt
INIT HARVESTS = 0

CROPNOW = PULSE(1,15,5)-(1.)
TREEMASS(t) = TREEMASS(t - dt) + (GROWTH - MORTALITY - HARVEST) * dt
INIT TREEMASS = 0

GROWTH = GRAPH(AGE)
(0, 0) (5, 2.8) (10, 18) (15, 12.5) (20, 12) (25, 12) (30, 12) (35, 12) (40, 12) (45, 12) (50, 12)
MORTALITY = TREEMASS*NATURAL
HARVEST = CROPNOW*TREEMASS*PROPORTION
YIELD(t) = YIELD(t - dt) + (HARVEST) * dt
INIT YIELD = 0

HARVEST = CROPNOW*TREEMASS*PROPORTION
AGE = TIME-YOUTHF*HARVESTS*PROPORTION*PROPORTION
PROPORTION = 0.5
YOUTHF = 20
NATURAL = GRAPH(TREEMASS)
(0.00, 7.77e-18), (25.0, 0.0105), (50.0, 0.0235), (75.0, 0.039), (100, 0.0545), (125, 0.0705), (150, 0.07), (175, 0.0705), (200, 0.0705), (225, 0.0695), (250, 0.0695)

Text Box 2. Equations generated by STELLA software to implement the mangrove model.

Using this data it is the possible to build a model of the change in forest biomass with time as a result of different harvesting strategies (Figure 2). Using STELLA the state variables (squares), flows (arrows), processes (circles) and sinks are identified and their quantities are estimated. STELLA converts graphic representations such as shown in Figure 2 to mathematical equations such as shown in Text Box 2. It is then possible, without too much expenditure of time and effort, to run the model and predict standing biomass and the amount of wood that could be harvested from the forests over a period of time (Radford, 1990). From the model, predictions can be made of what will happen if the thinning regime or the harvest cycle is modified. Since data on the nutrient content of the trees are available, it is also be possible to run a model based on nitrogen and phosphorus and thus get a good idea of the transformation of inorganic to organic nutrients.

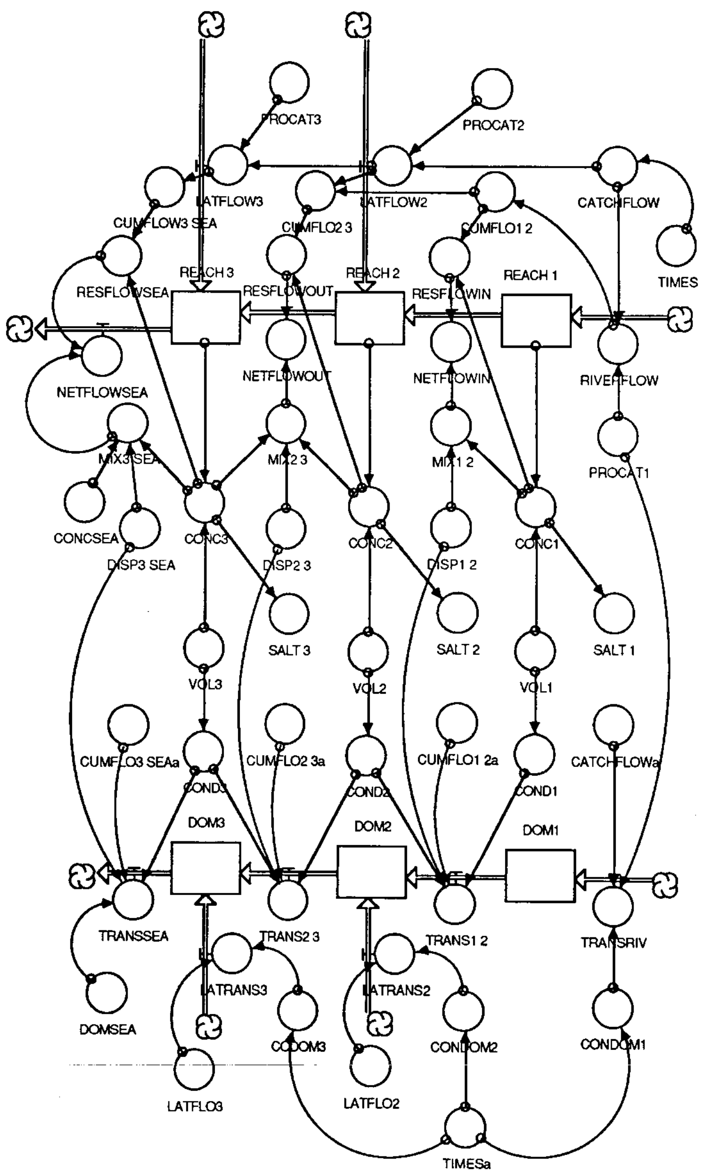


Figure 3. Complex system model of the Merbok Mangrove system generated using STELLA software.

The second example deals with a more complex three-compartment model looking at the flow of water, salt (conservative) and dissolved organic matter (non-conservative) through the estuary. Although there are not enough data to run this model, STELLA provides a useful way of identifying the main compartments of the ecosystem that might require quantification. Figure 3 shows how complex the model can become and also shows that by going through such an exercise, it is possible to identify exactly what types of data are required, thus the model helps in the conceptualisation as well as the design of the experiment. By developing such a conceptual model it is possible to avoid the unnecessary collection of considerable quantities of irrelevant data. In many cases the use of simple modelling software such as STELLA may be usefully applied at the very start of a new project.

5. RESPONSE TO FIRST LOICZ MODELLING REQUIREMENT - QUANTIFY FLUX

5.1 Describing Physical/Biological Systems and Defining Natural Boundaries

In order to build a budget model, it is necessary to define the spatial domain to be modelled. The definition of the land boundary is usually relatively easy; it is likely to be defined by the shore line or the limit of tidal excursion. Except for systems which are dominated by intertidal habitats (for example, mangroves or salt marshes), this exact position is not likely to be critical. The open, or "oceanic," boundary of in-shore waters may not be so readily chosen. To a great extent, breaking the world's coastal zone into typological units implies the recognition of classes of systems which might be useful in building an inventory of systems to be modelled within the context of LOICZ (LOICZ, 1995d). Regions will, however, be modelled at different spatial resolutions depending on a number of local and regional considerations. Many factors may need to be considered in defining the open boundary of the model domain: topography, habitat type, current system, and the distribution of material concentrations (Table 1).

In the case of topography, shelf edge, bay or estuary mouth, and sills between topographic basins are obvious candidates for definition of a "natural" open boundary. Particularly in the case of benthic dominated systems, habitat type (coral reef, seagrass bed, etc.) may provide useful boundaries. If there is no characteristic topography or habitat type in the model domain, it may be necessary to consider the current system or gradients of material concentration. For example the tidal excursion, the boundary between horizontal residual circulation water masses, and the frontal structure of material concentration are additional candidates for natural boundaries.

5.2 Defining the Questions to be Addressed

For the preparation of wider regional and global syntheses and estimates, the LOICZ Project requires data on carbon fluxes, but these guidelines show that it is more efficient to approach estimates of carbon flux through nutrient fluxes. Hence, the budget models discussed here will deal with fluxes of carbon, nitrogen, and phosphorus (CNP).

Within the context of LOICZ biogeochemical modelling, the primary questions to be addressed concern the role of the coastal zone as a source or sink for carbon, nitrogen, and phosphorus. Clearly, individual regions may function as sources or sinks for different materials, and equally clearly, the role of the coastal ocean, or parts thereof, may vary temporally between being material sources and material sinks. For example, many aquatic ecosystems take up dissolved inorganic carbon during the day (are sinks) and release inorganic carbon during the night (are sources). There are also clear seasonal cycles in biogeochemical fluxes within many systems. Scientific and management interest in the role of a system as a source or sink operates across a range of time and space scales. For example, systems receiving heavy nitrogen loading from sewage input may have primary production which is not nitrogen limited. With distance away from the nitrogen sources, primary production in many marine ecosystems may become nitrogen limited. Daily or seasonal changes in the biogeochemical performance of a system may provide information on the temporally varying cycles (for example, light and temperature) controlling such performance. It is necessary to identify the time and space scales and the processes by which such variations occur.

For the purpose of supplying data for global biogeochemical models, it is proposed that the flux estimates generally be aggregated into time steps of months to years. In some cases long-term steady state estimates may be all that are feasible or required. The smallest spatial scale which seems likely to be justified within the context of LOICZ in most instances is probably about 1 km, with space scales of 10's to 100's of km providing adequate resolution in many instances. It is often easier to develop robust budgets of systems at the larger spatial scales than the smaller spatial scales, because of decreased temporal variability of grid-averaged data. At the same time, the coarser spatial scales may sacrifice the ability to resolve the data by habitat or to extract detailed process-related information from the budgets. Final selection will depend on a balance of these considerations.

A total-system mass-balance budget is a simple class of mathematical models that tends to provide robust estimates of integrated ecosystem performance on the time and space scales of interest here. This class of model is little more than an ordered, objective description of what is known about the system in question. In many instances, collection of data which can be used in a budget may have occurred incidentally to other studies. Conservation of mass is, of course, a fundamental principle of nature. Therefore a comprehensive budget of the inputs of materials into the system of interest, outputs from that system, and amount in the system is an objective description that goes beyond simple tabulation of such data. While such budgets provide neither direct experimental nor direct theoretical information about how the system works, the budgets can describe the system at space and time scales which may not be amenable to experimentation or detailed simulation modelling. One result is that the descriptive output from budgets can be used in a statistical sense to evaluate and compare how systems work and how the parts of the Earth system are linked together.

5.3 General Methodological Background

In this chapter, a class of mass balance budgets are presented which are called here "stoichiometrically linked water-salt-nutrient budgets." The nutrients of specific interest here are carbon (C), nitrogen (N), and phosphorus (P), all of which are essential to life.

Stoichiometrically linked water-salt-nutrient budgets actually comprise a series of budgets which are solved in a prescribed order as described in Text Box 3. There is progressively more information about ecosystem performance to be derived by proceeding in the prescribed order. A note of caution seems warranted at this point. There are, in the ecological and geochemical literature, many so-called "budgets." Some of these are only partial budgets, and there may be more misinformation than information in a budget which is either partial or otherwise sloppily constructed. Consequently, any person constructing a budget should proceed in a careful fashion, with attention to completeness, and any person studying other persons' budgets is wise to consider just how carefully that budget has been constructed. At the same time, it should be appreciated that the construction of usable budgets requires judgements of what is (or is not) quantitatively important. A further point is that an overall "recipe" for the preparation of stoichiometrically linked budgets can be developed here, but the flavour of the eventual product will reflect the seasonings added by the individual cook working with the ingredients which are available.

1. **Water budget:** Establish a budget of freshwater inflows (such as runoff, precipitation, groundwater, sewage) and evaporative outflow. There must be compensating outflow (or inflow) to balance the water volume in the system.

2. **Salt budget:** Salt must be conserved in the system. Therefore salt flux not accounted for by the salinities used to describe the freshwater flows in Step #1, above, must be balanced by mixing. If there is no salinity difference between the system of interest and adjacent systems, or if the pattern of water exchange is too complex to be amenable to be described by the combined water and salt budgets, some more complex form of circulation analysis will be required. Steps #1 and #2 describe the exchange of water between the system of interest and adjacent systems by the processes of advection and mixing.

3. **Budgets of nonconservative materials:** All dissolved materials will exchange between the system of interest and adjacent systems according to the criteria established in Steps #1 and #2, above. Deviations of material concentrations from predictions based on these two previous steps are quantitatively attributed to net nonconservative reactions of materials in the system.

4. **Stoichiometric relationships among nonconservative budgets:** It can often be assumed that the nonconservative flux of dissolved inorganic phosphorus is an approximation of net metabolism at the scale of the ecosystem, because there is no gas phase for phosphorus flux. Nitrogen and carbon both have other major flux pathways (notably denitrification, nitrogen fixation, gas exchange across the air-sea interface, and [in some systems] $CaCO_3$ reactions). The deviation of the fluxes of these materials from expectation based on C:N:P composition ratios of reactive particles in the system can be assigned to other processes in a quantitatively reproducible fashion.

Text Box 3. Summary of sequential steps in budgetary modelling analysis.

In general terms, the sequence of budgets for use in stoichiometrically linked CNP budgets follows four steps: water budgets, salt budgets, nonconservative materials and stoichiometric linkages among nonconservative budgets.

Water Budgets: The concept of the hydrological cycle is well established, and is often presented (both globally and locally) in terms of water budgets. The conceptual model may be represented by a simple box diagram (Figure 4). An accounting of freshwater inflows to a coastal marine system (such as runoff, precipitation, groundwater) and of evaporation from the system is often rather easy to accomplish. The fundamental concept behind the budgets, of course, is the conservation of water mass. 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;" there are likely to be other flows, but the difference between inflows and evaporative outflow must be balanced by this residual flow. As examples of judgement 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. Simple calculations can usually be made to estimate whether terms such as these are likely to be significant above the errors in the other terms.

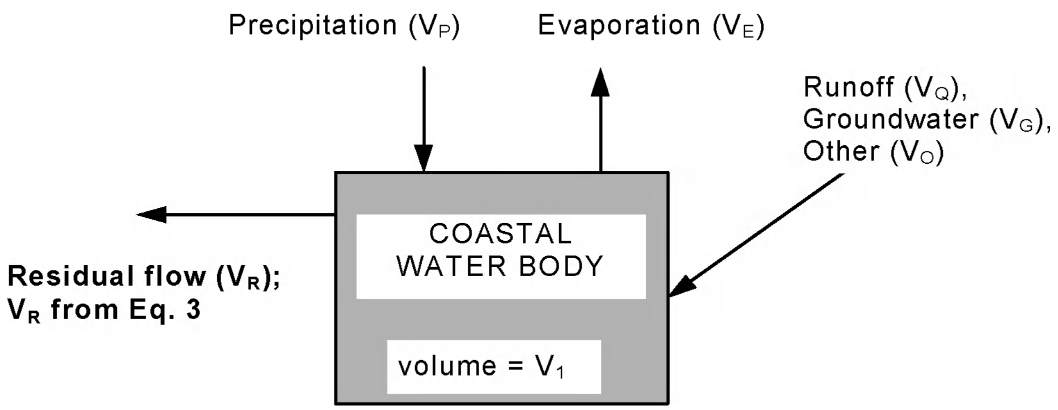


Figure 4. Generalised box diagram illustrating the water budget for a coastal water body. The arrows show the net water flow associated with each process. Quantities which are generally measured are shown in light typeface, while the quantity which is calculated to balance the budget (that is, V_R) is shown in bold typeface. In systems with net freshwater inflow, V_R will be negative (that is, out of system). System volume (V_1) is in units of volume, while all flow volumes are in units of volume per time.

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 5) which includes these exchange flows in addition to residual flow. These exchanges are often modelled as mixing, rather than as advection. The salinity balance accounts for these additional exchange flows. In this case, note that any material in the water which is not changing by internal reactions within the system (in general, the salt of any abundant, highly soluble material) can be used in place of salinity. "Salinity", as defined by oceanographers, is in effect the sum of those 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. Specific materials with similarly non-reactive properties (chloride is a common example) are said to be "conservative" with respect to salinity.

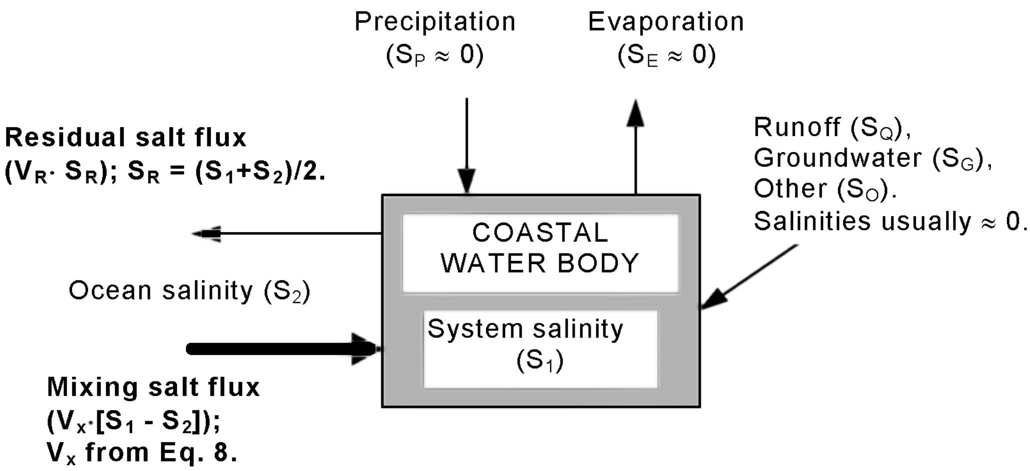


Figure 5. Generalised box diagram illustrating the salt budget for a coastal water body. The arrows show the net salt flux associated with each process. In general, residual flow (that is, $V_R \cdot S_R$) is negative indicating flow from the system. Under such conditions, mixing (V_X) is likely to transport salt into the system. Quantities which are generally measured are shown in light typeface, while quantities which are calculated within the budget are shown in bold typeface.

The concept of "conservative" should be treated with some caution. On some time scales all of the salts in the ocean react. Therefore no salt dissolved in water is truly conservative with respect to water. Systems which include significant evaporite deposits may exhibit very nonconservative behaviour of salinity. In low salinity systems, ion ratios may vary significantly; the entire concept of "salinity" becomes qualitative. In such systems it may be safer to use a property which is more explicitly defined (for example, Cl). Having pointed to these cautionary notes with respect to salinity, it is useful to realise that salinities of streams or groundwater flowing into estuarine systems or the slight salt content of precipitation can be ignored in most cases. Again, simple calculations to evaluate this assumption are a useful precaution.

In the absence of salinity gradients or adequate data to establish salt budgets or, in the presence of spatial distribution patterns which are too complex for simple water and salt budgeting, it may be feasible to develop 2 dimensional or 3 dimensional numerical models of water circulation (Haidvogel and Beckmann, submitted). The output from such numerical circulation models may subsequently be substituted for water and salt budgets in order to estimate water exchange.

Budgets of nonconservative materials
The next step in the budgeting exercise is to consider materials which may not behave conservatively with respect to salinity (Figure 6). These budgets may be termed budgets of nonconservative 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. Water exchange, defined by the water and salt budgets, describes the exchange fluxes of these elements along with salt. Clearly, total C, N, and P are conserved, but these elements may be transformed from measured, such as dissolved, to unmeasured, such as particulate or gaseous, phases. All dissolved phases of these materials are known to be involved in biochemical and abiotic reactions, so they are not likely to be conservative with respect to salinity. In the case of salinity, the budget is exactly balanced by water exchange. In the case of dissolved C, N, and P, the budgeted exchange fluxes are likely to leave some residual flux which is not balanced by these calculations. This residual for each element is a measure of the net internal fluxes (that is, sources minus sinks) of these materials. In fact, "conservative behaviour" of these materials with respect to salt would be taken to reflect one (or perhaps both) of two conditions: either the exchange rates of these materials in the water are fast relative to the internal fluxes, or the "conservative behaviour" represents the sum of uptake and release fluxes which cancel one another out. If turnover dominates over net flux in the cycle of a particular material, then the proportionality between salinity and this material is likely to be accompanied by a great deal of scatter in the data, reflecting rapid turnover but little net change (see examples in Imberger *et al.*, 1983).

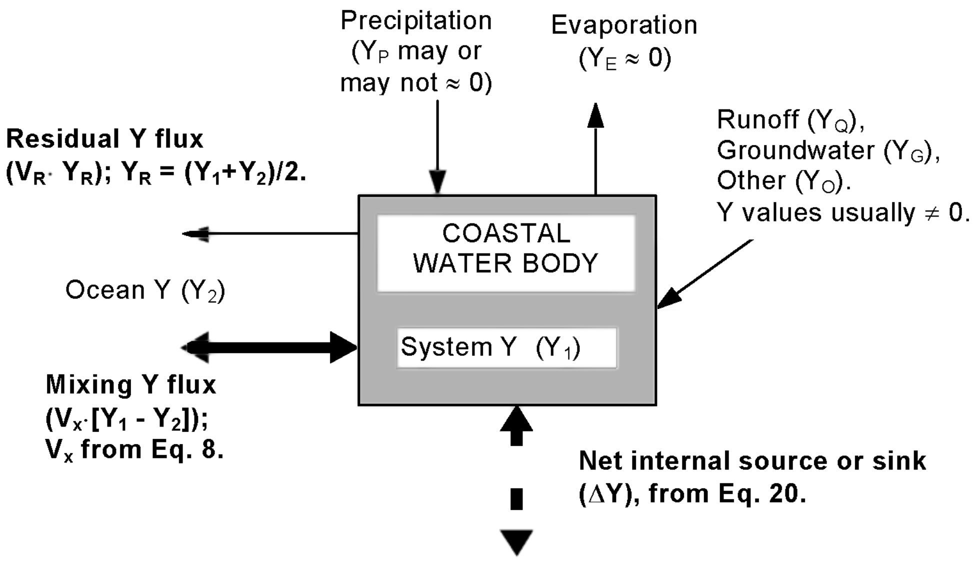


Figure 6. Generalised box diagram illustrating the budget for a nonconservative material, Y, in a coastal water body. The arrows show the net flux of Y associated with each process. Mixing (V_X) may be to or from the system. Quantities which are generally measured are shown in light typeface, while quantities which are calculated within the budget are shown in bold typeface. ΔY denotes the nonconservative flux of Y, and can be positive or negative with respect to the system.

Two other cautions are in order here. Firstly, it was pointed out above that water input from processes like groundwater and sewage could often be ignored, and that the contributions of these terms to the salt balance could likewise usually be ignored. It is clearly not the case that the nutrient content of this water can be ignored; that should never be done for systems receiving significant sewage input and should be done only with some caution for groundwater and precipitation. If there is runoff, the nutrient input from that runoff must be included in the budget.

Secondly, the budgets present here generally involve only dissolved materials. While there are methods to construct very useful budgets for particle fluxes, for example, sediment input by streams and deposition within the system, in general, salinity-based budgets must be treated with great caution in constructing budgets for particulate materials in shallow water systems. The reason is relatively simple. Dissolved materials have no gravitational component of flux within the water while particles do. Therefore particle distribution in the water column is likely to be extremely “patchy,” with respect to both time and space, in areas subject to heavy loading with stream sediments, as well as in systems where wave mixing or active bioturbation is stirring the bottom sediments up into the water column. These processes can generate great heterogeneity in estimates of particle concentrations. While budgetary calculations for particles can be made according to the procedures to be outlined here, sampling artefacts may make the results quantitatively unreliable. As a result, the use of salt and water balance calculations are not generally useful to estimate particle budgets. It is worth recalling, however, that conservation of mass is a fundamental law of nature. Therefore, for materials without a gas phase, any deviation of dissolved forms of that material from conservative behaviour must represent net uptake or release with respect to particles. This point is used in the interpretation of output from the budgets.

Stoichiometric linkages among nonconservative budgets

The next step involves developing the stoichiometric linkages among nonconservative budgets. The basic assumptions here 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. This point will be developed in the case studies, below.

For the sake of linking the C, N, and P budgets, phosphorus 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 nitrogen and carbon have prominent gas phases, and carbon and nitrogen 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 nitrogen and carbon (Figure 7).

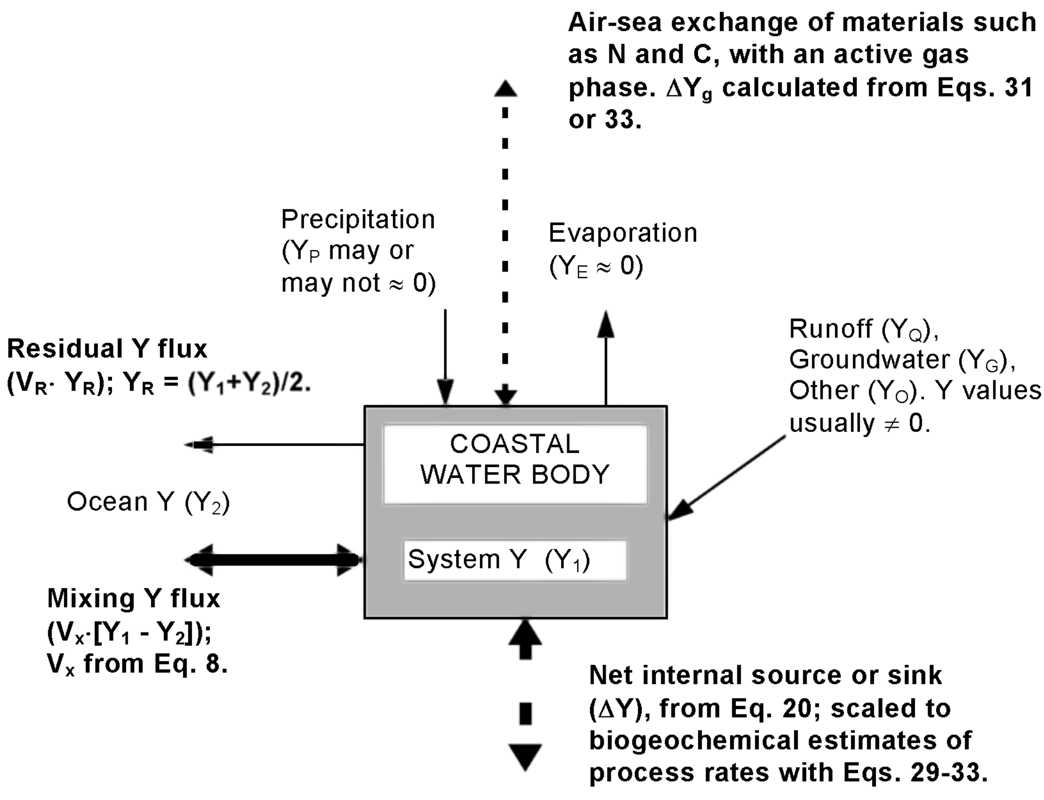


Figure 7. Generalised box diagram illustrating the budget for a nonconservative material, Y, which has an active gas phase in a coastal water body. In this case, appropriate stoichiometric linkages are used to scale the nonconservative fluxes (ΔY's) to system-scale estimates of internal biogeochemical processes. The arrows show the net flux of Y associated with each process. Quantities which are generally measured are shown in light typeface, while quantities which are calculated are shown in bold typeface.

In the case of nitrogen, the gas-phase reactions require biochemical activity to transfer nitrogen between fixed inorganic (NO_3, NH_4, and small amounts of NO_2) and organic (dissolved organic nitrogen (DON) and particulate nitrogen (PN)) pools and gaseous nitrogen (dominated by N_2). These reactions may be taken to represent the net difference between nitrogen fixation (represented in simplified form here as $N_2 \rightarrow$ organic nitrogen) and denitrification (in simplified form, $NO_3 \rightarrow N_2 + N_2O$). N_2 and N_2O) are not generally measured in seawater. In any case, the amount of N_2 in seawater is so large in comparison to all other forms of nitrogen that transfers to or from the fixed nitrogen pools are insufficient to affect N_2 measurably (generally << 1% change in N_2, even though the changes in the other pools may be large). 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 nonconservative fluxes of nitrogen in coastal systems. Therefore this stoichiometric procedure is a relatively robust way to estimate the difference between nitrogen fixation and denitrification. See, for example, Webb (1981) and Carpenter and Capone (1983) for discussions of nitrogen biogeochemistry and chemical ecology in the marine environment.

In the case of carbon, the transfers between the gas phase (CO_2 and its hydrated form H_2CO_3) and the dissolved phase are rapid responses to thermodynamic equilibration. Moreover, in the case of carbon, the gaseous phase is not large and is typically either measured or calculated thermodynamically. Further, the gaseous CO_2 content of seawater is typically measurably out of equilibrium with the atmosphere, so that gas exchange processes are constantly tending to cause CO_2 flux across the air-water interface. Deviations of carbon flux with respect to predictions based on phosphorus are therefore measures of the exchange flux of CO_2 across the air-sea interface. As was pointed out with nitrogen, the carbon fluxes which are not proportional to phosphorus are often large and are therefore useful measures of this gas flux. These and other complications in the carbon fluxes are considered in the case studies. Skirrow (1975) and Smith (1985) provide syntheses of the chemistry and chemical ecology, respectively, of CO_2 in aqueous systems.

5.4 Mathematical Structure of the Budgeting Procedure

With this background on the budgeting sequence, a very generalised mathematical description of the budgeting procedure can be laid out. The general procedure cannot deal with all of the details encountered in real-world situations, so the user of these guidelines is urged to gain a sufficient understanding of these rules to be able to use common sense in developing budgets. Following this section on the general mathematical structure of budgeting and the next section on information requirements, specific case studies are presented in which the mathematical formulation and other aspects of model development are explored in more detail. Officer (1980) provides a detailed and comprehensive review and analysis of calculating both water and salt budgets and nonconservative fluxes according to box models. The analysis presented here is a greatly shortened version of Officer's literature review and algebraic analysis. Officer also discusses the relationship between such box models and mixing diagrams widely used by geochemists to characterise materials which are not conserved relative to salinity. In this latter context, the short paper by Officer (1979) is a particularly clear explanation of the algebra behind mixing diagrams. Officer and Lynch (1981) and Loder and Reichard (1981) discuss, via numerical analysis, apparent nonconservative behaviour which can be generated as analytical artefacts if mixing diagrams are used to describe the distribution of materials in systems which are not at steady state. Kaul and Froelich (1984) give a specific example of this point. Formal extension of the nonconservative flux calculations to stoichiometric linkages and explicit numerical treatment of data not at steady state have been explored by Smith and his colleagues (Smith *et al*, 1991; Smith and Atkinson, 1994).

5.4.1 Water budget

Water is conserved. Therefore, the water volume entering a system must equal water volume storage within the system minus the water volume flowing out of the system (Figure 4). Inflows include stream runoff (V_Q), direct precipitation (V_P), and groundwater (V_G). There might be other inflows (V_O) such as sewage. There is also hydrographically driven advective inflow (V_{in}). Removals include evaporation (V_E) and advective outflow of water from the system (V_{out}). Water storage may be represented by the change in system of interest with time (dV_1/dt):

$$\frac{dV_1}{dt} = V_Q + V_P + V_G + V_O + V_{in} - V_E - V_{out} \tag{1}$$

In concept, Equation (1) is simple enough. For the purposes of actual budgeting, the equation may be difficult to implement. In practice, in any situation, there may be multiple source terms for V_Q, V_G, and V_O. In a large system, precipitation and evaporation may vary over the area of the system. These complications of multiple terms are relatively easily dealt with, if the data base is adequate to sum up the parts. V_{in} and V_{out} are the only terms in Equation (1) which are not readily measured. By rearrangement of Equation (1):

$$V_{in} - V_{out} = \frac{dV_1}{dt} - V_Q - V_P - V_G - V_O + V_E \tag{2}$$

It is useful to consider the difference between V_{in} and V_{out} as the residual flow driven by the water budget; This is identified as V_R. Further, in many cases dV_1/dt may be considered constant, simplifying the equation. V_{out} and V_{in} cannot be solved individually from this equation, but they can be used to evaluate V_R.

All of these terms have the units of volume per time (in most examples presented here represented by $m^3\ d^{-1}$). V_Q, perhaps V_G, and perhaps V_O are likely to be measured directly in units of volume per time. Precipitation (P) and evaporation (E) are typically measured in units of length per time ($mm\ d^{-1}$); volumetric estimates (that is, V_P, V_E) are derived by multiplying P and E (in length per time units) by system area (that is, the map area of the water surface being budgeted). In general, V_Q is likely to be the largest term on the right hand side of Equation (2) and is unlikely to be estimated to closer than 5-10% accuracy. Therefore any term much smaller than 5% of V_Q, or, if V_Q is not the largest term, of the largest term in the equation, can be ignored as being within the noise of the data. In most applications, V_O and probably V_G are sufficiently small to be ignored in the water budget; in many applications, V_Q may be the only term large enough to figure in the estimation of V_R. All freshwater inputs minus evaporation are combined into a single term (V_{Q^*}). Equation (2) can be simplified accordingly:

$$V_R = V_{in} - V_{out} = \frac{dV_1}{dt} - V_{Q^*} \tag{3}$$

While 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. V_R remains as the “residual flow” required to balance the water budget. Note that V_R is positive only in systems with evaporation in excess of precipitation and river inflow; that is, residual flow is into the system. The more usual case where freshwater input dominates, yields a negative value for V_R. The ratio of the absolute value of the system volume to the residual flow, that is, $|V_1/V_R|$ with units of days, is sometimes referred to as the freshwater residence time, or the hydraulic residence time, of the system. The total water exchange time is usually much shorter than the freshwater residence time, as demonstrated below.

5.4.2 Salt budget

Tidal or wind-induced inflows and outflows are not important to the water budget because they tend to balance out over time. However, these flows do exchange salt and other materials between the system of interest and the “outside world,” so they are important to the budgets of these materials. In effect, these exchange fluxes can be considered to be mixing terms (Figure 5). The horizontal exchange flux is represented by V_{in} and V_{out}. Dimensionally these fluxes, like the terms in the water budget, have the units of volume per time. 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 is designated by subscript 1; water outside the system is designated by subscript 2. These conventions lead to the following equation:

$$\frac{d(V_1S_1)}{dt} = V_{Q*}S_{Q*} + V_{in}S_2 - V_{out}S_1 \qquad (4)$$

Equation (4) can be simplified somewhat. For most applications, all salinities except S_1, and S_2 are likely to be small and can be considered to be 0. If there is doubt about the validity of this simplifying assumption, the investigator should evaluate the sensitivity of Equation (4) to that assumption with sample numerical values. Dropping the terms with small salt addition is useful for discussion without sacrificing anything in the algebra:

$$\frac{d(V_1S_1)}{dt} = V_{in}S_2 - V_{out}S_1 \qquad (5)$$

In Equation (5), the mixing exchange terms (V_{in}, V_{out}) remain as the unknowns. By combining Equations (3) and (5) and expanding the term $d(V_1S_1)$, V_{in} and V_{out} can now be evaluated individually:

$$V_{in} = \frac{1}{(S_2 - S_1)}\left[V_{Q*}S_1 - V_1\frac{dS_1}{dt}\right] \qquad (6)$$

and

$$V_{out} = \frac{1}{(S_2 - S_1)}\left[V_{Q*}S_1 - V_1\frac{dS_1}{dt}\right] - \frac{dV_1}{dt} + V_{Q*} \qquad (7)$$

It can be seen that Equations (6) and (7) simplify considerably if either dS_1/dt or dV_1/dt, or both, can be treated as constant. In particular, if $dV_1/dt = 0$, $V_{in} = V_{out} - V_{Q*}$. That is, V_{in} and V_R move water back and forth with respect to the system, with the difference between these terms being $-V_{Q*}$, the residual flow (Equation 3). It is therefore convenient to redefine V_{in} as the water exchange flow, V_X. Moreover, because the residual flow (V_R) can be either out of the system, that is, a system in which freshwater inflow exceeds evaporation, or into the system, that is, net evaporation, the appropriate salinity to use for residual flow is the salinity at the boundary between boxes 1 and 2. This salinity at the boundary is defined as S_R, the average of S_1 and S_2. By rearrangement of Equation (6) and use of the notation V_R and S_R for residual flow and the salinity of that flow:

$$V_X = \frac{1}{(S_1 - S_2)}\left[V_1\frac{dS_1}{dt} + V_RS_R\right] \qquad (8)$$

In many cases, system volume (V_1) is treated as constant; V_1 can be taken outside the derivative on the left side of the equation. If S_1 is also constant, then the salt content of the system is said to be at steady state. The entire derivative ($d(V_1S_1)/dt$) becomes 0, and the equation simplifies. This steady-state solution is the most common solution encountered in the literature for marine system; in lakes or other very confined water bodies, volume and/or salinity may vary with time. The full derivative term in the algebraic analysis will be retained, although most of the case studies presented will consider only the steady-state solution.

Total water exchange time is given by the ratio $V_1/(V_R + V_x)$. Note that this value will in general be smaller than freshwater residence time, often much shorter. 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_1 and S_2. In practice, the absolute value of this term should deviate from 0 by at least several tenths (p.s.u.) in order to achieve a robust estimate of V_x. In time trend data, V_x values which are large (positive or negative) with respect to their neighbour values are likely indicators that the term (S_1-S_2) is not reliably different from 0. Note that the exchange terms are readily derived if there is only one external salinity (S_2) mixing with the system salinity (S_1).

This 0-dimensional structure developed is readily expanded into a 1-dimensional series. Moreover, because many aquatic systems are stratified, it is often useful to lay out a two-layer analysis. The basic analytical structure which will be developed corresponds to surface outflow of less saline water and deep inflow of more saline water, with vertical mixing in each sub-basin. This model corresponds closely with both the classical analysis by Knudsen (1900) for the water and salt balance of the Baltic and the general concept of two-layer estuarine circulation (Pritchard, 1969), as presented in the form of box models by Officer (1980). In the following expansion, only the case where both volume and salinity of each box remain constant with time, that is, dV/dt = dS/dt = 0, is considered. This assumption simplifies the algebra but is by no means required. For more detail, the reader is referred to Wulff *et al.* (1994).

Each of n sub-basins (with n = 1 being the closest to shore) is divided into a surface box (s) and a deep box (d). At steady state, vertical entrainment ($V_{ent(n)}$) of water from the deep to the surface box of basin n equals the difference between water flowing horizontally to and from the deep box (i.e., $V_{in\rightarrow d(n)}$ - $V_{out\rightarrow d(n)}$). For the surface box, horizontal outflow - inflow ($V_{out\rightarrow s(n)}$ - $V_{in\rightarrow s(n)}$) equals freshwater inflow ($V_{Q*(n)}$) plus vertical entrainment. Further, the salt exiting the surface box ($V_{out\rightarrow s(n)}S_{s(n)}$) equals the salt input to the deep box ($V_{in\rightarrow d(n)}S_{s(n+1)}$) . Vertical mixing exchange ($V_{z(n)}$) between each surface and deep box also occurs and balances the salt budget.

$$V_{ent(n)} = V_{in\rightarrow d(n)} - V_{out\rightarrow d(n)} \tag{9}$$

$$V_{ent(n)} + V_{Q*(n)} = \left[V_{out\rightarrow s(n)} - V_{in\rightarrow s(n)}\right] \tag{10}$$

$$V_{out\rightarrow s(n)}S_{s(n)} = V_{in\rightarrow d(n)}S_{s(n+1)} \tag{11}$$

$$V_{s(n)}\frac{dS_{s(n)}}{dt} = V_{in\rightarrow s(n)}S_{s(n-1)} - V_{out\rightarrow s(n)}S_{s(n)} + V_{ent}S_{d(n)} + V_{z(n)}\left[S_{d(n)} - S_{s(n)}\right] \tag{12}$$

$$V_{d(n)}\frac{dS_{d(n)}}{dt} = V_{in\rightarrow d(n)}S_{d(n+1)} - V_{in\rightarrow d(n)}S_{d(n)} - V_{ent}S_{d(n)} - V_{z(n)}\left[S_{d(n)} - S_{s(n)}\right] \tag{13}$$

In this system of equations, surface inflow to the nth basin equals surface outflow from basin n-1; deep inflow to the nth basin equals outflow from basin n+1. For the first basin (n=1), surface inflow and deep outflow = 0. As with the 0-dimensional case, salinity differences between horizontally adjacent water masses are required to be non-0 values.

5.4.3 Estimates of water exchange via numerical modelling

It is, of course, possible to develop nutrient budgets in the absence of salt budgets. Examples of this include the classical “flow respirometry” measurements across coral reef flats (Odum and Odum, 1955) and budgets of materials flowing in and out the mouths of tidal channels (Kjerfve *et al.,* 1981; Wattayakorn *et al*., 1990). In such instances it will be necessary to turn to an alternative estimate of water exchange, possibly including complex 2 or 3 dimensional numerical circulation models in order to describe the exchange terms. It is beyond the scope of this report to discuss this array of methodology in detail (see, for example, Haidvogel and Beckmann, submitted), but a brief review is helpful.

From the physical viewpoint, the magnitude of horizontal mixing V_x is determined by the dominant current system around the open boundary of the model area. If the tidal current is dominant, the effect of tidal mixing is the largest for the determination of the magnitude of V_x. If the density-driven current or the wind-driven current is dominant, the effect of water exchange due to the vertical gravitational circulation or that of water exchange due to the horizontal residual circulation is the largest for the determination of the magnitude of V_x respectively. In the case where the open boundary is the shelf edge, the effect of the boundary current is frequently dominant in addition to the three currents system mentioned above. The water exchange between the shelf and the open sea due to frontal eddies, which is generated by the instability of the boundary current, mainly determines the magnitude of V_x.

The results of direct current measurement around the open boundary of the model area are separated into tidal current, density-driven currents, and wind-driven currents by statistical analysis and harmonic analysis. The magnitude of V_x can then be estimated with the current data, as follows.

For the contribution from tidal currents ($V_{x(t)}$):

$$V_{x(t)} = \frac{2 \cdot a \cdot U \cdot L \cdot l}{\pi} \tag{14}$$

Here a (0 < a < 1.0) denotes the mixing rate of water mass during one tidal cycle. The magnitude of ‘a’ depends upon the horizontal geometry and bottom topography around the system. It ranges between 0.2-0.4 in narrow straits and 0.1 on wide shelves (Yanagi, 1989). U is the vertically averaged tidal current amplitude, L is the tidal excursion, and l the horizontal length of the open boundary of the model area.

For density-driven currents ($V_{x(d)}$):

$$V_{x(d)} = \frac{U_u \cdot h \cdot l}{2} \tag{15}$$

Here, U_u denotes the current speed of the density-driven current in the upper layer; and h is the water depth.

For wind-driven currents ($V_{x(w)}$):

$$V_{X(w)} = \frac{U_w \cdot h \cdot l}{2} \tag{16}$$

Here U_w denotes the maximum speed of barotropic wind-driven current normal to the open boundary.

For frontal eddies ($V_{x(f)}$):

$$V_{x(f)} = b \cdot r \cdot D \cdot C \tag{17}$$

Here b (0 < b < 1) is the entrainment ratio of shelf water in the frontal eddy, r is the wave length of frontal eddy, D is the thickness of frontal eddy and C is the phase speed of frontal eddy. The magnitude of b ranges from 0.01 to 0.05 (Lee *et al.*, 1981).

The terms may then be linearly superimposed to derive an overall estimate of V_X:

$$V_X = V_{x(t)} + V_{x(d)} + V_{x(w)} + V_{x(f)} \tag{18}$$

In the real world of the coastal sea, the residual flow field is not steady. Tidal currents and tide-induced residual currents are nearly steady throughout the year with the spring-neap tidal cycle modulation. The density-driven current, however, varies seasonally in temperate and high latitudes, and strong episodic density-driven currents are sometimes generated by high freshwater inflows from flooding. The most variable component of residual flow is the wind-driven current due to the wind above the sea surface. It is difficult to estimate an appropriate "typical" V_x when the residual flow field is highly variable and complex around the open boundary. In such case, some averaging procedure on the residual flow field is carried out in order to estimate a correct V_x for material transport under particular circumstances.

5.4.4 Summary of conservative material balance

It follows from the above analysis that the balance, or budget, of salt in the system of interest is defined by the following general equation describing the mass of material S in the system (dVS/dt), where ΣV_{in} and ΣV_{out} represent all of the hydrographic inputs and outputs (including in this case exchange flow in and out) of each water type and S_{in} and S_{out} represent the salinity of those water inputs and outputs:

$$\frac{d(VS)}{dt} = \sum V_{in}S_{in} - \sum V_{out}S_{out} \tag{19}$$

Expanding this equation:

$$V\frac{dS}{dt} + S\frac{dV}{dt} = \sum V_{in}S_{in} - \sum V_{out}S_{out} \tag{20}$$

Steady state assumptions of either dS/dt or dV/dt may simplify Equation (20). It is worth remembering at this point that various of the water sources entering the system are likely to have a salinity near 0 (p.s.u.).

5.4.5 Budgets of nonconservative materials

Equation (20) represents a salt balance for the system, whether determined by means of a water and salt budget or direct estimates of water advection and mixing. Materials which are not conservative with respect to water and salt can be assumed to be represented by the same hydrographic inputs and outputs as govern the water and salt. Thus, the advection and the mixing exchange derived for water and salt are equally well applied to these other materials (Figure 6). For any material Y, Equation (20) is modified to include the sum of the nonconservative processes acting in the system to add and remove Y (that is, ΔY). It is assumed that the concentration of Y in evaporating water is 0, but it is not assumed that inputs of Y in the other water sources are 0.

$$V\frac{dY}{dt} + Y\frac{dV}{dt} = \sum V_{in}Y_{in} - \sum V_{out}Y_{out} + \Delta Y \tag{21}$$

Again, steady state assumptions may allow one or both of the derivatives on the left side of the equation to be dropped. In some cases individual fluxes may be directly available, rather than being the product of concentration and flow. For example, sewage input of Y may be directly known, without data on sewage volume. The summed nonconservative fluxes (ΔY) are the information desired and are derived by rearrangement:

$$\Delta Y = V\frac{dY}{dt} + Y\frac{dV}{dt} - \sum V_{in}Y_{in} + \sum V_{out}Y_{out} \tag{22}$$

The units of ΔY are mass per time; generally presented in this report as moles (mol) or kilomoles per day. Note two aspects of this equation. In the first place, this derivation gives no information about the processes leading to ΔY, either the number of processes or the general form of those processes. Physical, abiotic chemical, or biotic chemical processes may contribute to ΔY, and they are indistinguishable from this derivation. Such information is derived through other considerations, as discussed in the next section and exemplified in the case studies. Some terms, again sewage is an example, may be directly entered as known values in Equation (22), or may be part of the term ΔY.

In the second place, while this budgeting procedure based on a salt balance is in principle applicable to any material in many situations, it often cannot be applied with much quantitative success to particulate materials. The concentrations of these materials tend to be so patchy both spatially and temporally in response to sedimentation and resuspension that they are not adequately sampled in the context of a budgetary procedure derived for application to tidally averaged data.

In general is useful to express ΔY per unit area, by dividing the value estimated according to Equation (22) by the system area, often expressed as mol or mmol m^{-2} d^{-1}.

5.4.6 Stoichiometrically linking the nonconservative CNP budgets

One procedure for gaining insight into the processes leading to the nonconservative fluxes is to examine the "stoichiometric linkages" between the fluxes. The underlying assumptions behind this approach are firstly that a small number of processes can be enumerated which are likely to dominate these nonconservative fluxes, and secondly, that the underlying chemical stoichiometry of each of these processes can be approximated. Each of the nonconservative flux pathways likely to be important for these elements are considered in this subsection, proceeding from carbon fluxes, as the currency of primary interest, to the stoichiometric relationships among carbon, phosphorus, and nitrogen. In the remainder of this subsection, it is assumed that nonconservative fluxes of dissolved C, N, and P have been derived as discussed above. The nonconservative fluxes are here noted with the symbol "Δ."

Carbon fluxes
CO_2 in seawater moves among several dissolved inorganic ions according to rapid chemical equilibration reactions: $H_2CO_3 \leftrightarrow HCO_3^- + H^+ \leftrightarrow CO_3^{2-} + 2H^+$. The sum of these ionic forms is often written as "DIC" (dissolved inorganic carbon). Adequate measurement of the dissolved inorganic C system in water requires the measurement of two components related to the CO_2 system. Measurement of two components, plus temperature and salinity, allows a complete description of DIC partitioning. Realistic measurement possibilities include pH, total alkalinity (TA), DIC, and pCO_2. In practice, pH and TA are the most commonly measured variables; in principle, the most useful ones to use for budget calculations are DIC and TA. It is beyond the scope of this report to discuss the measurements further. Skirrow (1975) provides a detailed discussion of the theory and practice of measuring the CO_2 system in water.

Carbon fluxes in aquatic ecosystems include organic biogeochemical fluxes, inorganic biogeochemical fluxes, and abiotic fluxes controlled by physical-chemical considerations. The prevailing organic fluxes are primary production of organic matter and oxidation of organic matter via various pathways. It is convenient to represent primary production and aerobic respiration by an equation of the form:

$$CO_2 + H_2O \leftrightarrow CH_2O + O_2 \qquad (23)$$

The reaction proceeding from left to right represents a geochemical simplification of primary production, while the reaction proceeding from right to left represents respiration. Any budgetary analysis, including traditional flow respirometry or incubation techniques, measures the net of these processes over the budget period. It is thus concluded that the net reaction primary production minus respiration (*p-r*) with respect to carbon is equal to the net decrease in CO_2 according to Equation (23). Because CO_2 equilibrates rapidly among its dissolved ionic forms, change in DIC is the variable of immediate interest here. Decreasing DIC may indicate net production of organic carbon, while increasing DIC may indicate net consumption of organic carbon. Let us denote the change of DIC due to organic metabolism as ΔDIC_o.

DIC flux is involved in two other reactions which are likely to be important at the scale of the system. If the CO_2 partial pressure of the water ($pCO_{2(w)}$) differs from that of the air ($pCO_{2(a)}$), then there will be gas flux across the air-sea interface from high to low pCO_2. This change in DIC is denoted as

ΔDIC_g. DIC changes in the water also occur during the precipitation (DIC decrease) or dissolution (DIC increase) of $CaCO_3$ (ΔDIC_c). These three basic pathways account for most DIC flux in most aquatic ecosystems. Thus the total nonconservative change in DIC (ΔDIC_t) can be described as follows:

$$\Delta DIC_t = \Delta DIC_o + \Delta DIC_g + \Delta DIC_c \tag{24}$$

Note that there usually are some minor pathways of ΔDIC_o associated with respiration such as sulphate reduction (ΔDIC_s) and denitrification (ΔDIC_d). These, and other, usually even more minor respiratory pathways, are part of ΔDIC_o.

Total alkalinity flux (TA) is a useful component to estimate in CNP budgeting. The definition of TA can be simplified, leaving out the contribution of borate alkalinity, as TA ≡ $[HCO_3^-] + 2[CO_3^{-2}] + [OH^-] - [H^+]$. Although the contributions of OH^- and H^+ to TA itself are minor it will be seen that their contributions to ΔTA are significant.

Total alkalinity changes in response to calcification. The calcification reaction, or its reverse, $CaCO_3$ dissolution, may be written several ways, all of which have the same effect on TA. For example:

$$Ca^{2+} + HCO_3^- \rightarrow CaCO_3 + H^+ \tag{25}$$

This version of the reaction has been deliberately chosen to demonstrate that TA decreases in response to HCO_3^- consumption on the left side of the equation and H^+ production on the right. An alternative, apparently more straightforward way to write the reaction ($Ca^{+2} + CO_3^{-2} \rightarrow CaCO_3$) does not explicitly introduce H^+ but has the same ΔTA ($\Delta TA_c = 2\Delta DIC_c$).

There is a minor change associated with nutrient fluxes, as discussed below, but this can be explicitly corrected out of the measured TA and is ignored here (see Brewer and Goldman, 1976; Gaines and Pilson, 1972; Smith *et al.*, 1991). More importantly, there is also an alkalinity change due to net sulphate reduction; that is, sulphate reduction - sulphate oxidation (Berner *et al.*, 1970; Gaines and Pilson, 1972; Smith *et al.*, 1991):

$$2CH_2O + 2H^+ + SO_4^{2-} \rightarrow 2CO_2 + H_2S \tag{26}$$

According to Equation (26), or alternative versions of the reaction, $\Delta DIC_s = \Delta TA$. It is important to think of this reaction as a net reaction. H_2S is thermodynamically unstable in the presence of free O_2 and will rapidly oxidise back to SO_4^{2-}. However in the presence of metal ions, especially Fe, the H_2S will rapidly become bound into metal sulphides.

For each mole of ΔDIC_s released, there is 0.5 mole of sulphate reduced. Available studies have used alkalinity flux as either a measure of calcification or sulphate reduction. This is, in general, probably valid. Systems with high carbonate accumulation tend not to have much available terrigenous Fe, hence they tend to have most of the sulphate, which has been reduced to sulphide, oxidised back to sulphate, hence, $\Delta TA_s \sim 0$. Systems with high terrigenous load tend to have low accumulation of carbonate materials, hence, $\Delta TA_c \sim 0$. This topic, including a consideration of systems in which both ΔTA_s and ΔTA_c are significant, merits further investigation. For the present analysis, however, it is assumed that ΔTA can either be assigned to sulphate reduction or to calcification. With this caveat, ΔTA is interpreted according to the more important of these two processes in any particular system: $\Delta DIC_c = \Delta TA_c/2$; or $\Delta DIC_s = \Delta TA_s$.

It follows from the above description that, in any particular system, ΔTA is uniquely describing carbon flux associated either with calcification or with some portion of (*p-r*). However, a budget of ΔDIC and ΔTA cannot uniquely define ΔDIC_o and ΔDIC_g. Both of these fluxes are desired terms to extract from budgetary analysis.

Another component of nonconservative dissolved carbon flux can also be measured: the flux of dissolved organic carbon (DOC). While few such studies are available, it seems generally likely that the absolute value of ΔDOC is small compared to the absolute value of ΔDIC at the scale of total ecosystems. Note that the production or consumption of DOC represents conversion between DOC and either DIC or particulate organic carbon (POC).

General basis for stoichiometric modelling

A generalised equation for primary production and respiration is reported above in Equation (23). Because organic matter contains carbon, nitrogen, and phosphorus in an almost constant ratio within any one ecosystem, and tends to have a rather similar ratio, the Redfield C:N:P molar ratio of 106:16:1, throughout much of the ocean, the reactions of primary production and respiration can be represented by somewhat more complex equations. It should be recognised that the equations are not intended to describe the actual chemical reaction which goes on, but they do appear to approximate the stoichiometric relationship among carbon, nitrogen, and phosphorus, and oxygen. For primary production, where NO_3^- is the nitrogen source and where the starting organic matter has a Redfield composition, the charge-balanced net reaction can be represented by an equation of the form:

$$\begin{aligned}&106CO_2 + 16H^+ + 16NO_3^- + H_3PO_4 + 122H_2O\\&\rightarrow (CH_2O)_{106}(NH_3)_{16}H_3PO_4 + 138O_2\end{aligned} \tag{27}$$

Various modifications have been offered to make the details of this stoichiometry more "biochemically reasonable" (Anderson, 1995). In general, these changes involve the oxygen and hydrogen content of the organic matter, not the carbon, nitrogen, and phosphorus content. Because the interest here is in the carbon, nitrogen, and phosphorus relationships of the organic matter, the older formulation is retained without loss of generality in the analysis.

This reaction, or one like it to represent slightly different estimates of oceanic organic matter C:N:P ratios, is typically written for the open ocean. In the coastal ocean or other situations where NH_4^+ is the nitrogen source, the reaction may be written as:

$$\begin{aligned}&106CO_2 + 16NH_4^+ + 16OH^- + 90H_2O\\&\rightarrow (CH_2O)_{106}(NH_3)_{16}H_3PO_4 + 106O_2\end{aligned} \tag{28}$$

There are two points to laying out these two alternate equations explicitly. In the first place, although the two equations do involve different stoichiometries with respect to the relationship between free oxygen and CNP, the CNP stoichiometry being covered in the present discussion is unaffected. In the second place, coastal systems may have NH_4^+ as an externally supplied nutrient. This is in contrast to the upper water column of the open ocean, where NH_4^+ is almost inevitably associated with recycling (Dugdale and Goering, 1967). If the sum of NO_3^- + NH_4^+ is simply treated as "DIN," no assumption need be made about NH_4^+ as a new versus a recycled source of nitrogen.

The primary release of inorganic nitrogen during decomposition is as NH_4^+, that is, the reverse of equation (28). Nitrogen flux, as discussed below, is associated with denitrification and uses NO_3^-. Therefore, the process of nitrification is important:

$$NH_3 + 2O_2 \rightarrow HNO_3 + H_2O \tag{29}$$

The important point to note with this reaction is that carbon and phosphorus are not directly involved in the net reaction. Again this makes the point that the relationship between NO_3^- and NH_4^+ may be considered an "internal cycle" which need not be dealt with directly. The above reactions have been in terms of the uncharged forms of DIN. Note, however, that net uptake of one mole of NO_3^- consumes a mole of H^+ , while net uptake of a mole of NH_4^+ consumes a mole of OH^- (Equations 27, 28). These second-order corrections on ΔTA can be readily made.

A reaction which is of great importance to nitrogen cycling in benthic systems is denitrification (Seitzinger, 1988). This respiration pathway is minor with respect to total carbon oxidation, but can be of great significance with respect to nitrogen loss. Stoichiometrically this reaction can be represented by an equation of the form (see also, Smith and Hollibaugh, 1989; Richards, 1965):

$$\begin{aligned}&(CH_2O)_{106}(NH_3)_{16}H_3PO_4 + 94.4HNO_3 \rightarrow \\ &106CO_2 + 177.2H_2O + H_3PO_4 + 55.2N_2\end{aligned} \tag{30}$$

The important point to note in this reaction is that fixed inorganic nitrogen is consumed, but that the DIC:DIP flux ratio is preserved. A further nitrogen related process in many systems is nitrogen fixation. Although the biochemical process of nitrogen fixation is by no means the reverse of Equation (30), it is stoichiometrically useful to think of it in such a manner. That is, nitrogen fixation is the process by which N_2 gas is directly incorporated into organic matter. Again, the stoichiometry is preserved.

One final point needs to be made in this general treatment. Conversions back and forth between particulate and dissolved organic matter are clearly of potential importance in chemical ecology. The assumption is made for the sake of CNP stoichiometric budgeting that these conversions do not involve phase changes between organic and inorganic carbon.

The above discussion has been presented in terms of the familiar Redfield Ratio, because it is heuristically useful to work with "real numbers." In explicit situations where the reacting organic matter has a composition different from the Redfield Ratio, the stoichiometry can be modified accordingly. Atkinson and Smith (1983) report an example of such stoichiometry for benthic plants, which differ markedly from Redfield C:N:P composition, and Smith *et al.* (1991) give derivations in terms of algebraic expressions. While it is sometimes instructive to look at the full equations as laid out above, stoichiometric analysis at the ecosystem level can simply deal directly with the individual, local C:P and N:P ratios. These are discussed below.

Phosphorus-carbon stoichiometry

While the details of phosphorus chemistry are complex (Froelich, 1988), budgetary interpretations may be regarded as somewhat simpler than that of carbon. Analytically there is only a need to consider dissolved inorganic phosphorus, here denoted DIP, and dissolved organic phosphorus, DOP, conversions to and from particulate phosphorus. In general the nonconservative flux of DOP is small compared to the flux of DIP. Measurement and budgeting of ΔDOP data are advocated when available, but ΔDIP is of primary interest to the budgetary analyses.

The nature of particulate phosphorus becomes problematical, because there may be both organic matter and inorganic matter as part of the particulate phosphorus. To a great extent this problematical area can be avoided in budgets by the analysis of total particulate phosphorus (PP) in any particular compartment. In general, it appears that most conversion between dissolved and particulate phosphorus in open seawater involves organic material. Thus, the ratio of C:P in the particulate material $(C:P)_{part}$, multiplied by the nonconservative flux of DIP, becomes an estimate of organic matter (*p-r*):

$$\Delta DIC_o = \Delta DIP \cdot (C:P)_{part} \tag{31}$$

That is, ΔDIP scaled by $(C:P)_{part}$ ratio becomes a measure of net ecosystem metabolism. A system with ΔDIP > 0 is interpreted to be producing DIC via net respiration (*p-r < 0*), while a system with ΔDIP < 0 is interpreted to be consuming DIC via net organic production (*p-r > 0*). This assumption is most likely not to work in systems with an anaerobic water column, or with sediments anaerobic to the sediment-water interface. Under either of these conditions, redox-mediated phosphorus desorption from inorganic particles is likely to occur.

Conceptually, a carbon budget is what is likely to be of most immediate ecological or biogeochemical use. However, if Equation (31) is accepted, then ΔDIP, rather than ΔDIC, may be the best record of net system metabolism. It is suggested that ΔDIP be the first priority for ecosystem nutrient budgeting.

If both DIP and DIC data are available, Equations (24) and (31) can be further developed. If the system is a calcifying system, then:

$$\Delta DIC_t = \Delta DIP \cdot (C{:}P)_{part} + \Delta DIC_g + \frac{\Delta TA}{2} \tag{32}$$

Equation (30) can be rearranged and solved for ΔDIC_g:

$$\Delta DIC_g = \Delta DIC_t - \Delta DIP \cdot (C{:}P)_{part} - \frac{\Delta TA}{2} \tag{33}$$

If the system is interpreted not to be a calcifying system, then the ΔTA term drops out of Equations (32) and (33).

At this point, a useful check on Equation (30), and also on Equation (31), can be offered. It is possible to calculate $pCO_{2(w)}$ from the TA and DIC data, or other variable pairs in the CO_2 system. A generally accepted equation to describe gas flux across the air-water interface is:

$$\Delta DIC_g = K \cdot \alpha \cdot \left(pCO_{2(a)} - pCO_{2(w)}\right) \tag{34}$$

where K is the exchange rate coefficient (in m d^{-1}) and α is the CO_2 gas solubility in seawater as a function of temperature and salinity. K varies primarily as a function of wind speed and tends to range between about 0.5 and 5 m d^{-1}. Hartman and Hammond (1985) provide a particularly useful discussion of K. If everything else is known, it is possible to substitute DIC_g derived according to Equation (33) into Equation (34) and see if a reasonable value for K is derived. K derived in this fashion should, in general, be higher than would be predicted from the mean wind speed over the study period, because of the non-linear response of gas exchange to wind speed. An example of such calculations is found in Smith *et al.* (1991).

Nitrogen-phosphorus stoichiometry

Budgets of nitrogen fluxes include three forms of dissolved inorganic nitrogen (NO_2^-, NO_3^-, and NH_4^+) and dissolved organic nitrogen (DON). Typically, NO_3^- and NO_2^- are measured together and reported as "NO_3^-" which is usually the dominant form. For many purposes it is sufficient to group the inorganic forms into DIN. A characteristic of the nitrogen system which makes it very different from either the carbon or phosphorus system is the dominance of gaseous N_2 over other forms of dissolved nitrogen in seawater. Moreover, this N_2 gas is neither measured (because there is so much of it, at analytically nearly constant concentrations) nor in equilibrium with the other forms of nitrogen. Conversion from N_2 gas to organic nitrogen is termed "nitrogen fixation," while conversion from NO_3^- to N_2 is termed "denitrification." Both of these processes require biotic mediation (primarily by various forms of bacteria) and usually require locally anaerobic conditions to proceed in aqueous ecosystems. This discussion of the biochemistry of the nitrogen system is necessarily greatly oversimplified, but more detail is beyond the scope of these guidelines. The interested reader is referred to Webb (1981) for more detail. The important point for the sake of budgetary analysis is that significant amounts of nitrogen are transferred between so-called "fixed nitrogen" (DIN, DON, PN), which is measured, and gaseous nitrogen (N_2), which is not. The net effect of this transfer is here termed (*nfix-denit*) and is often quantitatively significant to the nitrogen budget.

Assuming that the N:P ratio of particulate material in the system $(N{:}P)_{part}$ is know, the dissolved nitrogen flux associated with production and decomposition of particulate material is the dissolved phosphorus flux ($\Delta P = \Delta DIP + \Delta DOP$) multiplied by $(N{:}P)_{part}$. It follows, that (*nfix - denit*) is the difference between the measured dissolved nitrogen flux ($\Delta N = \Delta NO_3 + \Delta NH_4 + \Delta DON$) and that expected from production and decomposition of organic matter:

$$(nfix - denit) = \Delta N - \Delta P \cdot (N{:}P)_{part} \tag{35}$$

ΔDON, ΔNH_4^+, and ΔDOP tend to be small relative to ΔNO_3^-. Hence, solution of Equation (33) without these terms is generally likely to introduce a rather small error in the estimation of (*nfix-denit)*.

Summary of stoichiometric analyses of nonconservative CNP fluxes

In general it is useful to derive nonconservative phosphorus fluxes first. If ΔDIP and $(C:P)_{part}$ are both known, then it is feasible to use Equation (31) as an estimate of net system carbon metabolism (*p-r*, or ΔDIC_o). If phosphorus data are available, it is likely that nitrogen data are available as well. With data on $(N:P)_{part}$, estimates can be made of (*nfix-denit*) from Equation (35). Adequate data for DIC and TA are less likely to be available. However, if they are available, then Equation (33) can be solved to derive an estimate of ΔDIC_g. If the system is a noncalcifying system, then ΔTA is an estimate of DIC release during sulphate reduction; if the system is a calcifying system, then $\Delta TA/2$ is an estimate of DIC uptake by $CaCO_3$ precipitation.

5.5 Preparation for the Case-Study Calculations

Examination of the case studies presented in the next sub-section, along with the cautionary lesson from the Merbok mangrove system (Section 4), provides insight into the application of this sort of budgetary modelling. The technique is widely, but by no means universally, applicable. First and foremost there must be some method to estimate the residence time of the water within the system of interest. In many instances a straightforward way of establishing water residence time is by means of combined water and salt budgets. Establishing such budgets, however, may not always be practical. In that case, the alternative approach is by means of a numerical model of water exchange. Detailed procedures for the establishment of such a numerical circulation model is beyond the scope of this report, although some background information has been provided. For the remainder of this discussion, it is assumed that some method to estimate water residence time in the system of interest is available.

Given an estimate of water residence time, there must be a net biogeochemical signal relative to material flux due to physical transport. Ability to extract a budgetary signal for any particular reactive material Y is determined by the absolute value of the ratio of net biogeochemical change of Y, in the earlier notation, the reaction rate, ΔY, multiplied by time, to the sum of the physical influxes, or effluxes, of Y, for example, $\Sigma V_{in}Y_{in}$; that is, by the ratio $|\Delta Y \cdot time/\Sigma V_{in}Y_{in}|$. If this "reaction ratio" is > 1, a change is readily measured by such budgets. However, the net change may have occurred rapidly initially, with little subsequent change. Resolution of the rate of change and location of change within the system has been lost. As the ratio falls below about 0.1, ΔY will become progressively less readily determined. The critical reaction ratio for determining ΔY cannot be more rigorously defined, because it will depend upon the precision with which Y can be measured and on various time scales of variation of both ΔY and $\Sigma V_{in}Y_{in}$.

The ecosystem budgetary approach may be viewed as a large-scale incubation. Therefore an experimental analogue to this situation is an incubation in which the starting water mass defines $\Sigma V_{in}Y_{in}$ and the difference in water composition over the incubation time defines ΔY, the reaction rate. A short incubation time defines the reaction rate under more or less constant conditions, but the incubation time must be sufficiently long to measure this quantity precisely. The experimental solution to the problem of a small reaction ratio is to increase the incubation time--with potential "chamber effects." If this ratio is too low in a natural system to be readily determined, again ΔY must be increased relative to $\Sigma V_{in}Y_{in}$. One obvious solution to the problem in many instances is to increase the size of the system being budgeted. If the volume flow rate through the enlarged system remains constant, $\Sigma V_{in}Y_{in}$ will remain constant. With more reaction time, $\Delta Y \cdot time$ is likely to increase, thus increasing the ratio. Note that this quantity will not necessarily increase as the time increases; ΔY, that is, the net reaction rate, may decrease over that greater time. The choice facing the ecologist or biogeochemist determining any such budget is between raising the ratio, hence improving the quality of its resolution, and losing both spatial and temporal resolution of ΔY.

With the above background in mind, what is actually necessary to apply the budgetary techniques laid out here? Basic requirements can be summarised under five categories: system definition, freshwater inputs, salinity of the water, nutrient concentrations and other nonconservative components in water and other relevant information. These requirements are summarised in Text Box 4.

1. **System definition:** The boundaries of the system should be clearly defined and based on physiographic properties or water composition. The area of the system, divided into subtidal and intertidal areas, in the case of systems with extensive emergent vegetation, and the water volume or average depth are required. The area of the watershed may be required if data on freshwater flow, described below, are not well known.

2. **Freshwater:** Estimates of total stream flow and, if volumetrically important, groundwater flow and other freshwater discharges into the system are required to establish the water budget. Lacking direct flow data, information on precipitation and evapotranspiration in the watershed may suffice as a first approximation.

3. **Salinity:** Salinity of the system itself and of adjacent systems is required. Inflow water from land can probably be assumed to have a salinity of 0 p.s.u. For a first approximation the data should be summarised into arithmetic means (either long term or, if available, into shorter time increments) for the system(s) of interest and the adjacent water bodies.

4. **Nutrients and other nonconservative components:** In order of decreasing importance, data are required for the following variables: dissolved inorganic phosphorus, nitrate, ammonium, dissolved organic nitrogen, dissolved organic phosphorus, total alkalinity, pH (or other secondary measurement in the aqueous CO_2 system), and dissolved organic carbon. These data should be handled the same as salinity, with the exception that the nutrient concentrations in land water sources should not be ignored.

It should be emphasised that item numbers 1-3, above are required to establish a water and salt budget for estimating water exchange. Item 4 is required to estimate aspects of net system metabolism, with the relative importance of the variables being the order listed.

5. **Other:** Data on C:N:P ratios of suspended materials, major primary producers, sediments, and inflowing materials are extremely useful. It is useful to have a general description of major biotic components and the proportion of the system covered by those components. Other ancillary information on component metabolism and other aspects of the system, such as sedimentation rate, will assist in interpretation of the budgets.

Text Box 4. Summary of requirements for budget modelling analysis.

System definition

It is essential to have a clear image of the system to be budgeted. What are its spatial boundaries, both in terms of its landward boundaries and the “open” or oceanic boundary? With respect to the oceanic boundary, and if there is more than one region of exchange between the system and adjacent ocean, what are the relative cross sectional areas at the boundaries? These are likely clues as to relative water exchange volumes. The area of the system and the average water depth should be known. If the system is divided into obvious sub-basins, distinct water depths, or spatially discrete habitat types, it may be useful, although by no means required, to have some knowledge of area and dept within subsystems of the overall system. That information may or may not be helpful for budgeting. High precision on this information is not required. Adequate information can usually be extracted from hydrographic charts.

All of the information to follow can be profitably approached in either of two fashions. If available data are very restrictive, then reliable mean values over some period of time, the longer the better, can be used to establish static or steady state budgets. If the available system has a large amount of data, then it becomes useful to use the data to establish some sort of averaged trend. Minimal smoothing is recommended. For example, in one result presented below in some detail, data are reported averaged into two-month blocks.

Freshwater Input
Given this general information on the system, the next point is to establish a water budget. Precipitation is monitored in many areas of the world. Much of this information ends up in various national or regional governmental agency files. Some may be maintained by local agencies or even private groups. Those data, for a period as long prior to the study time as available, are invaluable. In many instances, those same files may include either pan evaporation data or wind speed and relative humidity data from which evaporation can be calculated by long established techniques (see for example Sverdrup *et al.*, 1942). Lacking that information, even regional seasonal evaporation maps can be used. Other freshwater sources of possible importance are likely to be gauged streams, if the watershed area is as large as, or larger than, the system area. Such data tend to be maintained by national government agencies. If only part of the watershed area draining into the system of interest is gauged, one may use gauged to ungauged watershed area ratios, perhaps including estimates of relative precipitation in the two areas, to extrapolate the gauged data to a system average. Lacking runoff data, consultation with local terrestrial ecologists and hydrologists may lead to estimates of vegetation evapotraspiration rates which can be used to approximate runoff from precipitation. Data on groundwater flow may also be available. In terrestrial systems with high precipitation and highly permeable soil, this freshwater source may be important. More often it appears to be a second order correction to the water budget. There may be other freshwater sources such as sewage. Again these are not likely to be quantitatively significant to the water budget. Examination of equations presented in the previous sections makes it obvious that the main role of freshwater input and evaporative water losses is likely to derive information about the system water budget.

The data to follow are less likely to be available in general government documents. They may be in technical papers, either formal publications or “grey literature” such as environmental impact reports. While assembling any such data for budgetary analysis, some effort should be made to evaluate the quality of the data (precision, accuracy, etc.). Of course these are also the kinds of data which should be collected during any serious budgetary study.

Salinity of water masses
Salinity data should next be examined to see if a salt budget, and thus an estimate of water exchange rate, can be established. In general it is safe to assume that all of the freshwater sources described above, as well as the evaporative loss term, have a salinity of 0 p.s.u. Of course if salinity data are available for any of these sources, they can be used in the calculations. Salinity in the system of interest and in the adjacent, oceanic system(s) are required, and there must be a salinity difference between the system and the ocean. If there is a vertical salinity gradient, those data are useful. It is recommended that the data in such stratified systems be divided into two “boxes” representing surface and deep waters with an estimate of the thickness of each box. Salinity differences of less than about 0.3 p.s.u., vertically and between horizontally adjacent boxes, are likely to be insufficient for establishing quantitatively useful salt budgets; greater differences will, of course, lead to more robust budgetary calculations.

Nutrient concentrations and other nonconservative components
Having arrived at the data for the water and salt budgets, the next requirement is for information on nutrients. As an absolute minimum, data on DIP and NO_3^- are required. NH_4^+, DOP and DON data are also highly recommended. Data on the aqueous CO_2 system may also be of great use (with pH and total alkalinity being the most likely data to be available). DOC data are useful, although rarely available. Other materials, such as Si, can also be readily budgeted if the data are available. It should be stressed that for all of these variables, the best available accuracy and especially precision are needed, because one is often looking for relatively small differences in water composition between adjacent water masses. Clean techniques of collecting, preserving and analysing the nutrients should be employed and high-precision measurements of the DIC-related variables are required if the data are to be useful. None of this is difficult, even under rather rudimentary field and laboratory conditions, but it does require attention to detail.

It should not be assumed that most freshwater sources delivering water to the system lack nutrients, even though this assumption is generally reasonable for salt. In many cases the levels are likely to be very high, especially in stream water, groundwater and any sewage sources. In some cases, sewage data may be available as mass emission rates, either based on direct data of per capita discharge estimates, rather than as concentrations in a waste stream of known volume.

Other relevant information
It is highly desirable to have data on the suspended load C:N:P composition ratio. Although data on the concentrations of these suspended materials are not required for budgeting purposes, these data clearly are useful. For both suspended load and sediment composition, a serious research programme should measure these quantities but reasonable guesses can probably be made for preliminary budgetary calculations.

Finally, other ancillary information is likely to be useful for amplifying from the system-level budgets to the performance of components in the system: for example, primary production of phytoplankton or benthic plants; respiration rates of components in the system, sedimentation rate, etc. If the overall budgetary characteristics of the system are known and specific budgetary components are known, then other components may be considered by difference. Estimates of the number of humans in the watershed, the distributions of those humans, and major aspects of terrestrial vegetation, land use, and other activities in the watershed will be useful in interpreting the budgets.

5.6 Case Studies

Eight case studies have been chosen to illustrate the use of the general budgetary approach outlined above. Each is chosen to illustrate specific aspects of the use of budgets.

- **Bahia San Quintín, Mexico**, introduces the use of this approach as an exploratory exercise, in a coastal lagoon for which there are only very limited data.

- **Klong Lad Khao Khao, Thailand**, is a mangrove estuary for which an extensive general data set on salinity, nitrogen, and phosphorus is available. This system is used to present, in a step-by-step manner, an example of the budgetary calculations.

- **Tomales Bay, California**, **United States** is used to present non-steady state water, salt, and dissolved inorganic phosphorus budgets; then to discuss the stoichiometric approach in detail; and finally to demonstrate how one can compare total system metabolism with major metabolic components.

- **Gulf of Bothnia**, at the head of the Baltic Sea, illustrates a system in which the assumption of a constant water volume is not appropriate and in which temporal variation of water composition should also be considered.

- **The Baltic-Kattegat System**, illustrates steady-state analysis for a large estuarine sea which is divided into a horizontal series of basins with two-layer vertical stratification.

- **Spencer Gulf, Australia**, examines water, salt, and CNP budgets in a system dominated by calcification.

- **Tokyo Bay, Japan**, illustrates a water exchange budget for Tokyo Bay, established on the basis of a direct three-dimensional numerical model, rather than a salt budget to establish exchange.

- **East China Sea** illustrates the numerical analysis of two-dimensional pattern of water flow in a stratified system.

As a cautionary note, the Merbok mangrove system of Malaysia, discussed in Section 4, serves as an example where various techniques, including budgets based on measurement of tidally induced current flow, have been tried and have generally not worked well to describe nonconservative fluxes of carbon, nitrogen, and phosphorus.

It should be further noted that in these guidelines there is an attempt to be internally consistent in the application of the stoichiometric budgeting. One result is that some of the calculated rates differ slightly from previously published estimates. This brings up the point that it is important for the sake of detailed comparison that either consistent rules be applied, or that changes in the rules be clearly spelled out.

5.6.1 Bahia San Quintín: Exploratory steady-state NP budgets in a coastal lagoon

Bahia San Quintín (area = 42 x 10^6 m^2, volume = 90 x 10^6 m^3) (Figure 8) is a coastal lagoon in Mexico for which only a limited amount of salinity, nutrient, and weather data are available. This hypersaline system is presented as the first case study to show what insights can be gained by using limited data to generate biogeochemical budgets. In Figure 8, it is obvious that the Bay consists of two distinct sub-basins. Although more detailed studies will eventually develop calculations for the sub-basins individually, the present data set is not considered adequate for that exercise. Published weather maps demonstrate that this system is net evaporative most of the time. Precipitation data are available from a weather station slightly south of the Bay, and there is no significant surface runoff except during some major storm events. Groundwater in the watershed has been intensively studied, because it is the only freshwater source supporting extensive agriculture in the watershed. Although the groundwater is so heavily exploited that flow is reduced to near 0, estimates of groundwater input have been included for illustrative purposes.

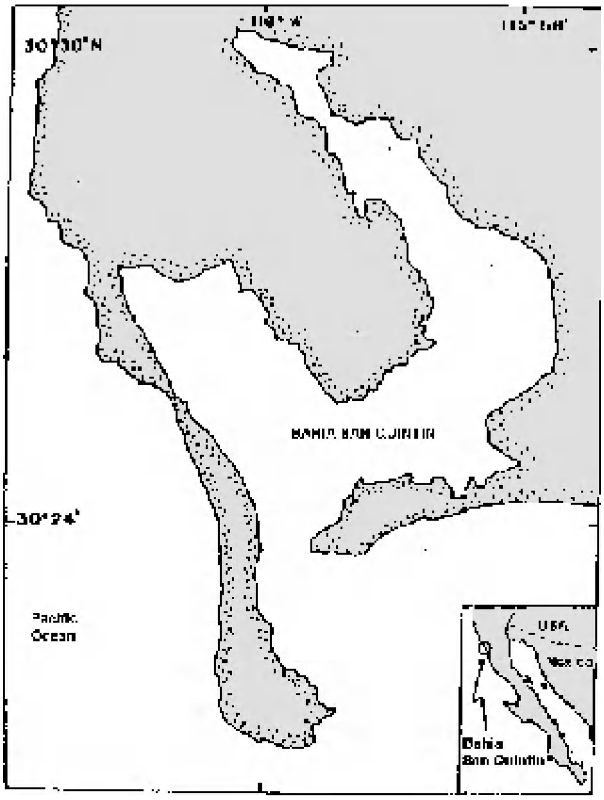
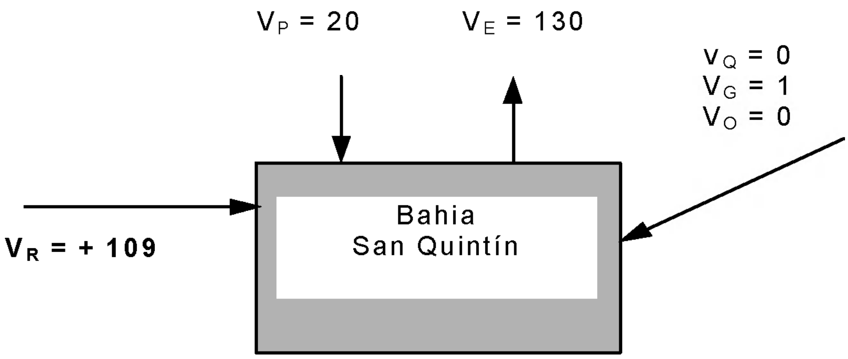
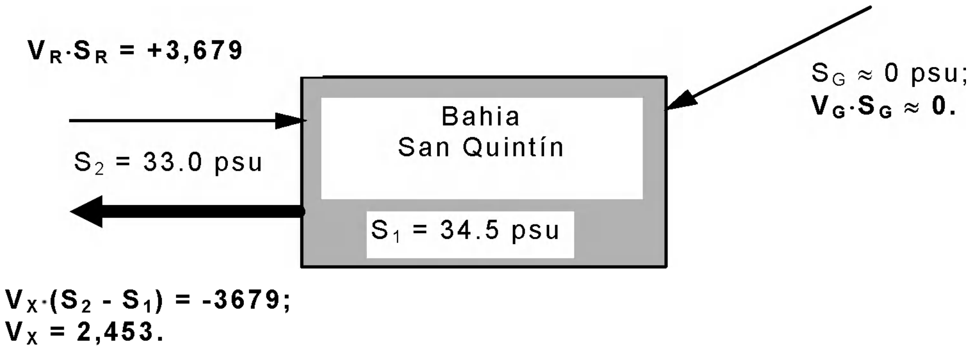


Figure 8. Location of Bahia San Quintin, Mexico.

Figure 9 illustrates the steady state water and salt budgets. Typically it is most useful to consider these budgets together. Precipitation is seasonal but averages about 170 mm yr^{-1}. Summed over the bay area, this is approximately 20,000 $m^3\ d^{-1}$ (V_P). Groundwater inflow (V_G) totals only about 1,000 $m^3\ d^{-1}$. Evaporation is by far the major term in the freshwater budget, averaging about 1,100 mm yr^{-1}. Over the bay area, this is equivalent to evaporative removal (V_E) of approximately 130,000 $m^3\ d^{-1}$. Thus there is a net freshwater loss of 109,000 $m^3\ d^{-1}$. According to Equation (2), there is seawater inflow into the bay to balance this loss; V_R is + 109,000 $m^3\ d^{-1}$. The hydraulic residence time of the system is given by the system volume divided by this residual flow: about 800 days.



Water Budget (fluxes in $10^3\ m^3\ d^{-1}$)



Salt Budget (fluxes in 10^3 kg d^{-1})

Figure 9. Steady-state water and salt budgets for Bahia San Quintín. Quantities estimated from data independent of the budgetary calculations are shown in light typeface; quantities calculated within the budget are shown in bold typeface.

The seawater inflow delivers salt to the system advectively, and the elevated salinity of the bay results in outward mixing of salt. The salinity of the inflowing seawater is taken to be the average of the bay and ocean salinity (that is, 33.75 p.s.u.), so the advective salt delivery is about 3.7 x 10^6 kg d^{-1}. V_X to remove this excess salt must be about 2.5 x 10^6 $m^3\ d^{-1}$. Thus the total exchange time for the system is the system volume divided by the sum of $V_R + V_X$: about 35 days.

Preliminary versions of the dissolved inorganic phosphorus and dissolved inorganic nitrogen budgets are presented in Table 2 and Figure 10. There are no data for dissolved organic nutrients, and the nitrogen budget does not include NH_4^+ (which is reported to be low and variable for this system). However, estimates derived from other systems (below) are used to conclude that the DIP and NO_3^- fluxes probably dominate. Nonconservative processes in the bay produce about 3,700 mol d^{-1} of DIP (ΔDIP) and 14,000 mol d^{-1} of DIN (ΔDIN).

Table 2. Nonconservative dissolved inorganic P and N fluxes in Bahia San Quintin.

PROCESS	RATE (mmol m^{-2} d^{-1})
area	42 km^2
ΔDIP	+0.09
ΔDIN	+0.33
(*nfix - denit*) [1]	-1.4 to -2.6
(*p-r*) [2]	-10 to -50

1) $(N:P)_{part}$ assumed to be between 16 (plankton) and 30 (seagrass).
2) $(C:P)_{part}$ assumed to be between 106 (plankton) and 550 (seagrass).

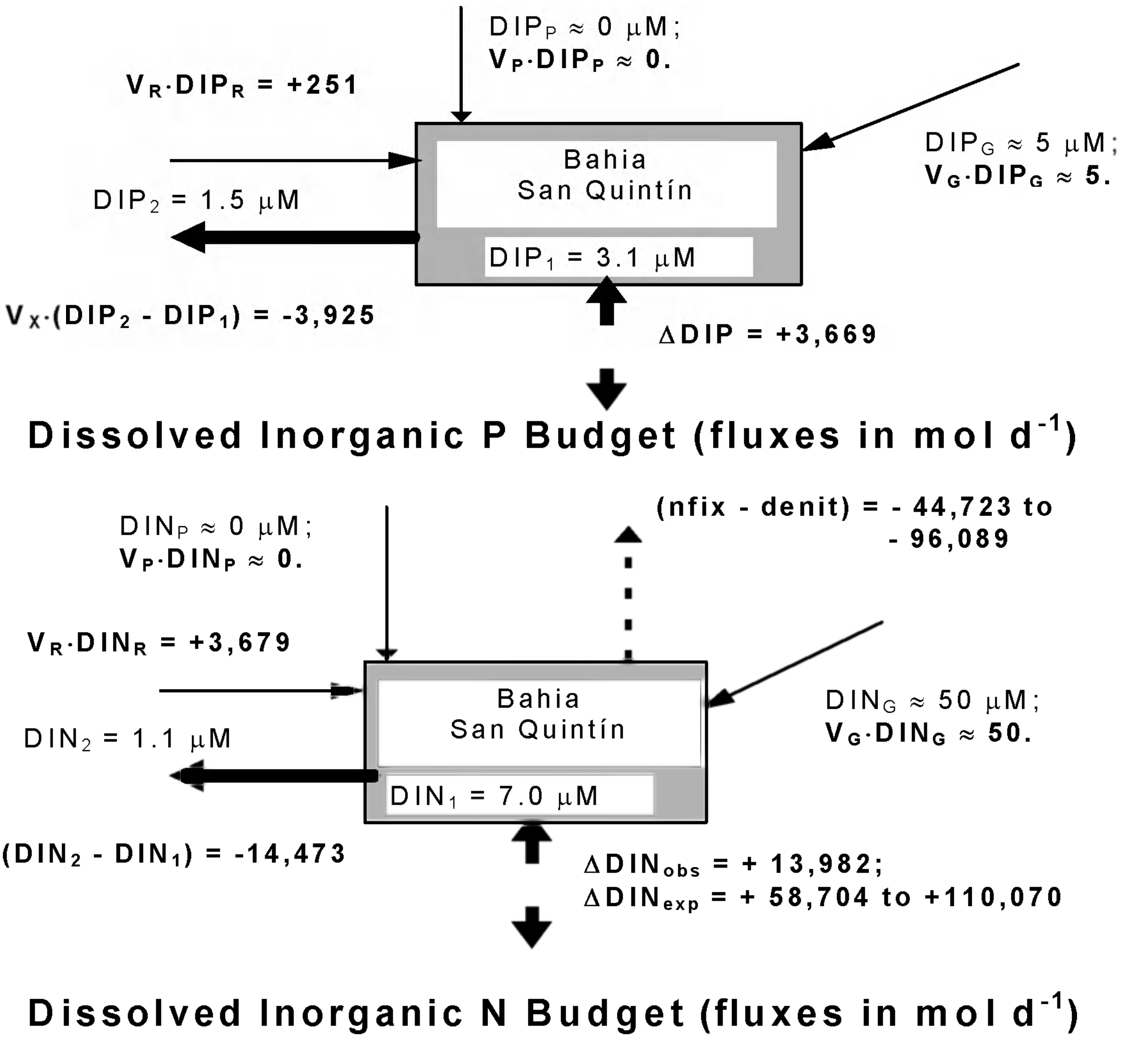


Figure 10. Steady-state DIP and DIN budgets for Bahia San Quintín. Quantities estimated from data independent of the budgetary calculations are shown in light typeface; quantities calculated within the budget are shown in bold typeface.

Independent estimates suggest that organic metabolism in this system is dominated by plankton and seagrass. Moreover, because terrigenous inputs to this system are small, inward drift of either plankton or benthic detritus is likely to dominate the net metabolism. The ranges of values for ΔDIN_{exp} from particle decomposition and (nfix - denit) are based on a range for $N:P_{part}$ between plankton ($N:P_{part} \approx 16:1$) and seagrass ($N:P_{part} \approx 30:1$), as plausible sources of particulate material to be accounting for decomposition. As a result ΔDIN is expected to range from 59,000 to 110,000 mol d^{-1}. Because the observed ΔDIN is only about 14,000, the remainder of the expected ΔDIN is assumed to be lost via (*nfix-denit*) of about 45,000 to 98,000 mol d^{-1}. Over the bay area, the average rates are between -1.1 to -2.3 mmol m^{-2} d^{-1}. This is well within the range of denitrification rates reported by Seitzinger (1988) for coastal marine systems.

Plankton and seagrass have C:P ratios of about 106:1 and 550:1, respectively. The value for ΔDIP is equivalent to DIP release of about 0.08 mmol m^{-2} d^{-1}. If plankton dominate input of organic matter from outside the system, then (*p-r*) is about 9 mmol C m^{-2} d^{-1}; if seagrass dominates, (*p-r*) is about 44 mmol Cm^{-2} d^{-1}. Limited data on primary production in this system suggest that *p* is near 160 mmol carbon m^{-2} d^{-1}. *r* can be estimated to be between about 170 and 200 mmol m^{-2} d^{-1}. If the stoichiometric assumptions are valid, this system is net heterotrophic ($r > p$) by about 5 to 20%.

Thus, from very limited data on the freshwater budget and the salinity and nutrient composition of this system, it has been possible to construct a preliminary estimate of how fast the system processes dissolved nutrients.

5.6.2 Klong Lad Khao Khao: Exploratory steady-state NP budgets in a mangrove estuary

The following case study was developed during the SARCS/WOTRO/LOICZ Workshop on Biogeochemical Modelling held in Penang, Malaysia (4-8 December 1995) to try out an earlier draft of these guidelines (LOICZ, 1995c). Data from 11 field sites in Southeast Asia were examined according to the draft guidelines, and it was felt that having one of the participants in the workshop (Dr. Gullaya Wattayakorn, Chulalongkorn University, Bangkok) work through the procedures in detail would further clarify the use of these budgetary methods. Therefore this section is presented with only limited modification of Dr. Wattayakorn's working notes, modified to correspond to the general outline presented in Text Box 4.

System definition: Figure 11 is a map of the area. The mangrove + waterway area occupies approximately 6×10^6 m^2; the waterway itself occupies about 10% of this area (6×10^5 m^2). Mean water depth in the waterway is about 6 m, while the average depth in the mangroves themselves is about 1 m. Thus, the average depth of the entire mangrove/estuary system is approximately 1.5 m. The watershed is estimated to be about 10 times the mangrove/waterway area, that is about 60×10^6 m^2.
Freshwater: Stream flow is not well monitored, but precipitation is estimated to be about 2,600 mm yr^{-1}, or about 7 mm d^{-1}. Evapotranspiration from similar areas in Queensland, Australia, is estimated to be about 5 mm d^{-1}. Data on groundwater flow or sewage discharge directly into the mangroves is not available.
Salinity: Salinity of precipitation and stream inflow is assumed to be 0; average estuarine salinity is about 29 p.s.u.; coastal seawater averages about 33 p.s.u.
Nutrients and other nonconservative components: Data are available for DIP, DOP, NO_3, NH_4, and DON in this system (Table 3).
Other: Mangrove litter is estimated to have a C:N:P molar ratio of about 1,300:11:1. It is assumed that this is also the approximate ratio of C:N:P in sediments delivered from the watershed. Plankton seem unlikely to be a major component because of high water turbidity in the open waterway. Mangrove primary production is typically about 8-10 tons ha^{-1} yr^{-1} of leaf litter and an equivalent amount of woody material (a total of 18 is used here). If this material is 40% carbon, it is equivalent to approximately 160 mmol C m^{-2} d^{-1}.

From these data it is possible to go through the sequence of budgetary analysis presented in Text Box 4.

Table 3. Average nutrient concentrations (μmol) for components of the Klong Lad Khao Khao system.

Nutrient	Seawater (Y_2)	System (Y_1)	Freshwater (Y_Q)
DIP	0.3	1.5	0.4
DOP	0.3	0.6	0.7
NO_3	0.2	0.4	2.6
NH_4	0.9	1.5	1.7
DON	97.0	170.0	220.0

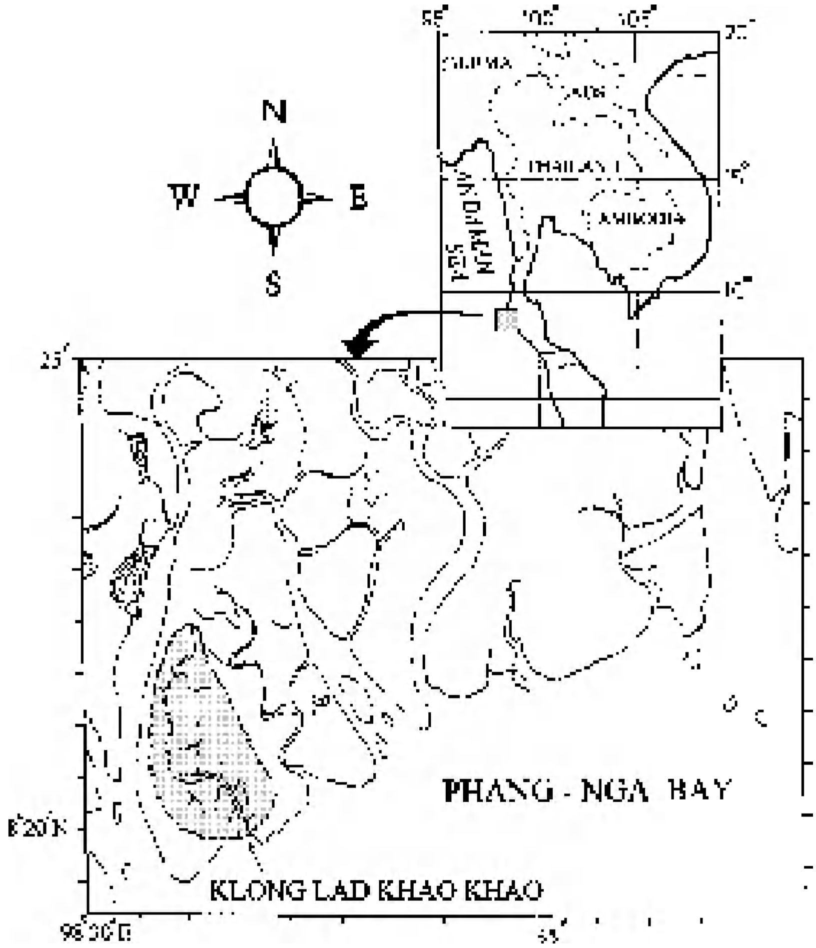


Figure 11. Location of Klong Lad Khao Khao, Thailand.

Water budget: Figure 12 illustrates the water budget for Klong Lad Khao Khao. Freshwater flow (V_Q) is estimated as P - E (2 mm d^{-1}) multiplied by the watershed area: 120,000 m^3 d^{-1}. Direct precipitation (V_P) and evaporation (V_E) are estimated as 42,000 and 30,000 m^3 d^{-1}, respectively, based on the mangrove + waterway area. Other components of inflow (V_G, V_O) are assumed small. It is also assumed that, averaged over a tidal cycle, system volume remains constant. From Equation (2):

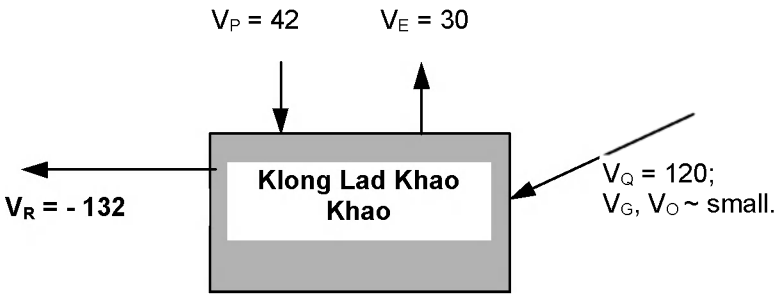
$$V_R = \frac{dV_1}{dt} - V_Q - V_P - V_G - V_O + V_E =$$

$$0 - 120{,}000 - 42{,}000 - 0 - 0 + 30{,}000 = -132{,}000 m^3 d^{-1}$$

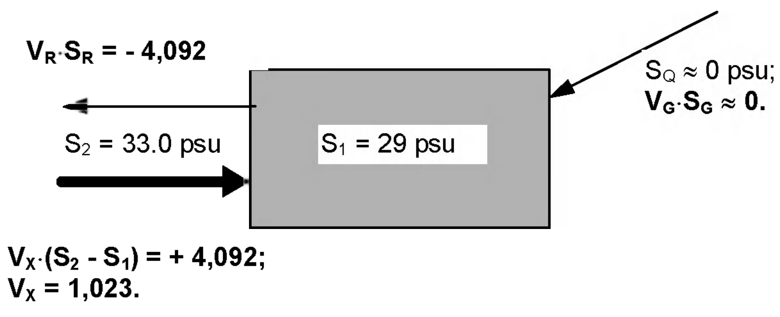
That is, V_R is negative, indicating residual outflow.

Salt budget: Figure 12 also summarises the salt budget. Residual outflow water has a salinity which is the average of estuary and ocean salinity, that is, 31 p.s.u., so salt export is $V_R S_R \approx 4.1 \times 10^6$ kg d^{-1}. Exchange of estuary water with ocean water must replace this salt export. The simplified version of Equation (8) (with $V_1 dS_1/dt = 0$) becomes:

$$V_X = \frac{1}{(S_1 - S_2)} V_R S_R = \frac{1}{(29 - 33)} (-132{,}000) \cdot 31 \approx 1.02 x 10^6 m^3 \cdot d^{-1}$$



Water Budget (fluxes in 10^3 m^3 d^{-1})



Salt Budget (fluxes in 10^3 kg d^{-1})

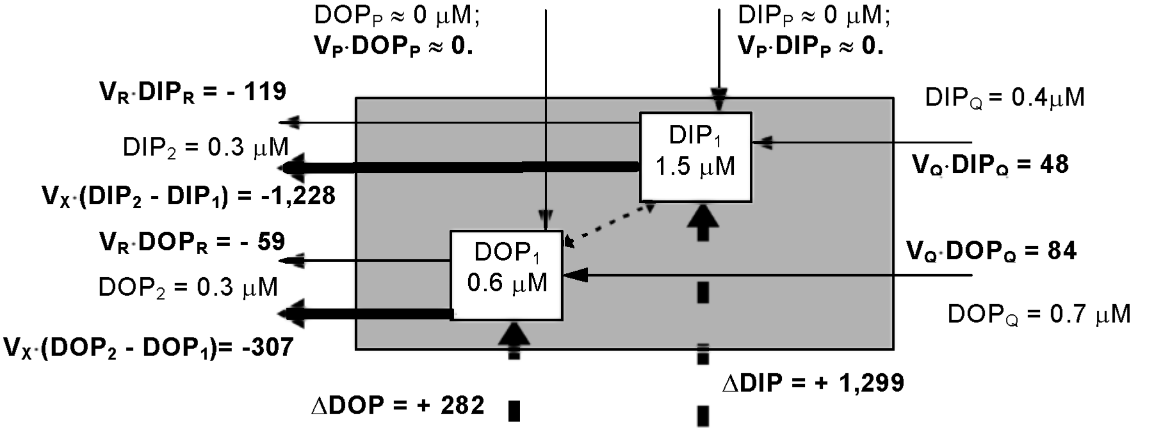
Figure 12. Steady-state water and salt budgets for Klong Lad Khao Khao. Quantities estimated from data independent of the budgetary calculations are shown in light typeface; quantities calculated within the budget are shown in bold typeface.

Budgets of nonconservative materials: Figure 13 summarises the dissolved P and N budgets for this system. NO_3^- and NH_4^+ are lumped into DIN. First consider DIP. Stream inflow delivers 48 mol DIP d^{-1} ($V_Q \cdot DIP_Q$); residual outflow removes about 119 mol d^{-1} ($V_R \cdot DIP_R$, where DIP_R is the average of the ocean and estuary DIP); mixing removes an additional 1,228 mol d^{-1} ($V_X[DIP_2 - DIP_1]$). In order to support this net export, there must be a positive value for ΔDIP. Solving Equation (20) at constant volume and DIP concentration:

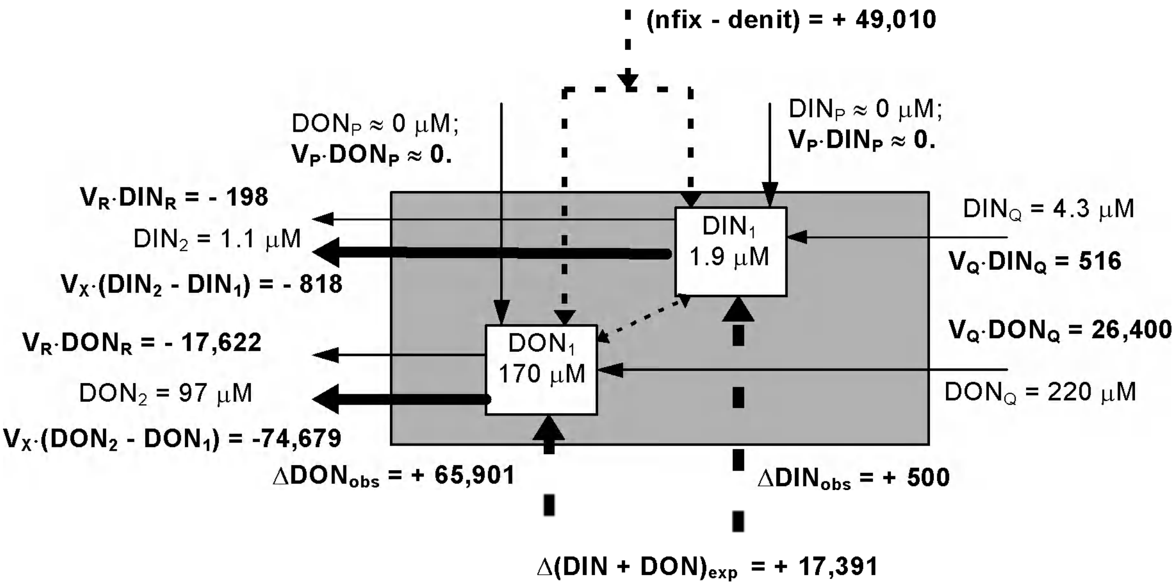
$$\Delta DIP = V\frac{dY}{dt} + Y\frac{dV}{dt} - \sum V_{in}Y_{in} + \sum V_{out}Y_{out}$$

$$= 0 + 0 - 48 + 119 + 1{,}228 = 1{,}299 \; mol \cdot d^{-1}$$

The other components are calculated similarly: ΔDOP = + 282 mol d^{-1}; ΔDIN = +500 mol d^{-1}, ΔDON = +65,901 mol d^{-1}.



Dissolved Phosphorous Budget (fluxes in mol d^{-1})



Dissolved Nitrogen Budget (fluxes in mol d^{-1})

Figure 13. Steady-state dissolved phosphorus and nitrogen budgets for Klong Lad Khao Khao. Quantities estimated from data independent of the budgetary calculations are shown in light typeface; quantities calculated within the budget are shown in bold typeface.

Stoichiometric relationships among nonconservative budgets: At the outset, several problems might occur here. There is the potential of either groundwater contamination with nutrients or direct discharge of sewage effluent into the system. Secondly, and perhaps more importantly, sediments are very organic rich and largely anaerobic. As a result, dissolved nutrients, especially phosphorus, may be released either from the organic matter itself or from inorganically sorbed materials on the mineral surfaces.

Initially, decomposition of mangrove litter is considered to be the most obvious source of CNP release. Upon reflection, that is not the case. That material was produced in the system, so there was initial uptake of nutrients into the litter. While there could be lags between uptake and release, and those lags might show up in a time series analysis, the assumption behind the steady state analysis is that average conditions in a system are being described with unchanging composition. Nevertheless the incoming terrigenous material is assumed to have a composition near that of the mangrove litter, a C:N:P ratio of 1,300:11:1.

First consider the ΔN expected from the decomposition of organic matter into DIP + DOP. The expected value from particle decomposition (nfix - denit) based on a $N:P_{part}$ ratio of terrigenous material of 11:1, is about $\Delta N = 11\cdot(\Delta DIP + \Delta DOP) = 11\cdot(1{,}299+282) = 17{,}391$ mol d^{-1}. The observed ΔN flux, overwhelmingly dominated by ΔDON, is 66,401 mol d^{-1}. From Equation (33) it can be calculated that:

$$(nifx - denit) = \Delta N - \Delta P \cdot (N\!:\!P)_{part} = (500 + 65{,}901) - (1{,}299 + 282)\cdot 11 = 49{,}010\ mol \cdot d^{-1}$$

The solution to this equation is positive, so it represents apparent net nitrogen fixation. If this rate were occurring throughout the entire mangrove + waterway area, it would yield a net nitrogen fixation rate of about 8 mmol m^{-2} d^{-1}. This rate seems too high in comparison with limited data for mangrove nitrogen fixation rates and more extensive data for other rapidly fixing environments (typically 2-5 mmol m^{-2} d^{-1}, from summary data in Capone, 1983). Note that even if ΔDIP is abiotic, rather than metabolic, it would have relatively minor effect on this calculation. One possible explanation for this high ΔDON, which should be closely examined in this system, is substantial DON input in groundwater or sewage.

Next consider ΔDIP as an estimate of (*p - r*) in the estuary, assuming that the decomposing material is dominated by terrigenous material with a C:P ratio similar to mangrove detritus (that is, 1,100:1). Applying Equation (31):

$$\Delta DIC_o = \Delta DIP \cdot (C\!:\!P)_{part} = 1{,}299 \cdot 1{,}100 \approx 1.4x10^6 mol \cdot d^{-1}$$

Dividing by mangrove + waterway area, a rate of about 230 mmol m^{-2} d^{-1} can be calculated. Because this rate is almost 50% higher than the net primary production of the mangroves, it is probably not a correct representation of (*p - r*) in this system. This would require a very large import of organic matter from outside the system. Plausible alternative explanations include desorption of phosphorus from sedimentary particles, a large input of P in groundwater or sewage, or the possibility that terrigenous material entering the system has a substantially lower C:P ratio than assumed here.

The budgetary calculations for this system appear algebraically robust. Shifts in the compositions of the various boxes or in the freshwater flow would need to be large in order to alter the budgetary calculations significantly. However, the calculated nonconservative fluxes yield stoichiometric implications about both (*p - r*) and (*nfix - denit*) which appear somewhat too high. There are at least two plausible alternative explanations for this discrepancy. Either there are additional inputs of nutrients, at a minimum DIP and DON, which are not being included in the budgets, or the organic-rich sediments exhibit substantial releases of these materials which are not directly accounted for by these metabolic pathways. In either case, the budgets point to directions which should be investigated further in order to understand the processes accounting for CNP fluxes in this system.

5.6.3 Tomales Bay: Time-varying CNP fluxes in a well mixed estuary

Tomales Bay, California (Figure 14), has been the site of intensive studies of total ecosystem metabolism (Hollibaugh *et al.*, 1988; Smith *et al.*, 1991; etc.). This budget for a temperate climate estuary illustrates time-varying, non steady-state, calculations. Only the inner two thirds of the bay area is included in this budget, because the outer third has water composition similar to that of the coastal ocean.

Non-steady state water, salt, DIP, DOP, NO_3^-, NH_4^+, DON, TA, DIC, and DOC budgets were established for the inner portion of this bay at two-month intervals between 1987 and 1994. Some of these data are illustrated for the period up to mid 1991. Specifically, the two-month time steps of calculated water exchange flux (V_X) and ΔDIP, are presented in order to illustrate the calculations in a system for which time series data are available. Secondly, the average nonconservative fluxes for each of the above materials is used over the period from 1987 to 1991 in order to illustrate the stoichiometric calculations of the metabolically related processes discussed in Sections 5.4.6. Finally, ancillary data on component metabolism is used to further elaborate the total system metabolism and to show how the budgets can be used in conjunction with such additional data.

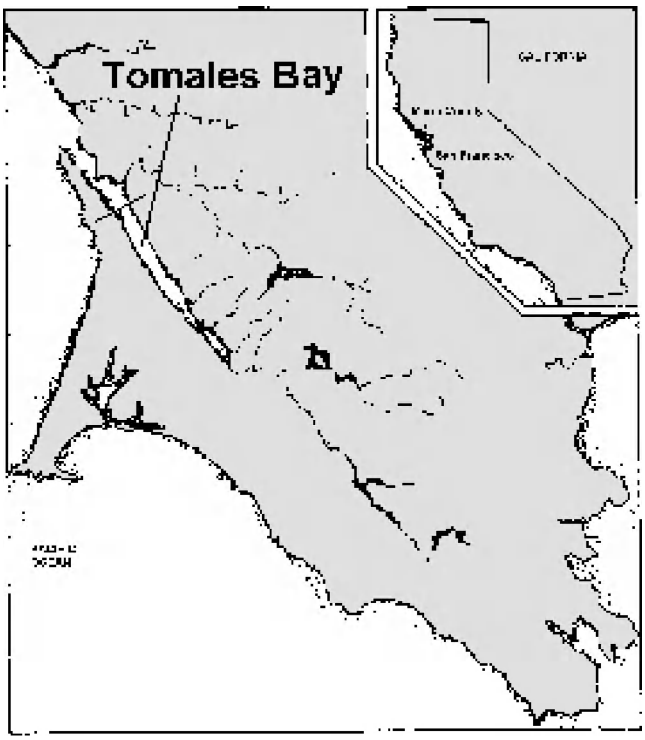


Figure 14. Location of Tomales Bay, California, United States.

The inner bay (area = 16 x 10^6 m^2; volume = 48 x 10^6 m^3) is treated as a single well-mixed system receiving inputs from stream runoff and precipitation, losing water to evaporation, exchanging water with the outer bay, and having internal reactions which vary over time. Tables 4-6 summarise the data used here to describe the freshwater fluxes and water composition over time. Precipitation and evaporation rate (P, E, in mm d^{-1}; Table 4) are converted to volume fluxes (V_P, V_E; Table 5) by multiplying the area of the Bay. Note that time-varying data for ocean, bay, and stream water composition are available. Because precipitation was not sampled on a regular basis, a constant value of 0.20 is used for DIP flux due to precipitation. It is obvious from inspection of the data that this assumption does not seriously affect the budgets. This is not always true; for example, in some systems precipitation is a significant source of nitrogen delivery. From separate studies it has been determined that groundwater is quantitatively insignificant to these budgets, and that there are no other significant water or nutrient sources such as sewage discharge.

Table 4. Stream flow (V_Q) , precipitation (P), and evaporation (E) data for Tomales Bay, July 1987-July 1991, at two-month increments.

Year	V_Q (10^3 m^3 d^{-1})	P (mm d^{-1})	E (mm d^{-1})
87.500	14	0.01	3.11
87.667	5	0.00	3.10
87.833	6	0.55	1.81
88.000	223	5.92	0.57
88.167	461	3.89	0.41
88.333	44	1.42	2.57
88.500	17	0.85	3.52
88.667	10	0.01	3.76
88.833	10	0.25	2.16
89.000	95	5.87	0.61
89.167	87	2.19	0.44
89.333	563	6.66	1.26
89.500	24	0.14	3.00
89.667	11	0.00	3.77
89.833	24	2.19	1.59
90.000	52	1.33	0.60
90.167	232	4.97	0.53
90.333	75	1.30	1.53
90.500	62	3.15	2.95
90.667	13	0.00	3.23
90.833	11	0.10	1.20
91.000	41	1.40	0.42
91.167	83	3.07	0.36
91.333	518	9.74	0.90
91.500	25	0.17	2.71

Table 5 and Figure 15 present the water volume exchange rates (V_X) over time as calculated from the salt and water budgets according to Equation (8). With real world data, some adjustments may be needed in order to generate realistic results. It was found that, for months with (S_1-S_2) < 0.3 p.s.u., calculated exchange rates were highly variable and often < 0 which is a physical impossibility. Salinity in this system alternates between slightly above oceanic during the summer to below oceanic during the winter. Hence, there were two times in the year when the difference between the bay and the ocean is close to 0 which yields unstable estimates of V_x. For these times, when (S_1-S_2) was below this cut-off, the value for V_x was set to the value from the preceding time step. Two time steps adjacent to those adjusted by this procedure gave negative values for V_x. These adjacent values were set equal to the preceding time step. It should be noted that this particular problem is less likely to arise in systems which are consistently above or consistently below the ocean in their salinities.

Table 5. Water circulation, residual flow and water exchange rates as calculated from the water and salt budgets for Tomales Bay, July 1987-July 1991. The subscript "Q" indicates streams; "P" is precipitation; "E" is evaporation, "1" is the Bay, "2" is the ocean. As discussed in the text, two versions of the daily exchange volume are provided: the uncorrected exchange volume ($V_{X(unc)}$), and values corrected ($V_{X(cor)}$) to the previous two-month interval for those periods when the difference between bay and ocean salinity was less than 0.3 p.s.u.

Year	#days	V_Q	V_P	V_E	S_2 p.s.u.	S_1 p.s.u.	S_Q p.s.u.	S_P p.s.u.	$V_{X(unc)}$ $m^3 d^{-1}$	$V_{X(cor)}$ $m^3 d^{-1}$
87.472		14	0	50	33.83	34.03	0.00	0.00		
87.650	65	5	0	50	33.62	34.68	0.00	0.00	997	997
87.850	73	6	9	29	33.27	33.74	0.00	0.00	2,313	2,313
88.005	56	223	95	9	32.19	28.35	0.00	0.00	1,233	1,233
88.190	68	461	62	7	33.11	31.63	0.00	0.00	12,850	2,850
88.368	65	44	23	41	33.67	32.81	0.00	0.00	2,018	2,018
88.536	62	17	14	56	33.99	34.74	0.00	0.00	-847	2,018Ŧ
88.724	68	10	0	60	33.68	34.67	0.00	0.00	1,776	1,776
88.839	42	10	4	35	33.46	34.25	0.00	0.00	1,508	1,508
89.016	65	95	94	10	32.71	30.70	0.00	0.00	1,519	1,519
89.175	58	87	35	7	32.13	29.77	0.00	0.00	1,182	1,182
89.348	63	563	107	20	32.87	31.51	0.00	0.00	16,360	6,360
89.521	63	24	2	48	33.95	33.96	0.00	0.00	-111,966	16,360*
89.685	60	11	0	60	33.71	34.62	0.00	0.00	1,259	1,259
89.852	61	24	35	25	33.46	33.17	0.00	0.00	-29	1,259*
90.016	60	52	21	10	33.31	32.08	0.00	0.00	966	966
90.173	57	232	80	8	32.33	29.96	0.00	0.00	3,242	3,242
90.355	66	75	21	24	33.68	32.89	0.00	0.00	5,731	5,731
90.567	77	62	50	47	33.63	33.65	0.00	0.00	-133,018	5,731*
90.671	38	13	0	52	33.59	34.19	0.00	0.00	1,066	1,066
90.839	61	11	2	19	33.40	34.13	0.00	0.00	342	342
90.996	57	41	22	7	33.33	32.89	0.00	0.00	1,841	1,841
91.159	60	83	49	6	30.91	27.47	0.00	0.00	191	1,841Ŧ
91.333	63	518	156	14	32.80	30.69	0.00	0.00	11,092	11,092
91.528	71	25	3	43	33.86	34.10	0.00	0.00	-7,482	11,092*

* $|S_{sys}$-Socn$| < 0.3$; V_x set to previous month.
Ŧ Unreasonable value of V_x; value set to previous month.

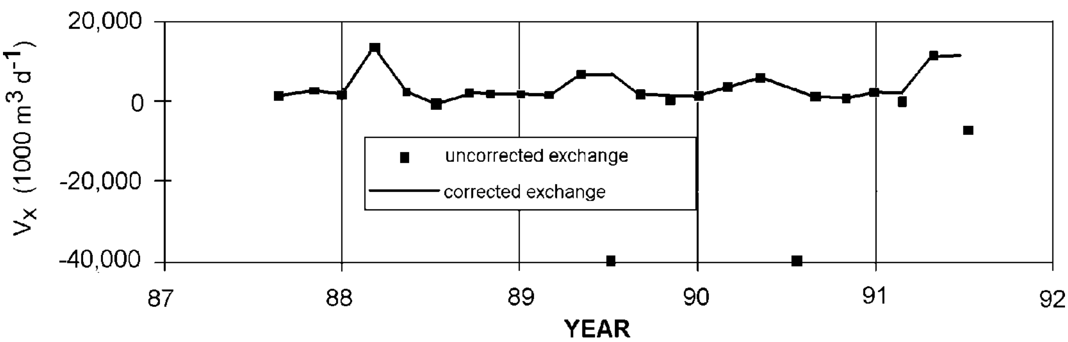


Figure 15. Time series of daily water exchange volume (V_X) between the inner and outer portions of Tomales Bay. The difference between the uncorrected and corrected values for V_X is discussed in the text.

Table 6 and Figure 16 give one example of calculated nonconservative fluxes for DIP. Similar budgets are available for other forms of dissolved phosphorus, nitrogen and carbon. To aid the comparison of biogeochemical rates among systems, it is convenient here to scale the nonconservative rates obtained by the system area. The system is a nonconservative source of DIP (ΔDIP) averaging +0.16 mmol m^{-2} d^{-1}. The seasonal variation in ΔDIP ranges from 0.0 mmol m^{-2} d^{-1} in December-January to greater than +0.4 mmol m^{-2} d^{-1} in June-July. Based on the assumption that DIP release largely represents decomposition of organic matter, these data indicate that the system *p-r* indicates net respiration, and that this occurs during most of the year.

Table 6. Nonconservative flux calculations for DIP in Tomales Bay, July 1987-July 1991. Notation as in previous table; Y_P = 0.20.

Year	#days	V_Q	V_P	V_E	$V_{X(cor)}$	Y_2	Y_1	Y_Q	ΔDIP	
									kmol	mmol m^{-2} d^{-1}
87.472		14	0	50		1.29	2.01	0.47		
87.650	65	5	0	50	997	1.15	3.10	0.55	2,651	0.17
87.850	73	6	9	29	2,313	0.95	2.81	0.80	4,079	0.25
88.005	56	223	95	9	1,233	1.33	1.92	0.80	269	0.02
88.190	68	461	62	7	12,850	1.27	1.37	0.46	1,353	0.08
88.368	65	44	23	41	2,018	1.54	2.05	0.61	1,547	0.10
88.536	62	17	14	56	2,018	1.18	2.76	0.29	3,653	0.23
88.724	68	10	0	60	1,776	1.23	3.56	0.32	4,580	0.29
88.839	42	10	4	35	1,508	1.59	3.34	0.92	2,325	0.15
89.016	65	95	94	10	1,519	1.62	1.84	0.83	-561	-0.04
89.175	58	87	35	7	1,182	1.67	1.74	0.92	109	0.01
89.348	63	563	107	20	16,360	1.44	1.55	0.63	2,250	0.14
89.521	63	24	2	48	16,360	1.54	1.95	0.67	6,957	0.43
89.685	60	11	0	60	1,259	1.13	3.44	0.58	3,983	0.25
89.852	61	24	35	25	1,259	1.48	3.19	0.48	2,018	0.13
90.016	60	52	21	10	966	1.33	1.80	0.42	-586	-0.04
90.173	57	232	80	8	3,242	1.20	1.47	0.82	797	0.05
90.355	66	75	21	24	5,731	1.55	1.80	0.85	1,725	0.11
90.567	77	62	50	47	5,731	1.46	2.61	1.13	7,148	0.45
90.671	38	13	0	52	1,066	1.50	3.31	0.69	2,711	0.17
90.839	61	11	2	19	342	1.32	3.37	0.92	724	0.05
90.996	57	41	22	7	1,841	1.16	1.84	0.83	9	0.00
91.159	60	83	49	6	1,841	1.37	1.65	1.04	502	0.03
91.333	63	518	156	14	11,092	1.04	1.34	0.62	3,525	0.22
91.528	71	25	3	43	11,092	1.04	1.78	0.71	8,466	0.53

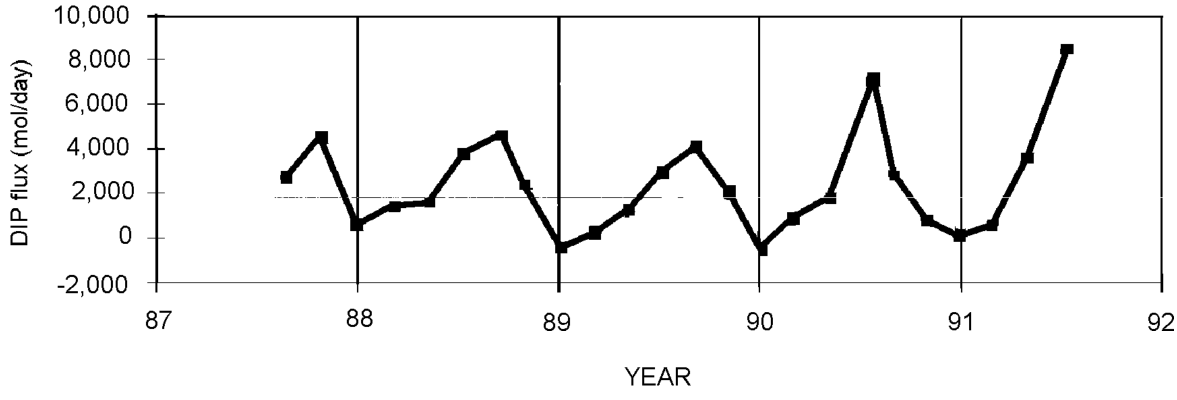


Figure 16. Time series of net nonconservative flux of DIP (ΔDIP) in Tomales Bay.

From the average ΔDIP of +0.16 mmol m^{-2} d^{-1}, the C:P ratio of organic matter, and Equation (31), ΔDIC_o can be calculated to be approximately ≈ +17 mmol m^{-2} d^{-1}. It follows that $p-r \approx -17$ mmol $m^{-2} d^{-1}$. From independent data (Cole, 1989; Hollibaugh, unpublished), plankton primary production in this system is known to average about 70 mmol m^{-2} d^{-1} over the study period. Other primary producers (benthic algae, seagrass) are estimated to contribute an additional 30 mmol C m^{-2} d^{-1}. Respiration exceeded primary production by an estimated 17 mmol m^{-2} d^{-1}, so $r \approx 117$ mmol m^{-2} d^{-1}. The *p:r* ratio of this system is thus estimated to be about 0.85. Note that obtaining *p-r* in this fashion is independent of direct estimates of either *p* or *r*, and that the *p:r* ratio is relatively insensitive to the value used for *p*.

Table 7 summarises the mean fluxes of dissolved forms of C, N, and P, and Table 8 gives the calculated stoichiometric characteristics of the system. One goal of this exercise is to apply stoichiometric reasoning in order to estimate the actual biogeochemical processes accounting for the calculated biogeochemical fluxes. Particulate material in this system has a C:N:P molar ratio approximating the Redfield Ratio (106:16:1).

Table 7. Average nonconservative fluxes for dissolved carbon, nitrogen, and phosphorus in Tomales Bay, July 1987 - July 1991.

VARIABLE	FLUX (mean ± standard error)
ΔDIP (mmol m^{-2} d^{-1})	0.16 ± 0.03
ΔDOP (mmol m^{-2} d^{-1})	0.02 ± 0.01
ΔNO_3^- (mmol m^{-2} d^{-1})	-1.46 ± 0.54
ΔNH_4^+(mmol m^{-2} d^{-1})	-0.07 ± 0.07
ΔDON (mmol m^{-2} d^{-1})	0.63 ± 0.19
ΔTA (meq m^{-2} d^{-1})	13.43 ± 3.51
ΔDIC (mmol m^{-2} d^{-1})	7.10 ± 2.59
ΔDOC (mmol m^{-2} d^{-1})	2.38 ± 0.88

This system accumulates little $CaCO_3$ in the sediments, so ΔTA is assigned to sulphate reduction (see Equation 26). ΔTA is 13 meq m^{-2} d^{-1}, so the estimated net rate of sulphate reduction, that is, gross sulphate reduction - sulphide oxidation, is $\Delta TA/2$, or about 7 mmol m^{-2} d^{-1}. This figure is somewhat higher than the burial rates of chromium reducible sulphur measured by Chambers *et al.* (1994) as 3 mmol m^{-2} d^{-1} at two subtidal sites in the bay, but lower than the rate of 30 mmol m^{-2} d^{-1} reported by those authors using ^{35}S incorporation rate experiments. The carbon decomposition associated with the budgeted rate of sulphate reduction is about 13 mmol m^{-2} d^{-1}, implying that about 12% of the respiration in this system is associated with sulphate reduction. Because this is not a calcifying environment, Equation (31) can be used here without the ΔTA term to estimate the rate of CO_2 gas flux across the air-water interface: $\Delta DIC_g = \Delta DIC_t - \Delta DIP \times (C:P)_{part} = 7 - 17 \approx -10$ mmol m^{-2} d^{-1}. This represents gas evasion from the water.

The changes in dissolved phosphorus and nitrogen, Table 8, the N:P ratio of local particulate organic matter (16:1), and Equation (35) are used to calculate (*nfix - denit*): (*nfix-denit*) = $\Delta N - \Delta P \times (N:P)_{part} \approx (-1.5 -0.1 + 0.6) - (0.16+ 0.02) \times 16 \approx -3.9$ mmol m^{-2} d^{-1}. That is, the system seems to be denitrifying about 4 mmol m^{-2} d^{-1} more nitrogen than it is fixing. How much would this number be altered by the absence of DON and DOP data? In that case, estimated (*nfix - denit*) becomes 5.1 mmol m^{-2} d^{-1}. Note also that the calculation is not particularly sensitive to NH_4 flux. In many cases, this term largely represents turnover, rather than net flux. Joye *et al.* (in press) have measured *in situ* subtidal denitrification rates between 1 and 9 mmol m^{-2} d^{-1} in this system. While nitrogen fixation does occur on some parts of the mud flats of this system with rates generally well less than 1 mmol m^{-2} d^{-1}, it appears to be spatially a restricted process (Joye and Paerl, 1993).

Table 8. Average stoichiometric fluxes in Tomales Bay, July 1987-July 1991, calculated from data in Table 7.

VARIABLE	FLUX (mean ± std. Error) (mM m^{-2} d^{-1})
(*p-r*) (BASED ON PARTICLE C:P OF 106)	-16.6 ± 3.3
(*nfix-denit*) (BASED ON PARTICLE N:P OF 16)	-3.9 ± 0.8
ΔDIC_s	+13.4 ± 1.8
CO_2 gas flux	-9.5 ± 3.1
plankton *p* (INDEPENDENTLY MEASURED)	70
other *p* (AS DISCUSSED IN TEXT)	30
r (*p* - [*p-r*])	81 ± 11

5.6.5 Gulf of Bothnia: NP Budgets in a System with Time Varying Volume

In a study of the nutrient budget of the Gulf of Bothnia (Figure 17) (area = 108 x 10^9 m^2; volume = 5,900 x 10^9 m^3), encompassing the two northern basins of the Baltic Sea, an intensive field programme was initiated during 1991 and yielded data with a monthly time resolution (Wulff *et al.*, 1994). This study is presented as a case in which it was possible to evaluate fluxes with a high temporal resolution, in which it was possible to follow both organic and inorganic nutrient fractions, and in which the temporal variation of water volume was important.

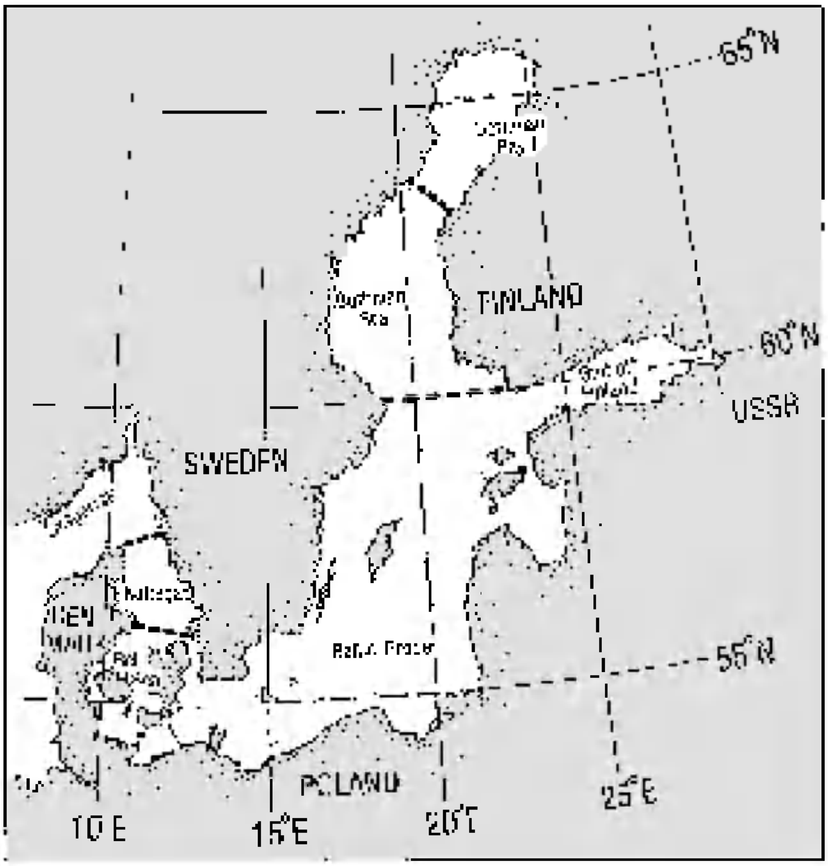


Figure 17. Location of the Baltic-Kattegat system.

In this study, it was found that it is not sufficient to use the variations in total amounts to estimate the fate of the nutrient load to the Gulf of Bothnia. The different fluxes between the sub-basins, that is the Bothnian Bay, the Bothnian Sea and between the Bothnian Sea and the Baltic proper, had to be estimated. The basic reasons for this were large differences in nutrient load, hydrography and biogeochemistry. The Gulf of Bothnia could then be represented by a simple two box model with only narrow connections between the sub-basins and to the Baltic proper. The water level variations were obtained from monthly means measured at several stations in each sub-basin. The net turbulent diffusive exchange between the sub-basins is included in the advective transports. The advective net volume exchanges are then estimated from volume and mass balances by using salt as a conservative tracer.

Volume changes, ΔV, in each sub-basin over monthly time increments have been derived from changes in average sea level (Figure 18). Those data, along with monthly average salinity, are used in Equations (6) and (7) in order to estimate water exchange between the two basins and between the Bothnian Sea and the Baltic Proper.

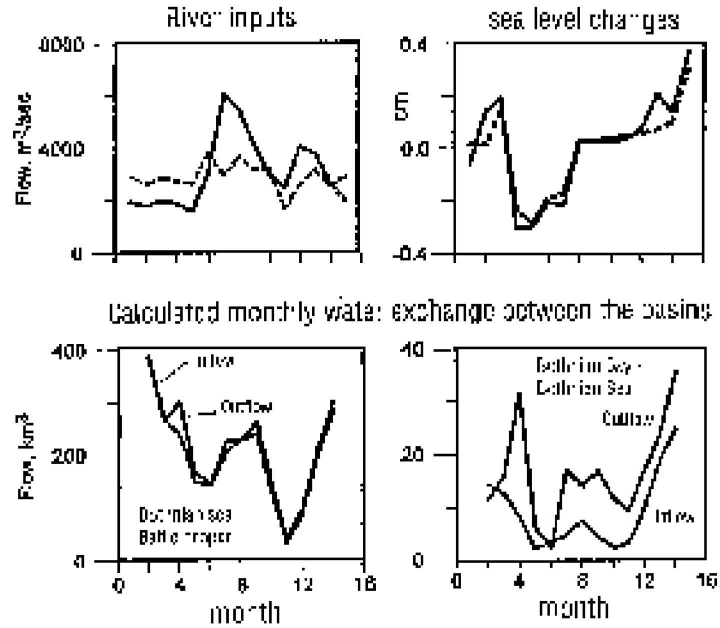


Figure 18. Monthly variations in freshwater inputs, water level, and water exchange in Bothnian Bay (solid) and Bothnian Sea (dashed).

The model parameters are, as mentioned above, assumed to be homogeneous within the basin. These volume-weighted averages are obtained using the calculated total amounts. The monthly mean salinity is obtained by interpolation of the averages based on relatively few observations. This interpolation will smooth events on the scale of a month or shorter. A simple scale analysis with regard to the time-dependent terms of water volume and salinity demonstrates that an average freshwater supply of 135 x 10^6 m^3 d^{-1}, which is about half the mean supply to the Bothnian Bay, will yield $\Delta h \approx 0.1$ m, if all the water were retained in the Bay over a month's time.

The significance of this calculation is that monthly water level changes on the order 0.1 m will have the same impact as half the mean freshwater input in the volume balance. A similar analysis in the salt balance yields

$$Qf_1S_1 \sim V_1 \frac{\partial S_1}{\partial t}$$

or

$$\Delta S \sim \frac{Qf_1 S_1 \Delta T}{V_1}$$

Typical data for Bothnian Bay give $\Delta S \sim 0.01$ p.s.u., which is a monthly change well within the observed range. An analogous analysis of the Bothnian Sea gives similar figures to that of the Bothnian Bay. The importance of this scaling analysis is that one cannot calculate monthly averaged fluxes in the Gulf of Bothnia without considering the time-dependent variations of the water level.

With the volume flows, loads and total amounts given, it is straightforward to estimate the sources and sinks in the system using Equations of the form of (21) and (22). The variables in the annual budgets are "organic" nitrogen and phosphorus, calculated as the difference between total nitrogen or phosphorus and the inorganic fractions (DIN or DIP).

From the monthly time-stepped nonconservative fluxes presented here, Figure 19, it is evident that the nitrogen and phosphorus cycles are neither constant over the year nor exactly balanced over an annual cycle in the Gulf of Bothnia. For the year illustrated, 1991, there is an accumulation of phosphorus, as organic phosphorus, and a loss of nitrogen, as inorganic nitrogen, in the water column reservoirs. There is also a redistribution between the dissolved inorganic and the organic (dissolved + particulate) fractions.

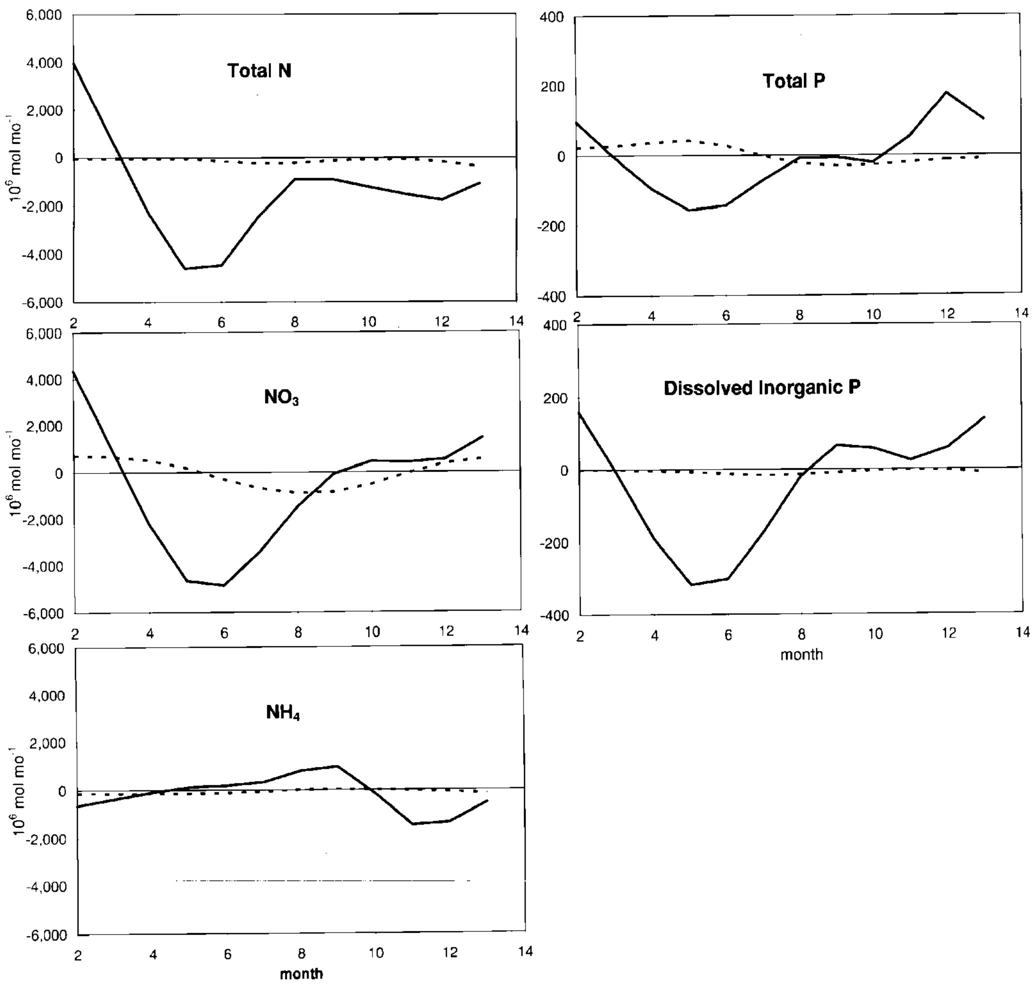
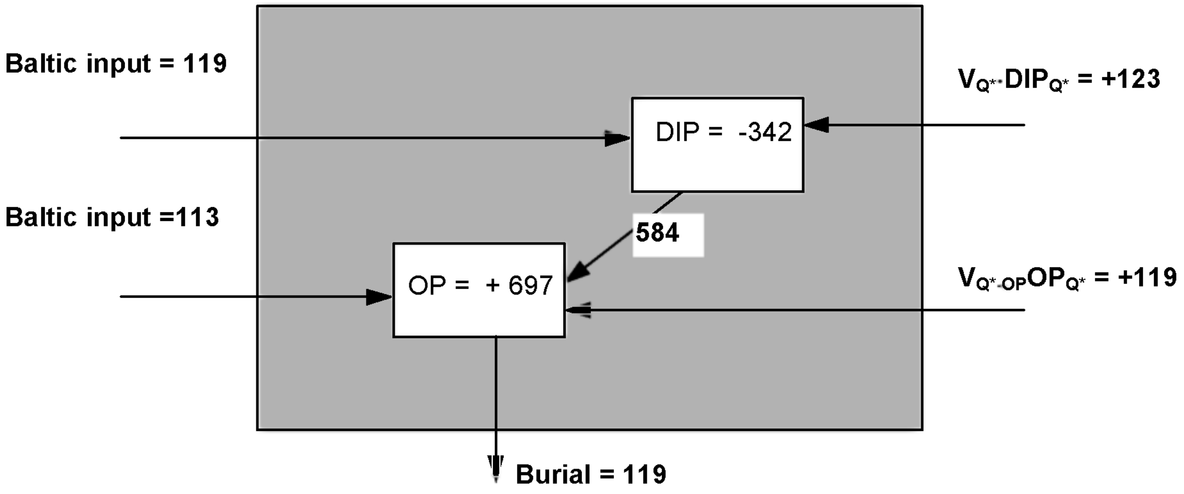
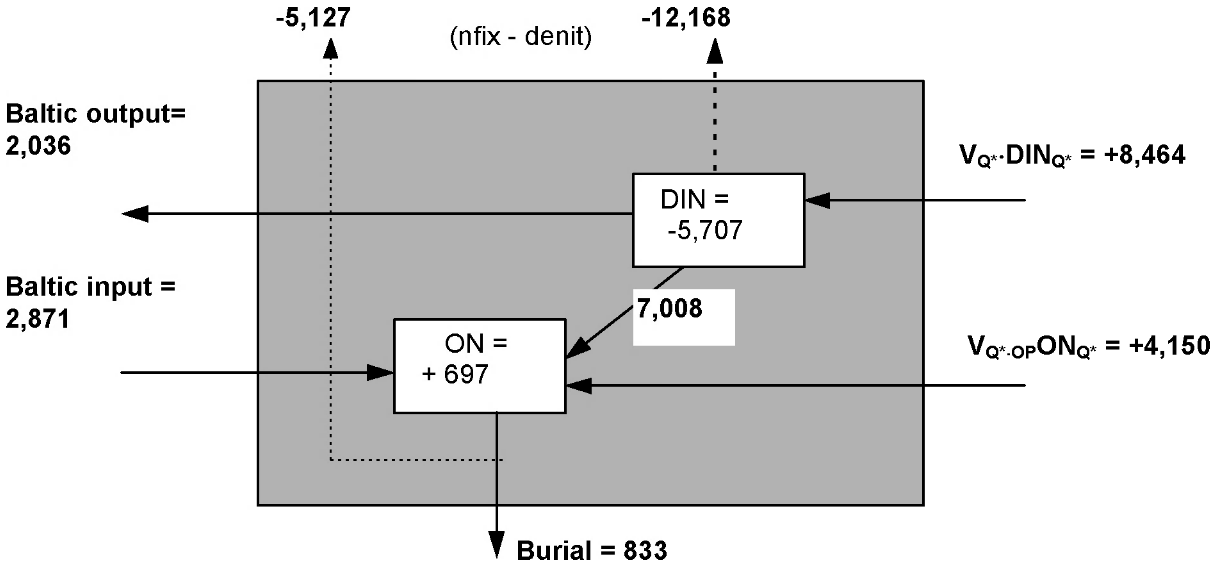


Figure 19. Monthly variations in the nonconservative fluxes of materials in Bothnian Bay (solid) and the Bothnian Sea (dashed).

Figure 20 shows fluxes to and from the Baltic including residual flow and mixing. DIN to organic nitrogen conversion is calculated from DIP to organic phosphorus conversion using an assumed $N:P_{part}$ of 12:1, and nitrogen burial is calculated from phosphorus burial with an assumed burial particle $N:P_{part}$ ratio of 7:1. The quantity (nfix - denit) (in both cases net denitrification) is then calculated to balance the nitrogen fluxes between DIN and ON and between ON and burial.



Phosphorus Budget (10^6 mol yr^{-1})



Nitrogen Budget (10^6 mol yr^{-1})

Figure 20. Annual budgets of phosphorus and nitrogen in the Gulf of Bothnia 1991. Quantities calculated within the budget are shown in bold typeface.

The phosphorus budget (Figure 20) shows a substantial import from the Baltic Proper, almost twice the load coming from the drainage basin to the Gulf. For the 1991 data, most of the phosphorus entering the Gulf remained in the water column. Phosphorus, not remaining in the water column or not exported hydrographically, is assumed to be exported to the sediments. The drainage basins are the major net source of nitrogen delivery; inorganic export to the Baltic Proper approximately balanced organic import (Figure 20). Nitrogen in the water column actually decreased over the budgeted year, with some nitrogen apparently accumulating in the sediments.

As demonstrated with Equations (27-31) and (35), the budgets for inorganic nitrogen and phosphorus involve transfer to and from organic matter due to assimilatory and respiratory processes. Qualitatively, the seasonal variation in ΔNO_3^-, ΔNH_4^+, and ΔDIP seems to be a common example of community production and regeneration. In the winter there is release of DIP, release of NO_3^-, and uptake of NH_4^+. This appears to represent net respiration of organic matter, with nitrification of released NH_4^+, Equation (28) proceeding in reverse, accompanied by nitrification according to Equation (27). Both DIP and NO_3^- are taken up in the spring, Equation (27), while NH_4^+ release during the late spring and summer reflects nitrogen recycling.

Although the annual budget estimates may give only a little information about the mechanisms behind these bulk fluxes, they can be used to assess the overall magnitude and significance of the different processes. By calculating N:P ratios of the different pools and fluxes (Figure 20), typically very high ratios are found for the inorganic pool in the Bothnian Bay and for the organic pools in both basins. Only the inorganic pool in the Bothnian Sea is close to the Redfield Ratio of 16:1. However, it is noteworthy that the N:P ratios for the net transfer of inorganic nutrients to organic are very close to the Redfield Ratio of assimilative nutrient uptake, in spite of the highly different ratios of the pools. This might imply that these calculated fluxes are actually related to the net primary production of these systems. Furthermore, net organic carbon production, calculated from these rates, are 4-6 mol C m^{-2}. Annual phytoplankton production measurements for these regions are comparable to these estimates considering that these estimates should be closer to 'new' production than to either gross or net primary production in the sense of Eppley and Peterson (1979).

Denitrification rates from these system level data can be compared with "direct" assays. Stockenburg and Johnstone (1994) measured denitrification directly in the Gulf of Bothnia during 1991. They obtained rates of 45-60 mmol m^{-2} yr^{-1} in the Bothnian Bay (1/3 of the Gulf area) and 100-350 mmol m^{-2} yr^{-1} in the Bothnian Sea. An area-weighted average of these figures is about 170 mmol m^{-2} yr^{-1}. The budgetary estimates yield an estimated *(nfix-denit*) equivalent to about 160 mmol m^{-2} yr^{-1}. Other denitrification estimates in the Baltic and adjacent marine sea areas (Koop *et al.*, 1990) have ranged between 140 and 660 mmol m^{-2} yr^{-1}. However, none of these studies has been in the Gulf of Bothnia.

The above fluxes for the Gulf of Bothnia provide some sense of seasonal variation in fluxes, the short-term importance of water column storage, and explicit treatment of exchange between the inorganic and organic phosphorus and nitrogen reservoirs. In the next case study, analysis of sub-basins within the entire Baltic-Kattegat system, treated as a steady-state system based on data over approximately 20 years is carried out.

5.6.6 Baltic-Kattegat: Steady-state NP budgets in the sub-basins of an estuarine sea

The Baltic Sea (Figure 17) is one of the most intensively studied marine areas in the world, and this wealth of existing information can be utilised to develop budget calculations and empirical models. These budgets give estimates of the relative importance of advective import/export, of inputs from the atmosphere and drainage basins and of internal sources and sinks for the concentration of nutrients and other substances in the basins. They also give estimates of the critical scales, such as the residence times of salt, water and other substances.

The Baltic Sea is an ideal system to use for this budget approach, due primarily to the long residence times of both water and of non-conservative substances, the possibility to use salt as a conservative tracer, and the long and extensive time series of data available. Using long time series of data on inputs and concentrations of salt and other substances in the basins, it should be possible to find empirical relationships between inputs and conditions in the sea.

Estimates of inputs of fresh water and nutrients combined with calculations of total amounts of salt and nutrients in different subregions of the Baltic have been used to develop nutrient budgets and models of the entire Baltic Sea (Wulff and Rahm, 1988; Wulff and Stigebrandt, 1989) and for sub regions like the Gulf of Riga (Yurkovskis *et al.*, 1993) and the Gulf of Bothnia (Wulff *et al.*, 1994). This approach has even been used in budgets and models of toxic substances, for example, the fate of pulp mill effluents (Wulff *et al.*, 1993; Wulff and Rahm, 1993).

The Baltic Sea, including several of its sub-basins, has been used to develop a detailed budget of dissolved nitrogen and phosphorus fluxes (Wulff and Stigebrandt, 1989). More recently, Smith and Richardson (in preparation) have developed a stoichiometrically based budget for the Kattegat. The combination of these two studies provides several interesting opportunities. The paper by Wulff and

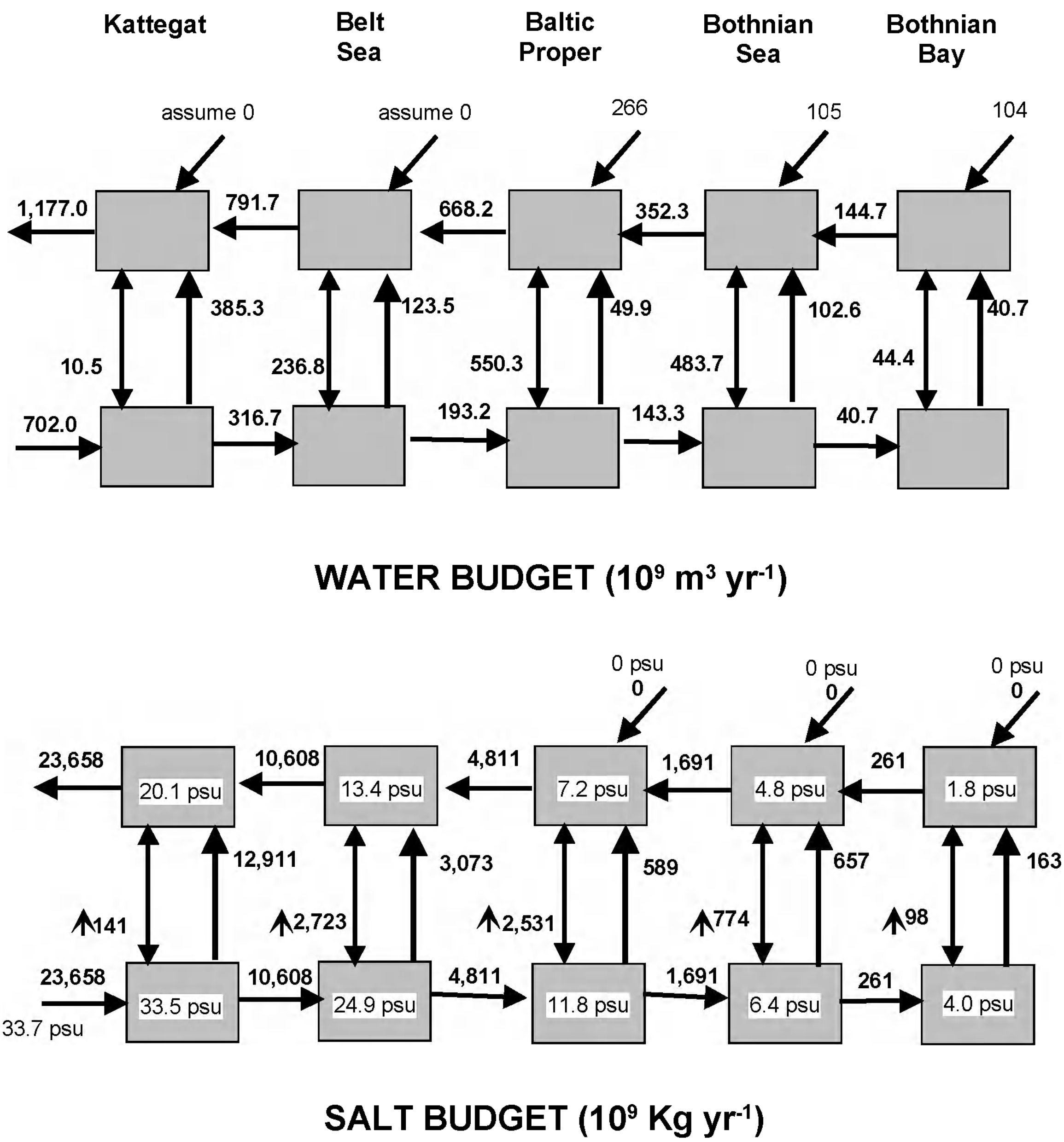


Figure 21. Steady-state water and salt budgets for the Baltic-Kattegat system to illustrate horizontal and vertical linkages between compartments. Quantities calculated within the budgets are shown in bold typeface. The slanted arrows in the upper boxes represent loading from land; the horizontal arrows illustrate advective flows between boxes; the single-headed vertical arrows indicate entrainment; and the double-headed vertical arrows illustrate vertical mixing.

Stiegebrandt (1989) provides an example of analysing three systems in series, Bothnian Bay, Bothnian Sea and Baltic proper, while the addition of the Kattegat actually adds two basins to the series, because the Belt Sea lies between the Baltic proper and the Kattegat (Figure 17).

Fluxes for any nonconservative material (Y) are calculated exactly as for the 1-layer case, by the addition of other known inputs, such as sewage, precipitation, groundwater, and $\Delta Y_{u(n)}$ and $\Delta Y_{d(n)}$ to Equation (21). One problem encountered by Smith and Richardson (in preparation) is that they did not have reliable data on DON and DOP for the Kattegat. However, both the Tomales analysis and data in Wulff and Stiegebrandt (1989) suggest that, while these terms may be important to the overall system hydrographic fluxes, they tend to be minor contributors to the nonconservative fluxes. In order to compare the two data sets, inorganic nitrogen and phosphorus data are used exclusively in the analysis presented here.

Figures 22 and 23 summarise the inorganic phosphorus and nitrogen balances for this system. In Figure 22 all of the upper boxes show ΔDIP to be negative (net uptake). It is assumed that this material falls out as particles, rather than either accumulating in the upper boxes or being removed as particle fluxes. Some of that material regenerates in the lower boxes (ΔDIP is positive). It is assumed that particulate fallout which does not regenerate is buried, rather than either accumulating in the lower boxes or being removed as particle fluxes. Vertical mixing (heavy, solid arrows between surface and deep boxes) are positive for net flux into surface box.

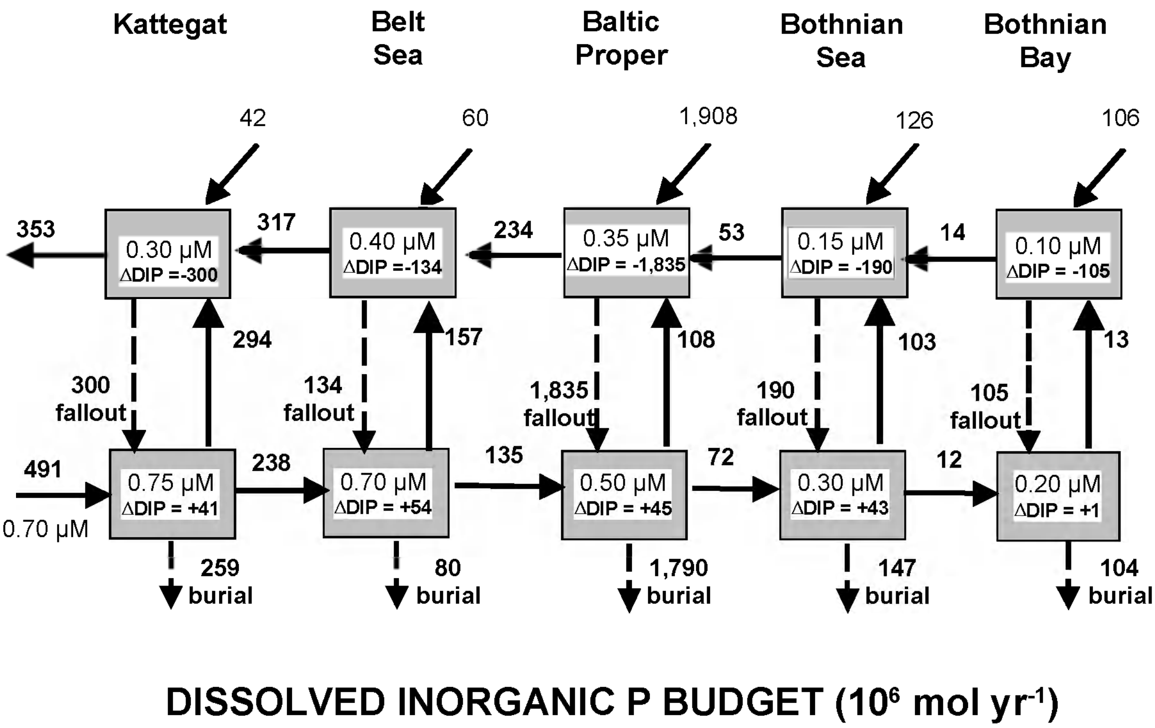


Figure 22. Steady-state dissolved inorganic phosphorus budget for the Baltic-Kattegat system. Quantities calculated within the budgets are shown in bold typeface. The slanted and horizontal arrows are the same as in Figure 21; the solid vertical arrows combine entrainment and mixing fluxes; the dashed vertical arrows indicate particle fallout from the surface boxes and burial flux from the bottom boxes, both inferred from the dissolved P fluxes.

In Figure 23, nitrogen fallout from the surface boxes is fixed by the $N:P_{part}$ ratio of 12:1. To account for the net loss, the remaining nonconservative DIN flux in the surface boxes is balanced with (nfix-denit). Nitrogen burial is fixed by the $N:P_{part}$ ratio of buried materials, 7:1, and the remainder of the nitrogen flux, gains or losses, in the deep boxes is balanced by (nfix-denit). Vertical mixing is represented by heavy solid arrows between surface and deep boxes, and are positive for net flux into surface box. Other assumptions and notations are as on Figure 22.

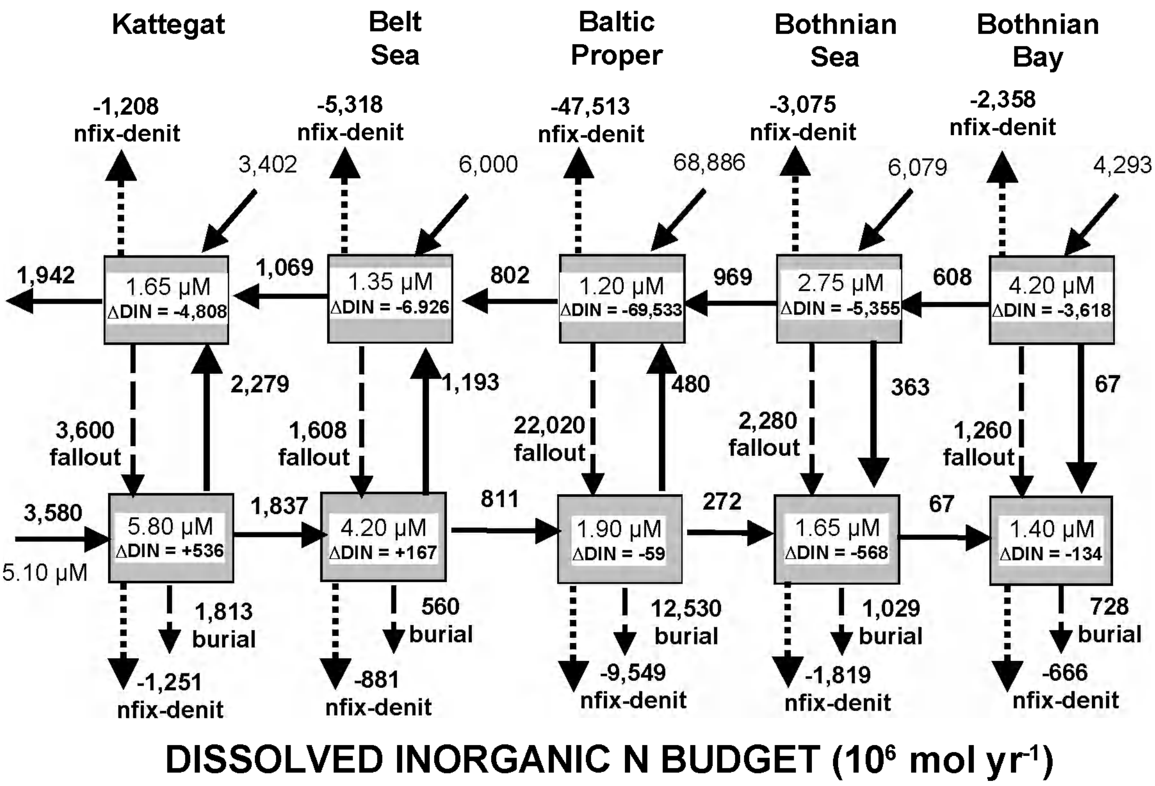


Figure 23. Steady-state dissolved inorganic nitrogen budget for the Baltic-Kattegat system. Quantities calculated within the budgets are shown in bold typeface. The slanted and horizontal arrows are the same as in Figure 21; the solid vertical arrows combine entrainment and mixing fluxes; the dashed vertical arrows indicate particle fallout from the surface boxes and burial flux from the bottom boxes, both inferred from the dissolved P fluxes. The dotted arrows represent (*nfix-denit*) inferred from the discrepancy between dissolved and particulate N fluxes.

In this case study, all fluxes, including the nonconservative fluxes, are most conveniently left as basinwide total fluxes, rather than being scaled per unit area, in order to describe the mass exchanges between sub-basins. However, Table 9 presents each sub-basin's nonconservative fluxes and the stoichiometrically derived rates scaled per unit area for ease of comparison.

Note that each basin shows an uptake of DIP in the surface box and a release in the deep box. This presumably represents net organic production in the surface and regeneration in the deep box. The pattern is somewhat more complicated for DIN. All surface boxes show net uptake, but the deep boxes are more variable. The stoichiometric balance is calculated by assuming that the phosphorus uptake in the upper box is matched by an nitrogen uptake which is 12 times as large, that is, $(N:P)_{part}$ = 12:1. This ratio is based on summary data by Smith and Richardson (in preparation) for the Kattegat and may not be entirely appropriate for the other basins; it is used here for illustrative purposes only. Nevertheless it is seen that the various sub-basins of the Baltic have rates of (*nfix-denit*) ranging from about -100 to -300 mmol m^{-2} yr^{-1}, that is, they exhibit net denitrification.

Table 9. Nonconservative nitrogen and phosphorus fluxes and stoichiometric calculations for sub-basins of the Baltic-Kattegat system (fluxes in mmol m^{-2} yr^{-1}).

	Kattegat	Belt Sea	Baltic Proper	Bothnian Sea	Bothnian Bay
Area (10^3 km^2)	21	20	267	72	36
$\Delta DIP_{surface}$ (1)	-14	-7	-7	-3	-3
Surface $\rightarrow$ Deep P fallout (2)	14	7	7	3	3
ΔDIP_{deep} (1)	2	3	0	1	0
P burial (3)	12	4	7	2	3
$\Delta DIN_{surface}$ (1)	-229	-346	-260	-74	-101
Surface $\rightarrow$ Deep N fallout (4)	171	80	82	32	35
(*nfix-denit*)$_{surface}$ (5)	-58	-266	-178	-42	-66
ΔDIN_{deep} (1)	26	8	0	-8	-4
N burial (6)	86	28	47	14	20
(*nfix-denit*)$_{deep}$ (4)	-59	-44	-35	-26	-19

(1) Net nonconservative flux in hydrographic budget.
(2) Assume all particles produced settle from that sub-basin's surface box to the deep box.
(3) Assume surface $\rightarrow$ deep fallout which does not regenerate is buried in that sub-basin.
(4) Assume N:P ratio of surface $\rightarrow$ deep particle flux = 12:1; calculate from phosphorus particle flux.
(5) Balance the nonconservative nitrogen flux.
(6) Assume N:P ratio of burial flux = 7:1; calculate from phosphorus burial flux

It is assumed that all particle formation settles from the upper box where formed, into the lower box for that basin. The deep DIP regeneration is derived from the settling particles, and the phosphorus not regenerated is assumed to accumulate in that basin. Again, using Kattegat data from Smith and Richardson (in preparation), the N:P ratio of sediment, 7:1, is used to calculate the burial flux of nitrogen. The nitrogen imbalance in this box is then attributed to denitrification.

Quantitatively, the nitrogen and phosphorus fluxes are not balanced without an additional nitrogen sink. The nitrogen fluxes are scaled via a particle uptake N:P ratio of 12:1 for p-r in the water and with a sediment N:P accumulation ratio of 7:1 (see section 5.4.6). Imbalances of the nitrogen budget are attributed to (*nfix-denit*). Some nitrogen and phosphorus are, of course, lost by being bound into refractory organic matter in the sediments. There is experimental evidence (Carman and Wulff, 1989) that DIP concentrations in the interstitial water are high enough to cause significant losses by adsorption to particles. This can be accounted for in the stoichiometric calculations by using the sediment N:P ratios. The stoichiometric calculations scaling nitrogen fluxes to phosphorus fluxes suggest that (*nfix-denit*) has consumed nitrogen both from the inorganic load in the water column and, primarily, nitrogen reaching the bottom as organic matter. The calculations suggest that about 70% of the nitrogen losses through denitrification occur in the sediments.

The points which emerge from this analysis are that the budgets of the individual sub-basins may be tied together, that the fluxes between the individual sub-basins must be retained in total mass units, but that the comparisons among the nonconservative fluxes are most constructively examined once scaled to rates per unit area. It is further noteworthy that the nitrogen fluxes can only be balanced relative to phosphorus fluxes if there is substantial nitrogen removal from the system via denitrification. The derived rates of denitrification are within the range of rates which have been independently estimated for portions of the Baltic-Kattegat system, suggesting that this procedure provides a robust assessment of denitrification for other coastal systems in general.

5.6.7 Spencer Gulf: Steady-state CNP fluxes in a calcifying hypersaline system

Nutrient budgets are available for Spencer Gulf, Australia (Figure 24) (Smith and Veeh, 1989). This hypersaline system dominated by calcareous sediments is used both to illustrate a simple 2-box linked model and also to illustrate calculation of $CaCO_3$ reactions from alkalinity fluxes. Modification of these budgets to the same stoichiometric framework discussed here provides further insight into the budgeting procedure. Spencer Gulf is a slightly hypersaline system, with salinity increasing from values near 36 p.s.u. in the ocean to salinities in excess of 45 p.s.u. at the head of the Gulf. There is insignificant surface inflow of freshwater, little precipitation, and apparently little groundwater inflow. The southern, or outer, portion of the system is a deep-water region, in which plankton are assumed to dominate primary production. The northern area is much shallower, with abundant seagrass.

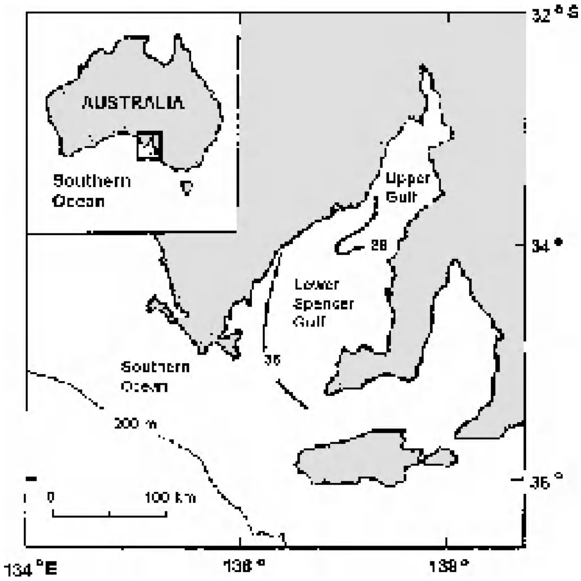


Figure 24. Location of Spencer Gulf, Australia.

Waters of the adjacent Southern Ocean are very low in nutrients, yet DIP decreases with distance from the ocean into the Gulf (Figure 25). The conspicuous break in the salinity-DIP plot near a salinity of 38 p.s.u. is used as basis to divide the Gulf into two hydrographic regions, denoted here as the Lower Gulf [area = 15.6×10^9 m^2; volume = 420×10^9 m^3], and the Upper Gulf [area = 6.1×10^9 m^2; volume = 30×10^9 m^3]. The evaporative water flux (V_E) is defined by evaporation (2.6 mm d^{-1}) and the area of the Gulf. The system is not vertically stratified, so the Lower and Upper Gulf boxes are linked by the 0-dimensional exchange and nutrient flux equations, Equations (1)- (22). Available data are sufficient for development of steady-state calculations, but insufficient to develop time-course calculations.

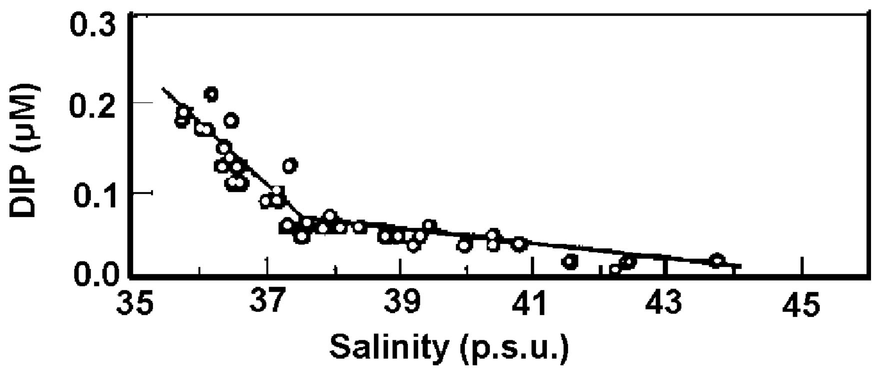


Figure 25. Distribution of DIP as a function of salinity in Spencer Gulf. The distinct slope break near a 38 p.s.u. is used to separate the Gulf into two regions.

Figure 26 summarises the water and salt budgets for the two regions. Precipitation and evaporation are grouped together into a single term of net evaporation (V_P - V_E). This flux pathway removes 16 x 10^6 m^3 d^{-1} of water from the Upper Gulf and 40 x 10^6 m^3 d^{-1} from the Lower Gulf. As a result of this removal, residual seawater inflow occurs to offset the evaporative loss. Residual flow (V_R) into the entire Gulf is thus 56 x 10^6 m^3 d^{-1}, with 16 x 10^6 m^3 d^{-1} of that residual flow moving northwards from the Lower to the Upper Gulf. Residual salt flux into the Upper Gulf from the Lower Gulf is 608 x 10^6 kg d^{-1}, and into the Lower Gulf from the ocean is 2,005 x 10^6 kg d^{-1}. From these fluxes V_X can be calculated between the Upper and Lower Gulf as 290 x 10^6 m^3 d^{-1}, and between the lower Gulf and ocean as 1,823 x 10^6 m^3 d^{-1}.

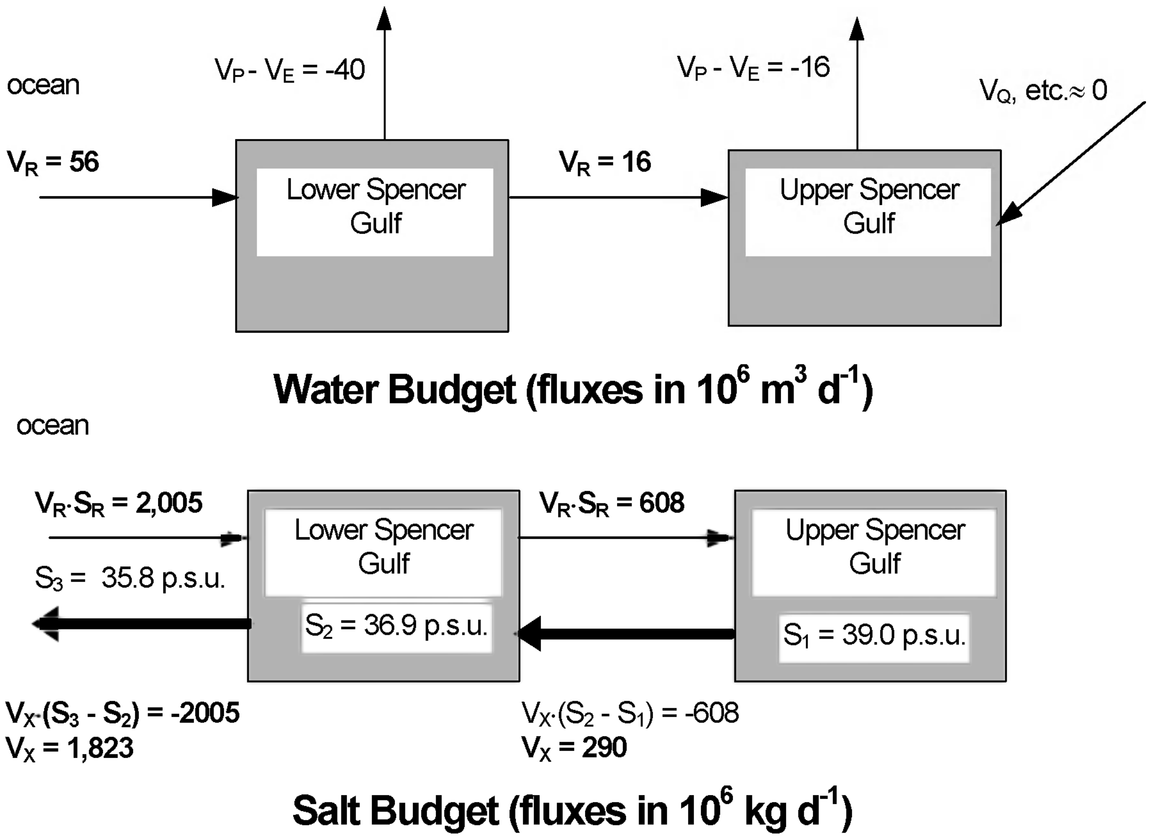
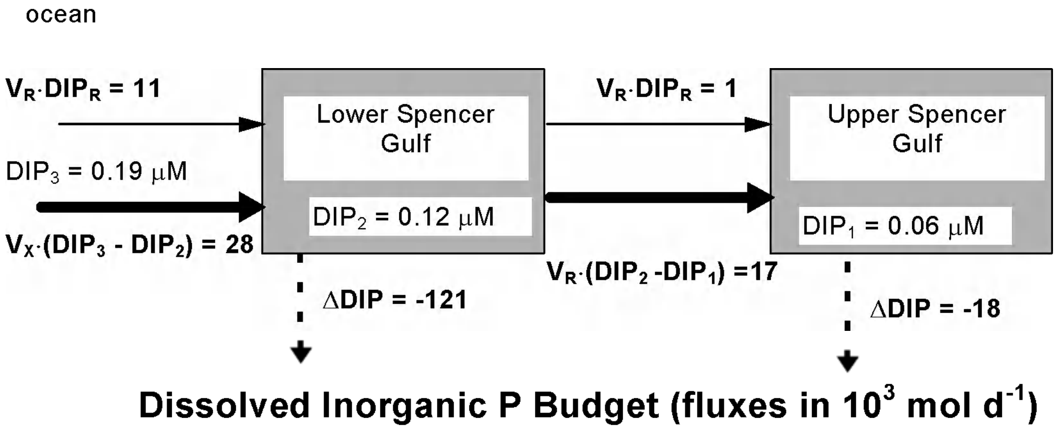


Figure 26. Steady-state water and salt budgets for Spencer Gulf. The heavy mixing arrows show the direction of net flux. Quantities calculated within the budget are shown in bold typeface.

Figures 27-29 summarise the dissolved C, N, and P budgets. The system is a net calcifying system, with little terrigenous material accumulating in the sediments. Hence, the change in total alkalinity (ΔTA) can be used as a measure of $CaCO_3$ precipitation (Equation 25), rather than of sulphate reduction in this system. The residual fluxes and exchange fluxes are calculated using the concentrations of these materials and the values for V_R and V_X. Nonconservative fluxes, that is, ΔY's for each of these terms, are calculated according to Equation 22, with all the freshwater inputs having values of 0. Although the various portions of each budget are included in the notation on the box diagrams, note that there is no gradient of DOP, NO_3, or NH_4 between the ocean and Gulf. The residual fluxes of these materials are small, driven by evaporative inflow of seawater, and the exchange fluxes are effectively equal to 0. DOC shows a slight increase from the ocean to the Gulf, but the calculated fluxes are small compared to TA and DIC. DIP, TA, DIC, and DON all show significant net nonconservative fluxes.



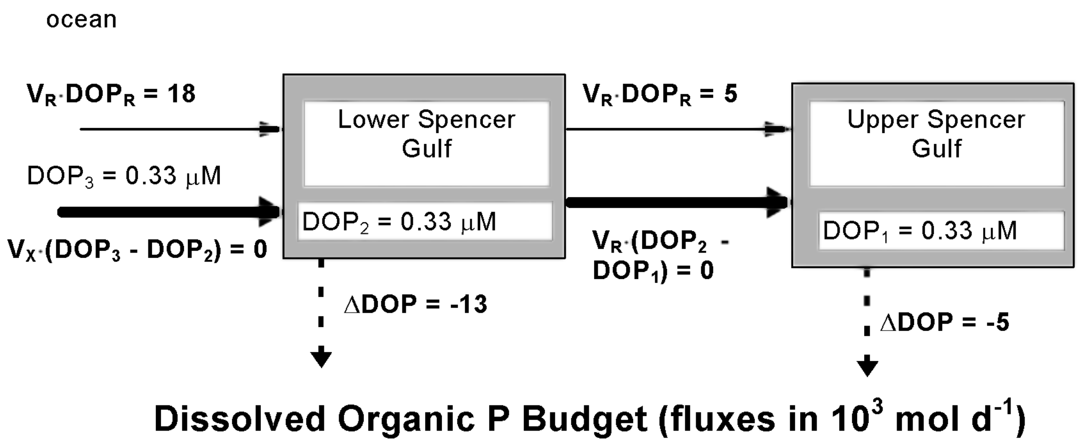
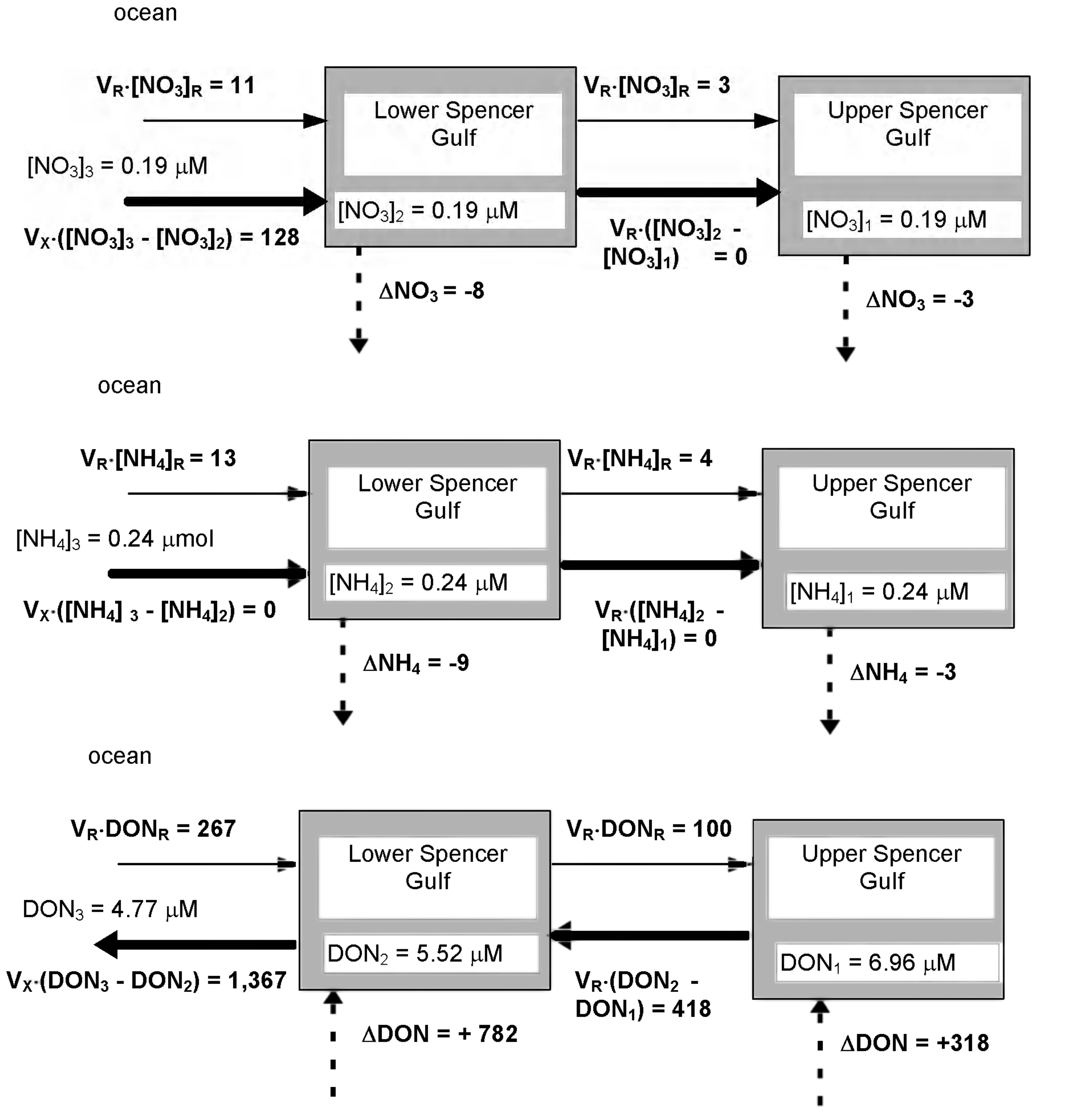


Figure 27. Steady-state dissolved phosphorus budgets for Spencer Gulf. Quantities calculated within the budgets are shown in bold typeface. Note that there is uptake of DIP in both boxes.



Dissolved Organic Nitrogen Budget (fluxes in 10^3 mol d^{-1})

Figure 28. Steady-state dissolved nitrogen budgets for Spencer Gulf. Quantities calculated within the budgets are shown in bold typeface. Note that there is very slight uptake of NO_3 and NH_4 and a large release of DON. There must be positive ΔDON (hence [nfix-denit] is positive) to balance the nitrogen budget.

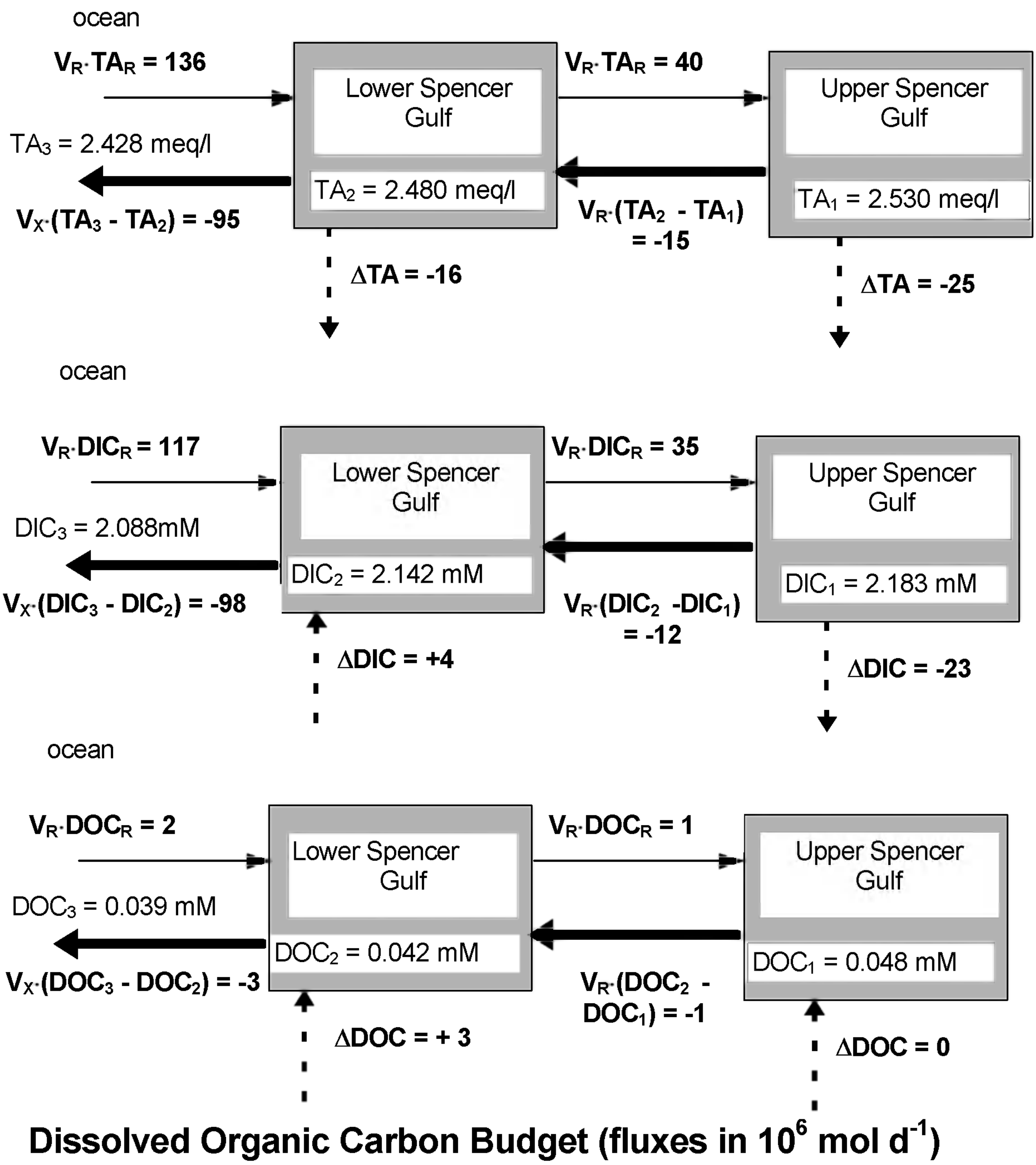


Figure 29. Steady-state fluxes of total alkalinity, dissolved inorganic carbon, and dissolved organic carbon in Spencer Gulf. Quantities calculated within the budget are shown in bold typeface.

Table 10 summarises the stoichiometric calculations based on the net fluxes of dissolved carbon, nitrogen, and phosphorus in this system. Based on ΔTA, scaled per unit area, the system apparently calcifies more rapidly in the Upper Gulf than the Lower Gulf. Based on the distribution of plant communities in the Gulf, it is assumed that the dominant primary producer shifts from plankton in the Lower Gulf to seagrass in the Upper Gulf. This shift and the composition shift of particulate material produced by these two plant groups are used to calculate (*p-r*) from the ΔDIP data. The two basins are calculated to be slight net producers of organic carbon. The stoichiometric calculations also suggest that the system (*nfix - denit*) is positive; the system appears to be fixing more nitrogen than is lost to denitrification. The net rates of (*nfix- denit*) appear reasonable in comparison with data for shallow systems of this kind (Capone, 1983).

Table 10. Nonconservative carbon, nitrogen and phosphorus fluxes and stoichiometric calculations for sub-basins of Spencer Gulf (fluxes in mmol m^{-2} d^{-1}, except TA, which is in meq m^{-2} d^{-1}).

	Lower Gulf	Upper Gulf
Area (km^2)	15,600	6,100
ΔDIP	-0.008	-0.003
ΔDOP	-0.001	-0.001
ΔNO_3	-0.001	-0.000
ΔNH_4	-0.001	-0.000
ΔDON	-0.050	-0.052
ΔTA	-1.03	-5.10
ΔDIC	+0.25	-3.77
ΔDOC	+0.19	+0.00
(*p-r*)	+1.0(1)	+1.7(2)
ΔDIC_c	-0.5(3)	-2.1(3)
ΔDIC_o	-1.0(4)	-1.7(4)
ΔDIC_g	+1.8(5)	0.0(5)
(*nfix-deniti*)	+0.23(6)	+0.13

(1) Lower Gulf is plankton dominated; ∴ (*p-r*) = -125 x ΔDIP (from local plankton C:P ratio).
(2) Upper Gulf is seagrass dominated; ∴ (*p-r*) = -660 x ΔDIP (from local seagrass C:P ratio).
(3) $\Delta DIC_c = \Delta TA/2$.
(4) $\Delta DIC_o = -p-r$.
(5) $\Delta DIC_g = \Delta DIC - \Delta DIC_c - \Delta DIC_o$.
(6) (*nfix-denit*) based on average N:P ratio of approximately 20:1.

5.6.8 Tokyo Bay: Numerical analysis of water circulation from current data

Tokyo Bay (area = 1000 km^2; volume = 17 x 10^9 km^3) provides an example of a system for which the circulation is estimated via numerical analysis of circulation, rather than water and salt budgets. At this writing sufficient data is not available to develop nutrient budgets of this system. The water exchange is estimated with a three-dimensional numerical model. The observed freshwater discharge from rivers and the estimated heat transfer through the sea surface from meteorological data in both the summer and winter are inputs to the model. Evaporation and precipitation at the sea surface are neglected because they are nearly balanced in Tokyo Bay. Groundwater inflow is also ignored because it is very small compared with freshwater discharge from rivers. Water from sewage is mainly loaded into rivers and it is included in the river discharge. The observed water temperature and salinity distributions are also given along the open boundary of the model basin. The interpolated sea surface wind field based on the observed wind on land is given to the model basin. The tidal stress, which generates the tide-induced residual current, is included in the momentum equation of this model on the basis of the results of tidal current calculations. The calculated quasi-steady residual flow field in the upper layers of Tokyo Bay are shown in Figure 30 (Yanagi and Shimizu, 1993). The residual flow consists of the density-driven current, the wind-driven current and the tide-induced residual current. Such results are verified by the limited observed data of current measurements in the field. It is possible to estimate V_X at the mouth of Tokyo Bay by using the results of the calculated tidal current and residual flow fields (Figure 31). Additional examples of the methodology and results can be found in Yanagi (1996).

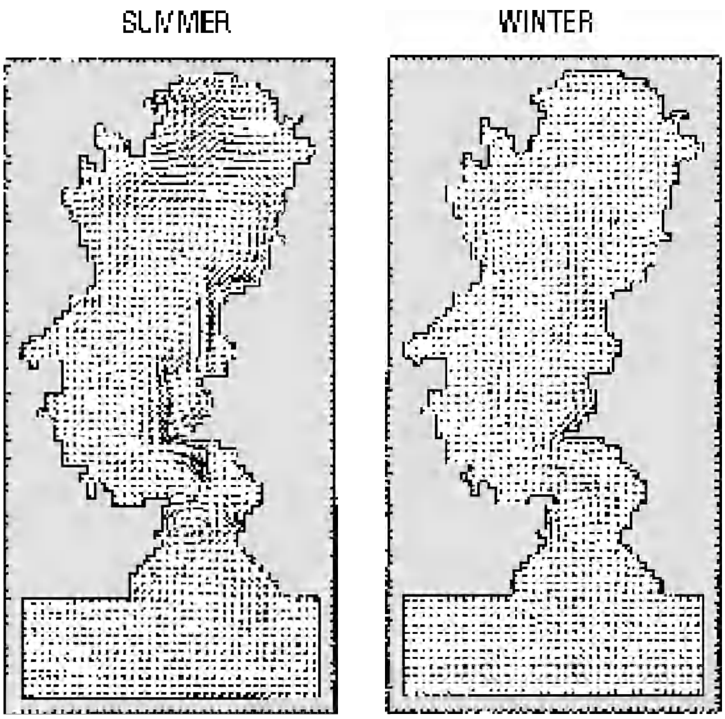


Figure 30. Calculated residual flow in the upper layers of Tokyo Bay in the summer and winter.

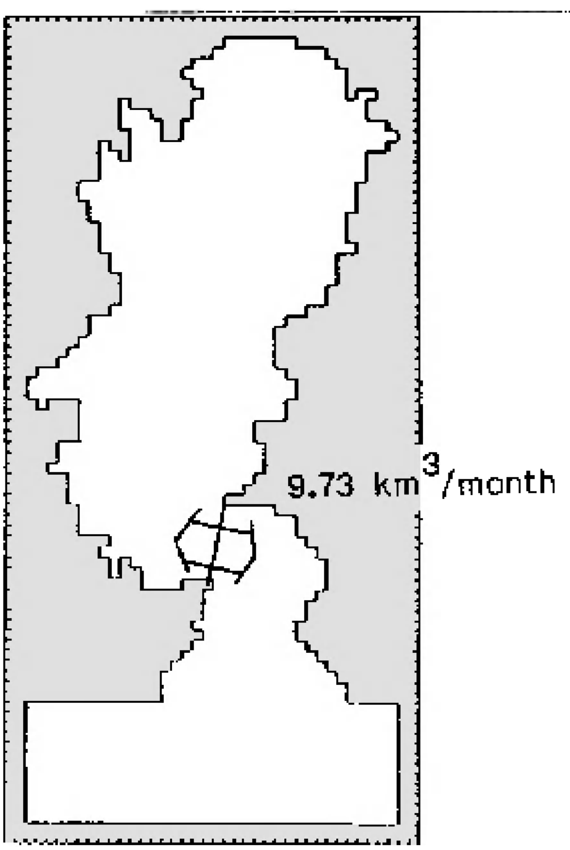


Figure 31. Estimated exchange flow (V_X) at the mouth of Tokyo Bay on the basis of calculated tidal currents and residual flow.

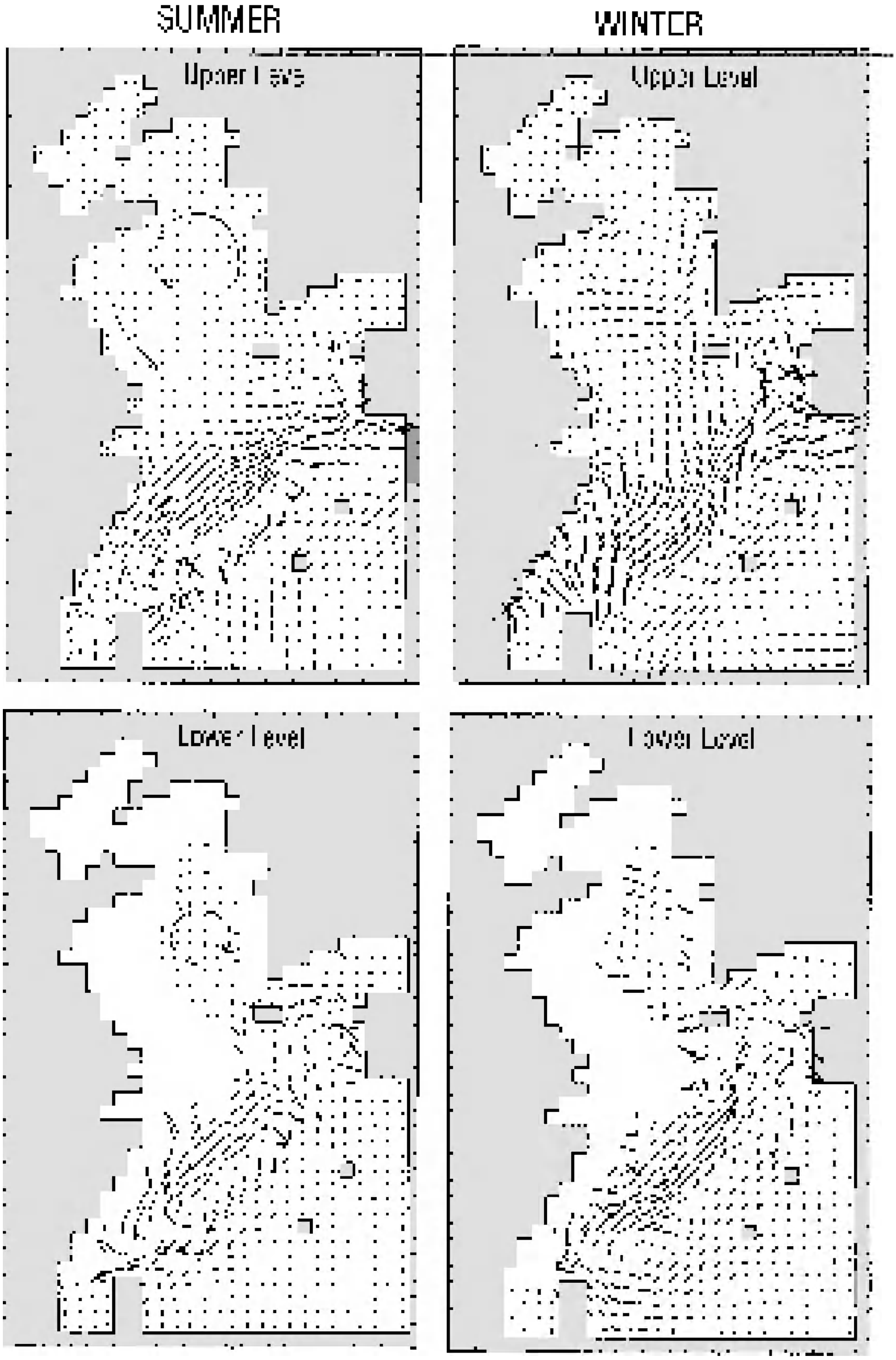


Figure 32. Calculated residual flow in the upper and lower layers of the East China Sea and the Yellow Sea in the summer and winter.

5.6.9 East China Sea: Numerical analysis of water circulation in a shelf sea estimated from the temperature and salinity field

In the East China Sea (area = 1.2×10^6 km^2; volume = 4.5×10^4 km^3), the seasonal variation of the three dimensional residual flow field is calculated by means of the robust diagnostic numerical model with the use of historically observed water temperature, salinity, and wind data (Figure 32). The estimated residual flow fields at the upper and lower layers in summer and winter are shown (Yanagi and Takahashi, 1993). Those in spring and autumn are similar to that in winter. It is nearly impossible to carry out the direct current measurements in order to obtain the whole current field in a coastal sea such as the East China Sea, because trawl fishing activity is very intense. However, the accumulation of water temperature and salinity data is relatively easy. The robust diagnostic numerical calculation technique is a very promising method for estimating the current field quantitatively in a coastal sea using observed water temperature and salinity data. This estimated current field then can be used to develop a water budget, such as here, for the East China Sea. Such results are a fundamental requirement for the subsequent development of regional budget models for salt, phosphorus, nitrogen, and carbon. For example, it is possible to estimate V_x across the shelf edge of the East China Sea.

This method is basically the same as that used for the ERSEM (European Regional Seas Ecosystem Model) developed for the North Sea (Lenhart *et al.* 1995). These authors calculated the seasonal and year-to-year variation of three dimensional current field in the North Sea from 1970 to 1992 with use of a general circulation model. Their circulation model was driven by implementing the observed meteorological data of sea surface wind, air pressure and sea surface temperature. They estimated the water budget in the North Sea on the basis of the calculated current field.

5.7 Summary of Case Studies

The various case studies have provided examples of the use of stoichiometrically linked water-salt-nutrient budgets in coastal marine systems, including some of the complications which can arise. Eight case studies are presented, each providing slightly different insight into budgeting material fluxes in such environments. The insights which emerge from these examples can be generally characterised as follows.

Preliminary data can be used to gain insight into how systems process carbon, nitrogen, and phosphorus as was done for Bahia San Quintín and Klong Lad Khao Khao Bay. The Klong Lad Khao Khao study developed as a workshop exercise while these guidelines were in draft stage and is worked through in explicit detail. In that system, the stoichiometric calculations yield results which may not be entirely reasonable. While more detailed assessment would be necessary to verify this apparent discrepancy and isolate the basis for it, the very existence of such potentially problematical results is itself insight into other processes which may be occurring in the system.

Two systems allowed examination of non-steady state salinity: Tomales Bay and the Gulf of Bothnia. The Gulf of Bothnia allowed further examination of changing system water volume. Because of rather detailed data available for both of these systems, they are further useful for the more detailed examination of stoichiometric linkages between carbon, nitrogen and phosphorus. These data are compared with available data for component metabolism in these two systems. In the case of Tomales Bay, time-stepped data for freshwater inputs and for the salinity and DIP concentration of the various water types are given so that the calculations may be duplicated in detail. Furthers point for that system are: 1) nonconservative total alkalinity flux in that system is used to estimate system-level rates of sulphate reduction; and 2) CO_2 gas flux is calculated to close the DIC budget.

Three cases of geographic linkages between systems were presented, Bothnian Gulf, Baltic-Kattegat, and Spencer Gulf. One of these, the Baltic-Kattegat, includes both horizontal linkages between adjacent basins and vertical linkages between surface and deep waters. Spencer Gulf was used to introduce the concept of nonconservative total alkalinity flux as a measure of calcification in actively calcifying systems.

Finally, two examples, Tokyo Bay and the East China Sea, were given in which numerical simulation models, rather than water and salt budgets, provide information on water circulation.

6. RESPONSE TO SECOND LOICZ MODELLING REQUIREMENT - PREDICTION

Budget calculations, however useful, describe essentially a static situation. By comparing budgets of similar systems under different environmental conditions or by following the same system over time under changing conditions, it is possible to derive empirical relationships useful for prediction. Thus budgets and empirical relationships can be merged into dynamic simulation models. This has been a very successful approach used in limnology (Vollenweider, 1969) and there are no reasons why such an approach could not be used for coastal systems as well. A good recent example is the analysis of North Atlantic shelf data made by Nixon *et al.* (in press) showing that the net fractional transports of nitrogen and phosphorus are inversely correlated with the mean residence time of water in the system. Examples of dynamic time-dependent empirical models are the nutrient budget of the Baltic Sea developed by Stigebrandt and Wulff (1989) and the modelling of Ver *et al.* (1994).

In the short term, budget calculations and empirical models are likely to have a greater value as predictive tools of different management strategies than the development of detailed mechanistic models. Mechanistic models serve initially as a 'workbench' where model evaluations can be compared with field measurements to improve our overall scientific understanding.

Empirical models are generally limited in their predictive capabilities to the range of observed data for which they were generated. As a result process oriented system models also need to be developed in order to evaluate the effects of perturbations outside the range for which there exists empirical data.

Most dynamic simulation models are 'mechanistic'. That is, they attempt to integrate existing knowledge derived from studies of different processes, into simulations for entire ecosystems. Experience to date shows that many mechanistic modelling projects, particularly those that attempt to replicate the functioning of entire ecosystems, have failed because they are often based on a 'bottom-up' approach. This has demonstrated that even a detailed understanding of various processes, expressed as sub-models and assembled into an 'ecosystem' model, is often insufficient to describe total system properties (see for instance Platt *et al*., 1981).

A holistic approach is required where the goals of the models and the critical scales are defined prior to model formulation and simulation. The model is in itself a hypothesis, and the numerical simulation is a tool to test this hypothesis, not a goal in itself.

From the LOICZ perspective, the question is how will the nutrient budget of a coastal system be affected by environmental change, primarily changes in climate and nutrient load. Thus, the LOICZ objective necessarily restricts the required model resolution from an infinite number of possible ecosystem components to a few important state variables. Even with this recognition, as noted in Section 3, there is a tendency to disaggregate unnecessarily, that is to add additional variables or data, simply because the information is available, or because researchers feel that the model cannot be developed without incorporating all available expertise.

What then are the minimum key processes that have to be included in a dynamic process oriented model of a coastal ecosystem? This chapter attempts to present these along with a few simple guidelines, illustrated by examples.

As has been described earlier in the section on budget modelling (Section 5.3), the basic differences between a conservative material, such as salt, and a non-conservative substance, such as nutrients, are the internal sources and sinks. Nitrogen, as inorganic nutrients, can be added through N_2-fixation and lost through denitrification. Phosphorus can be adsorbed to particles. In some systems, a large proportion of the nutrients is stored in living organic matter or in detritus in the sediments. A dynamic simulation model must therefore be able to describe the physical and biogeochemical processes that control the fluxes between inorganic and organic pools and the environment (inputs, internal sources and sinks).

As a simple first example, consider a simple well-mixed estuary where primary production is dominated by phytoplankton. In such a system, nutrients and suspended organic matter are exported (or imported) through water exchange. Additional inputs occur through river inputs, points sources and atmospheric deposition. Primary production and sedimentation of organic matter are then the key processes that deplete the water column of nutrients. From an offshore perspective, these are the key biological processes that have to be described. Nutrients are reaching the productive surface layer, assimilated and recycled and eventually lost through sedimentation. Models describing these processes in the open ocean are a key objective for Joint Global Ocean Flux Study (JGOFS) Core Project of the IGBP, where the biological model is incorporated into ocean circulation models (Fasham *et al.*, 1990; Sarmiento *et al.*, 1993). The models usually have a fixed stoichiometry, assuming a constant C:N ratio. Phosphorus is rarely included in ocean 'blue water' models where nutrient ratios generally follow the Redfield Ratios. The primary reason for this is that remineralisation is to a great extent occurring in the water column and little organic matter will eventually reach the sediments which are situated at great depths (> 1000 m). The basic flow structure that has to be resolved in an oceanic biological model is illustrated in Figure 33.

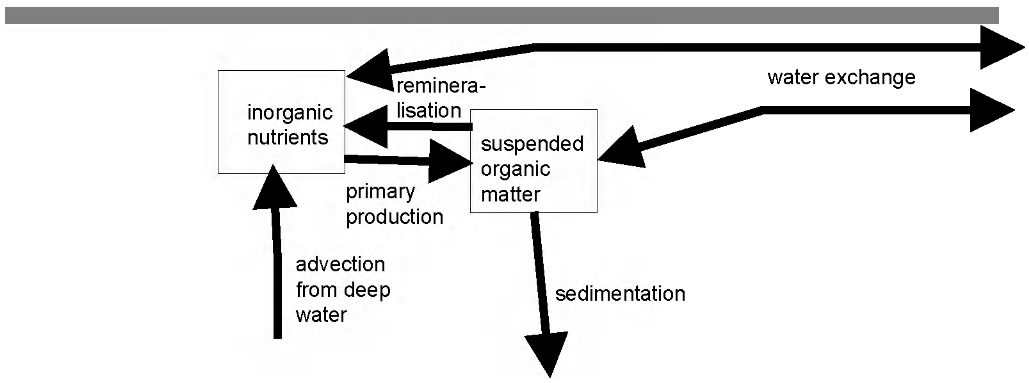


Figure 33. The basic flow structure that is resolved in most oceanic model of nutrient fluxes.

In the coastal zone however, a large fraction of the organic matter falls to the bottom where it is partly accumulated and buried and partly decomposed. Some of the nutrients are returned to the water column; some are lost through the internal sinks. One important difference between oceanic and coastal models is the role of sediment processes for the recycling of nutrients. Another important difference is that the sediment biogeochemical processes are likely to change nutrient concentration due to the fact that substantial proportions of the nutrient are buried as organic matter or lost through sinks, like denitrification for nitrogen and adsorption for phosphorus. These sinks will also change the N:P ratio since more nitrogen is usually retained compared to phosphorus in most marine sediments.

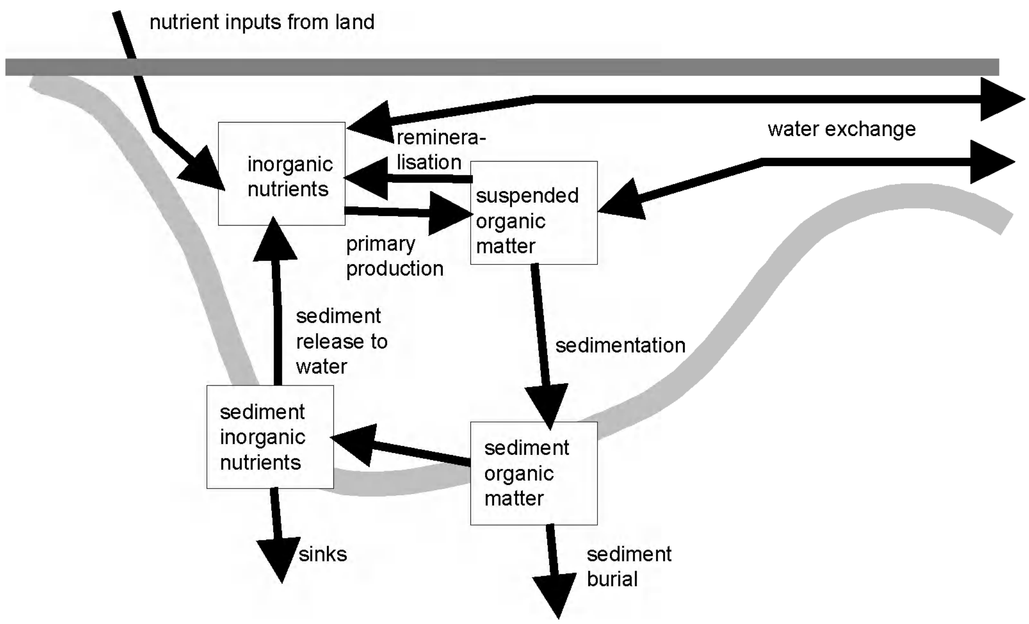


Figure 34. A simplified conceptual flow diagram of nutrient cycles in a coastal ecosystem.

The conceptual model of a coastal system must therefore include sediment processes as illustrated in Figure 34. The basic configuration is in principle the same, independently of which nutrient (CNP) we are describing, although the processes controlling the fluxes, particularly the internal sinks/sources are different.

This simple compartment flow diagram consists of only four state variables, the four boxes in Figure 34, and would be considered to be overly simplified by most ecologists. The immediate reaction for most ecologists is to disaggregate this further by adding additional boxes. However, for the present purposes, this may not be necessary as even this highly simplified system contains a complex flow structure. It may also be possible to validate such a simple model using data that is readily available. Simple standard measurements of inorganic and 'total' nitrogen and phosphorus in the water column may have already been made or may be possible with limited effort. Measurements of the concentrations of suspended and dissolved nutrient fractions are rarely available. Similarly measurements of both organic and inorganic CNP fractions in the sediment may be difficult to achieve. To carry out further disaggregation, it would be necessary to identify appropriate measurements of nutrient inputs from different sources on land, collected with the same methods as used for the water. The concentrations in the sea outside the bay would also have to be known. A common experience is that the compilation of data to support even a highly aggregated system such as this is difficult.

As a result, it is very important to ensure that a higher level of detail can be supported by available data before disaggregating. For instance, it is 'natural' for the plankton ecologist to describe phytoplankton-zooplankton interactions, the microbiologist to include all the interesting features of the microbial loop, and so on for other fields of coastal zone research. However, at each step, the decisive questions are: do we have sufficient quantitative data to address these issues, and is the inclusion of these issues relevant to the objective of the model?

After defining the compartments and basic flow structure of the system, the next step in the development of a dynamic simulation model is to define the processes that need to be included. As with the compartments, there is an infinite number that could be included. Again, the objective of the model and the specific characteristics of the system will determine what is to be included or excluded. In the simple example presented here, the effects of seasonal variation in temperature and insolation would be important and should be included only if the bay was situated on a temperate latitude. These effects would be irrelevant if the bay is located near the equator. Since, in this dynamic model, the aim is primarily to describe how the system changes with respect to time, the temporal resolution of the model must also be decided. For instance, if the purpose is to study the effect of climate change, it may be necessary to have data describing the bay for hundreds of years. If the purpose is to study the effect of changes in nutrient inputs due to the building of a sewage plant, it may only require measurements for a time period of a decade or less. If episodic events, like flooding and hurricanes, are important, the temporal resolution of the data may have to be as high as daily or hourly. In addition to the requirements set by the different questions to be asked, the behaviour of the system, such as the residence time of water and that of different nutrient compartments, as described in section 5.4, will also define the data requirements at the different temporal scales.

Figure 35 demonstrates some of the phenomena usually encountered in coastal and marine systems along with their spatial and temporal scales. The lower diagram shows the need to identify the model definition and the scale of interest. Phenomena that occur on other scales have to be parameterised or treated as external forcing functions. For instance, if a model is developed to follow the seasonal succession of the entire pelagic community it may not be necessary to resolve phenomena on shorter time scales such as the individual movement of an organism. The phenomena that occur on lower scales can be described in aggregated functional relationships, that is “parameterised”, relative to the scale of interest. For the same model it may not be necessary to describe all of the processes that control the system such as water temperature. These higher scale phenomena may be given as an “external function”.

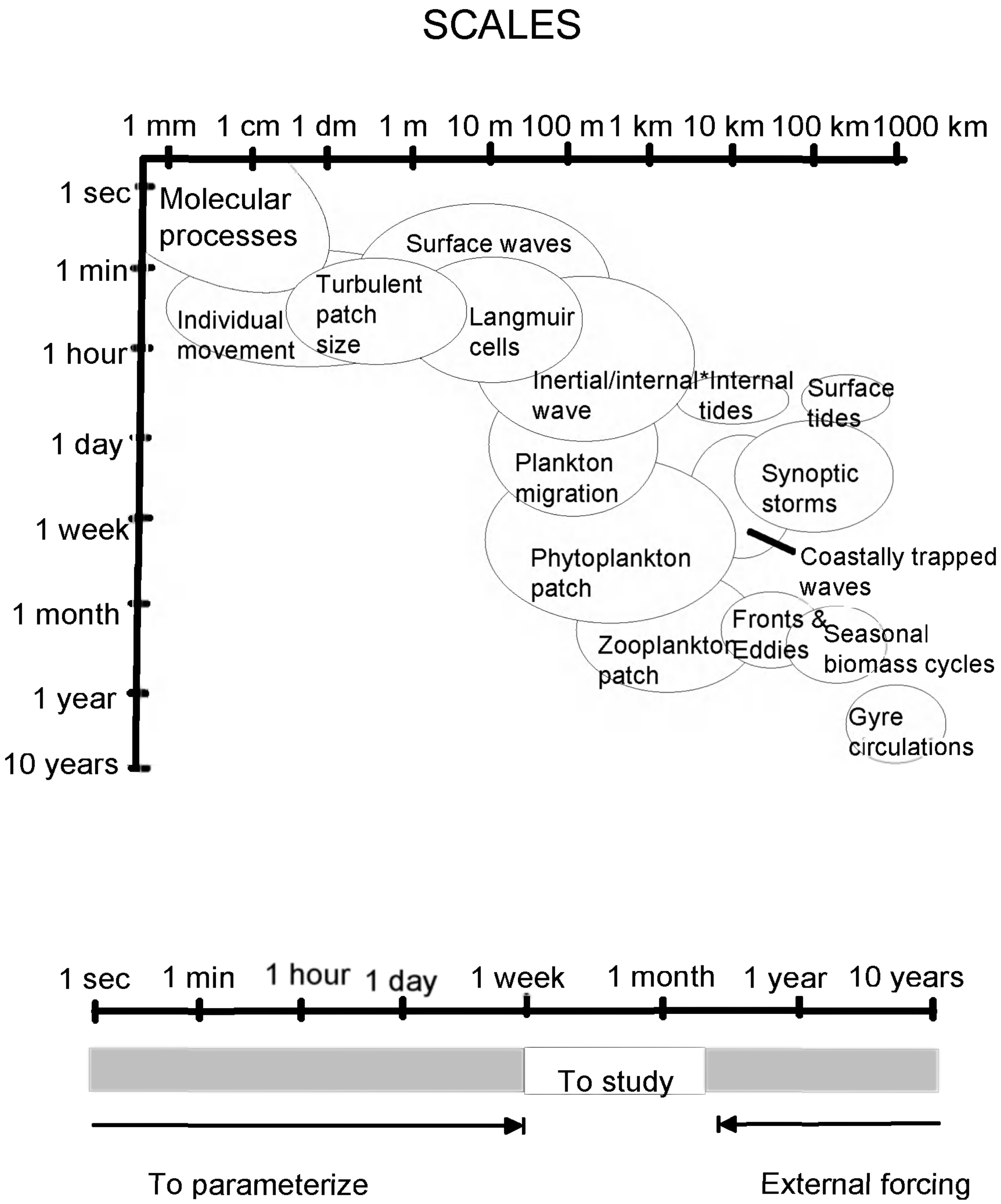


Figure 35. A schematic illustration of spatial and temporal scales of coastal and marine systems. A model aimed at describing a coastal ecosystem must resolve only a part on this entire spectra. Processes that occur on a lower scale will be parameterised while those on larger scales will be treated as external forcing functions.

The use of highly aggregated compartments in a simple model means that it is difficult to directly use field data and laboratory experiments to scale the functional relationships that the model aims to describe. However, these difficulties remain even if the model is disaggregated into 'functional' groups for which there are experimental data. As an example of this difficulty, one mistake that is often made in modelling the trophodynamics of coastal populations is to use data from zooplankton feeding rate experiments in models of phyto-zooplankton interactions. Such simulations show that the modelled zooplankton population will die because the phytoplankton concentration is too low to maintain the herbivores! The simple explanation for this result is that the model assumes that average concentrations of zooplankton feed on average concentrations of phytoplankton. This is not true in the 'real world' where various adaptive strategies and processes occur on spatial and temporal scales that are not included in the model. Figure 35 attempts to illustrate that it is imperative to consider these scaling arguments in the model development. A recent extensive treatment of the problem of scaling issues in modelling, as well as in general ecological research, can be found in Giller *et al.* (1994).

Traditionally, numerical modelling of complex systems required a considerable skill in mathematics, systems or control theory and computer programming. Although some tools now exist to aid development, this is still true and there are many technical and mathematics challenges in achieving the successful implementation of large numerical models. A good recent example of such a complex systems model which includes the variables and processes of interest to LOICZ and what is needed in terms of technical and logistic support is the ecosystem model of the North Sea (ERSEM). A detailed description of this model development and its results are described by Blackford and Radford (1995) and Ruardij *et al.* (1995).

6.1 The Development of a Dynamic Simulation Model - A Simple Demonstration

As stated previously, the process of model development is often as useful as the final model itself. It has also been stated that even a very simple model may contain features not easily understood without carrying out a simulation exercise. As a simple but concrete demonstration of this, a software modelling application, STELLA (see Annex 1 for reference information), is used here to implement and simulate the nutrient dynamics of the simple hypothetical bay illustrated in Figure 34. In this case, the focus for the simulation exercise is on the effects of water exchange on the net export of nutrients from the bay to the outside sea. The question to be asked is: Will an increased water exchange affect how much nutrient that is imported, exported or retained in the bay?

The initially step in building the model with STELLA is to place state variables (squares), flows (broad arrows) and processes (circles) in a flow diagram using the STELLA symbols (Figure 36).

To accurately describe the flows of nitrogen in this example, the minimum number of state variables are: DIN (dissolved inorganic nitrogen), PON (particulate organic nitrogen in the water column), sediment organic nitrogen and sediment DIN.

The processes that are controlling the fluxes between the state variables in the model are: assimilation, sedimentation, sediment burial, sediment mineralisation, denitrification, DIN release and input and water exchange of DIN and PON with the sea outside the bay.

For the 'Model Bay', assume that measurements are available showing that the maximum growth rate of PON is 50% per day under ideal conditions, with no factors limiting growth. The only limiting factors to be considered here are nutrients, DIN, and the light shading effect of biomass represented as PON. The difference equation showing the change in biomass of algae with respect of time (dt) is scaled as:

$$\frac{d[PON]}{dt} = growth - losses \qquad (36)$$

In the simple model, growth is equalised with (net) *assimilation* and *sedimentation.* A maximum assimilation rate of 3% per day is defined so that it is convenient to develop functional relationships for nutrient, called here N_{max},, and biomass shading, called here P_{max}, so that they attain values between 0 and 1. Thus, Equation (34) equation becomes:

$$\frac{d[PON]}{dt} = assimilation - sedimentation \tag{37}$$

Thus

$$assimilation = P_{max} \cdot N_{max} \cdot 0.5 \cdot PON \tag{38}$$

if the nutrient concentration is high and biomass is low enough to ensure that the algae grow at their maximum rate, P_{max} and N_{max} are equal to 1. If there are no nutrients and the biomass is very high, P_{max} and N_{max} are equal to 0. Thus, with this simplistic formulation the limitations due to multiple factors can be described. For instance, there will be no algae growth if there is a high nutrient concentration but P_{max} is 0. It remains to scale these functions for values between 0 and 1. For nutrients the classical Michaelis-Menten, also called Monod, relationship can be used. Assume that experimental data is available that show that the algae grow at half of their maximum rate at a DIN concentration of 0.5 µmol. The Michaelis-Menten equation for N_{max} is then

$$N_{max} = \frac{DIN}{0.3 + DIN} \tag{39}$$

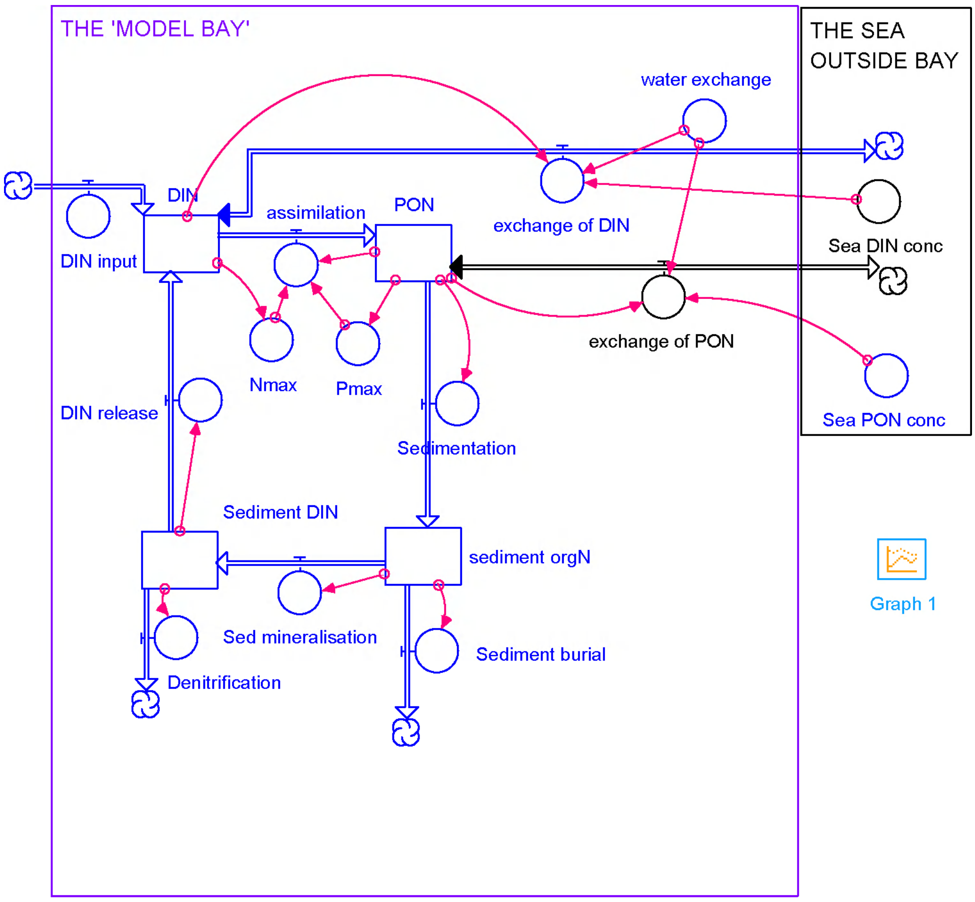


Figure 36. The graphical flow diagram of nutrient dynamic in the 'Model Bay' using STELLA software.

When the concentration of particles in the water column increases, less light will penetrate and the assimilation will become light limited. Assume that the assimilation will decrease to 50% when the concentration of PON reaches 2 μmol. Again, the Michaelis-Menten equation can be used, in this case inverted to formulate P_{max}:

$$P_{\max} = 1 - \frac{PON}{2 + PON} \tag{40}$$

Assimilation in this model is then a function of nutrient concentration and of PON. Measurements are available that show that 10% of the PON particles sediments out each day. Since the factors that affect the growth and loss is known, a *differential equation* can be written that describes PON change with respect to time:

$$\frac{d[PON]}{dt} = P_{\max} \cdot N_{\max} \cdot 0.5 \cdot PON - PON \cdot 0.10 \tag{41}$$

It is further assumed that 5% of the organic matter in the sediment is degraded per day. Of the nutrients that are released into the sediment, 50% is released into the water column and 10% is denitrified each day. Thus, the differential equations for all of the state variables can be written. With STELLA software, these equations are automatically generated when the flow diagram is drawn and the processes are defined. The equations generated by STELLA for the structure depicted in Figure 36 are listed in Text Box 5.

```
DIN(t) = DIN(t - dt) + (DIN_release + DIN_input - assimilation - exchange_of_DIN) * dt
INIT DIN = 10

DIN_release = Sediment_DIN*0.50
DIN_input = 0
assimilation = PON*Nmax*Pmax*0.5
exchange_of_DIN = water_exchange*(DIN-Sea_DIN_conc)
PON(t) = PON(t - dt) + (assimilation - Sedimentation - exchange_of_PON) * dt
INIT PON = .1

assimilation = PON*Nmax*Pmax*0.5
Sedimentation = PON*0.10
exchange_of_PON = water_exchange*(PON-Sea_PON_conc)
Sediment_DIN(t) = Sediment_DIN(t - dt) + (Sed_mineralisation - DIN_release - Denitrification) * dt
INIT Sediment_DIN = .001

Sed_mineralisation = sediment_orgN*.05
DIN_release = Sediment_DIN*0.50
Denitrification = Sediment_DIN*.0
sediment_orgN(t) = sediment_orgN(t - dt) + (Sedimentation - Sed_mineralisation - Sediment_burial) * dt
INIT sediment_orgN = 1

Sedimentation = PON*0.10
Sed_mineralisation = sediment_orgN*.05
Sediment_burial = 0*sediment_orgN
Nmax = DIN/(0.5+DIN)
Pmax = 1-(PON/(2+PON))
Sea_DIN_conc = 0
Sea_PON_conc = 0
water_exchange = 0.0
```

Text Box 5. The STELLA presentation of differential equations and processes of the Model Bay.

STELLA lists the differential equations in a format: X(dt) = X(t-dt) + inputs - losses, where dt is the timestep. The statements starting with INIT gives initial concentrations of the state variables. State variables are all scaled in mmol m^{-3} and rates are d^{-1}. For the sediment, assume that the average depth of the bay is 5 m. Thus, the sediment concentrations could be scaled to unit m^{-2}, simply by multiplying them with the area:volume ratio (5 in this case).

It is important to gradually develop the model. In this case, the first simulation is run without any inputs of nutrients to the system, nor any losses. This is done by changing the constants for sediment burial; denitrification, DIN input, and water exchange are all set to zero. Thus DIN can be used by PON, sedimentated out to sediment organic N (SEDN), or be mineralised and immediately returned to the water column. With the scaling used here, the simulation, running for one year, generates results shown in Figure 37.

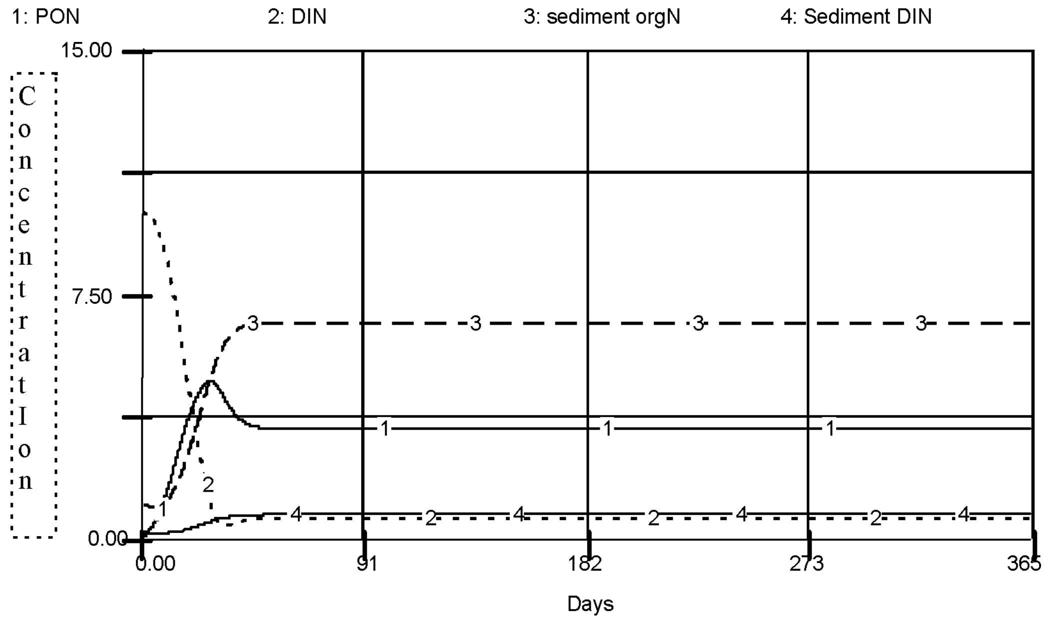


Figure 37. The change in concentration of nitrogen (μM) of the four state variables in the model when there are no inputs, water exchange nor internal losses through sediment burial or denitrification.

This simulation illustrates how inorganic nutrients (DIN) will rapidly decrease from the initial concentration (10 μM) to about 1 within 40 days. The rate of decrease is naturally a reflection of the scaling that has been applied to the assimilation function, transferring nutrient from DIN to PON. After the initial increase of PON and sediment organic N, a mirror of the DIN decrease, the increase of organic matter will continue. The system will reach a steady state with no change in concentration after about 60 days. The final concentrations are a sum of all the initial amounts found in all compartments. Thus, this first simulation can be used to check the consistency of the model and that the numerical solution scheme does not create numerical instabilities and 'leak' nutrients. There are several numerical methods (and variable time steps) that can be used in STELLA in order to ensure numerical stability.

In the second simulation, a check that the formulation of water exchange is consistent is carried out:

exchange_of_DIN=water_exchange*(DIN-Sea_DIN_conc)

Here the water exchange is changed from 0 to 1.2 % per day, in steps of 0.2 %. This is a kind of sensitivity analysis that shows that even very small variations are critical. These runs also confirm that the formulation of water exchange has the desired effect (Figure 38).

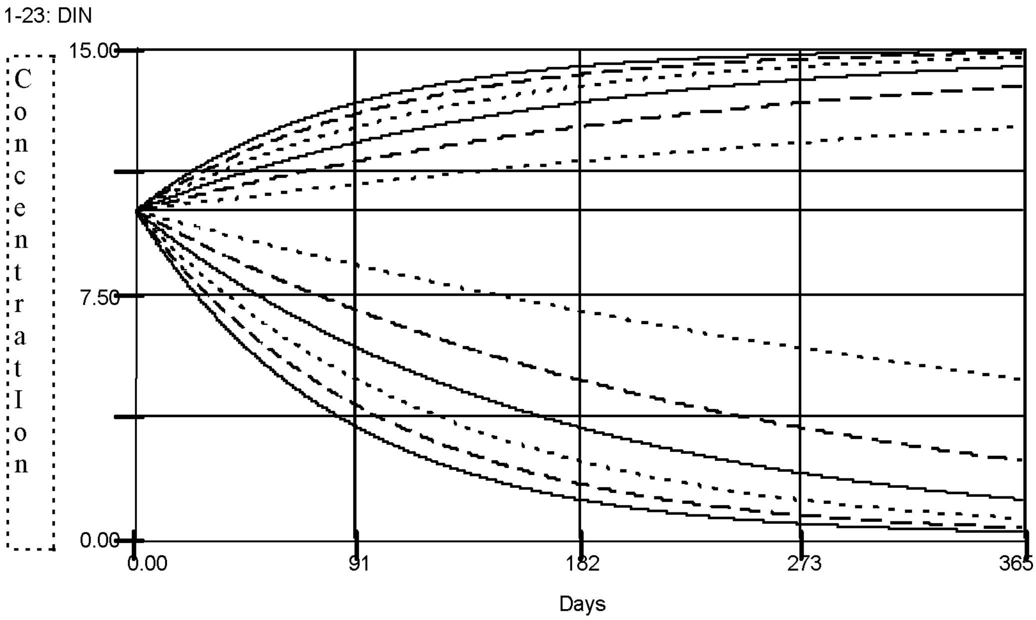


Figure 38. Variations with time in concentration of dissolved inorganic nitrogen, DIN, with different levels of water exchange, from 0 to 1.2 % per day. The straight line shows the concentration when there is no water exchange. The curves with decreasing concentration result from simulations where the external concentration is zero, the increasing concentrations result from simulations where the external concentration is set to 15 μM. In this sensitivity analysis the concentrations are not affected by processes other than water exchange (DINinput, Assimilation, DIN release are all set to zero).

By successively changing various parameters, continued checks can be made on the ability of the model to produce results that compare favourably with available data and understanding. This sensitivity analysis is presented only as an example of the methodology as the number of perturbations on even this simple model are too numerous to present in these guidelines.

In the "final" simulation, the original model formulation and rates are used (Text Box 5) with the exception that there is a daily DIN input of 0.1 μM. The model is then run until a steady state with a varying water exchange state is reached, here expressed in water residence time. From each of these simulations, the net export of nitrogen (DIN+PON) as percentage of nitrogen inputs per day is calculated when the system has reached steady state (Figure 39).

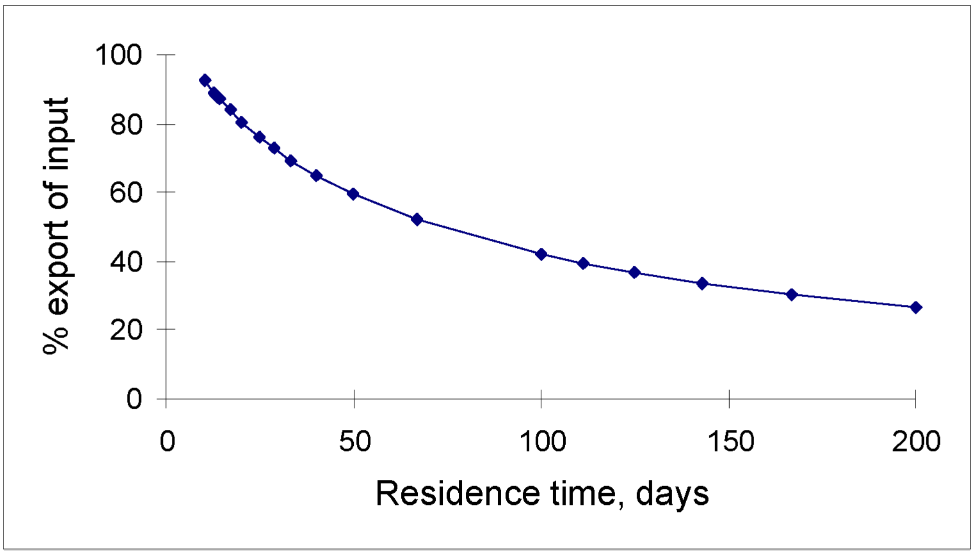


Figure 39. The percentage of inputs that are exported from the bay when the water residence time is changed.

With very short residence times, on the order of a few weeks, most of the nitrogen that enters the bay will be immediately exported. With longer residence times less nitrogen is exported. In the model this is apparently caused by an increasing importance of the internal losses, primarily through denitrification. A decreased water exchange means that inorganic nutrients will cycle through the four compartments of the system several times. For each time a nitrogen unit passes through the sediment DIN pool, there is a likelihood (10%) that it will be lost through denitrification. More recycling means that more is lost through this process. This simple model thus demonstrates the importance of considering the interactions between physics and biogeochemistry.

Model simulations can often be useful in the initial phase of a research programme before actual measurements are made. Although not all data are yet available, there is usually enough information to scale the system in terms of its physical dimensions and the concentrations of the state variables to be initially considered, as demonstrated in the example above. Literature information can often be used to formulate and scale initial processes. The scientists involved in the project can then use the model to test the importance of various processes and interactions. For instance, will the outputs change if the rate of denitrification is not constant but changes in relation to sedimentation of organic mater? Is it important to consider the “microbial loop” and nutrient recycling in the water column? Will the importance of internal losses versus exports change with increasing nutrient loads?

The modelling of dynamic systems on the computer has, with software like STELLA, become a real possibility for ecologists. A significant preparation in mathematics and programming was needed earlier to develop even a simple model like the example used here. This prevented many coastal and marine scientists from utilising modelling as a tool to formally describe and test hypotheses on the structure and functioning of the world around us.

In summary, modelling is an essential tool in the analysis and hypothesis testing of coastal and marine ecosystems. It is however, essential to remember that numerical simulation is only a tool, however powerful, and not a goal in itself. Some basic advice on how to best use this tool is summarised Text Box 6.

- Define objectives and goals for the simulation model. What are the problems to be study? If the system is complex, define subsystems and partial goals. Should the model be descriptive or predictive?
- Define spatial and temporal resolution for the model. What should be inside the model, what should be external?
- Define the state variables; as few as possible. Determine what units are going to be used.
- Describe the important flows in the system and those processes that control them. Define units and temporal resolution.
- Ensure that the model is consistent in term of units, conservation of mass, etc.
- Discuss how the model should reflect the real world situation before the simulation is carried out. Select a time period, check the integration method. Run the model.
- Carry out sensitivity analyses using different parameters and different values.
- Compare the model results with field and experimental data.
- Document each step.

Text Box 6. Basic advice for carrying out general system modelling.

7. MEETING THE GLOBAL BIOGEOCHEMICAL MODELLING OBJECTIVES OF LOICZ

It is anticipated that biogeochemical models of different parts of the world's coastal zone will be developed under LOICZ as part of national and regional programmes by following the guidelines outlined in this document. These guidelines recommend that at a minimum the new applications models should initially focus on mass balance budget models of carbon, nitrogen and phosphorus. However, as described earlier in this report, there is also the need in some situations to develop system models which can be used to increase understanding of the internal dynamics of the key environmental processes that control biogeochemical fluxes.

Since most model development under LOICZ is expected to be supported primarily at the national or regional level, the spatial extent will probably be relatively small in order to address important local management issues. The majority will presumably describe specific nearshore habitats (such as mangrove systems, seagrass beds, coral reefs, etc.) or particular estuaries and coastal embayments. Hopefully a number of studies will also describe relatively large areas of the continental shelf such as the North Sea and East China Sea.

In order to meet the long term, global objectives of LOICZ, it is essential to scale-up or compile the results of these local and regional models into global coastal zone models. This important activity, which marks the culmination of the LOICZ modelling strategy, Text Box 1, will be undertaken as a framework activity and a proposed programme of activities is outlined in the Implementation Plan (Pernetta and Milliman, 1995).

It is intended that budgets developed at the local and regional levels will be integrated into global estimates of fluxes and that local and regional system simulation models will be coupled to global atmosphere/ocean models. Both of these activities will require the coupling of models with relatively small scale, short term processes into models of large scale, longer term processes. The task of developing improved methods for assimilating fine scale models into large scale models and the task of developing global models of biogeochemical processes will be developed in conjunction with these guidelines and the results that they produce. The first step is the establishment of a limited number of common questions that can be addressed by comparable model outputs.

If there are good estimates of carbon, nitrogen and phosphorus fluxes to and from each type of coastal system identified in the LOICZ typology exercise, and estimates of the proportion of each type in each climatic zone are available, it would be a fairly straightforward matter to derive better estimates of global fluxes by weighted summation. It should be noted that integration of the fluxes from small units, such as the individual salt marshes or seagrass beds within an estuary can be achieved by constructing the budget model for the estuary as a whole rather than for its component parts. At the same time such an approach loses information on specific habitats of local interest.

Scaling up system simulation models will be a much more difficult endeavour because of numerous problems. Even within a single model, there are problems with the coupling of processes on very different time scales. For example, a model that has time steps short enough to represent the growth of bacterial populations on a scale of hours cannot readily accommodate parameters of fish populations that vary on a time scale of years. In general, longer time scales integrate variations on shorter time scales. Day-to-day fluctuations in the biomass of phytoplankton can be integrated into the rates of growth and reproduction of zooplankton that feed on the phytoplankton, but the details of the phytoplankton changes will not be represented. Similarly, week-by-week fluctuations in zooplankton populations can be integrated into the parameters of planktivorous fish populations.

The question of scale is also important in coupling physical oceanographic and biological processes. Large scale turbulence is progressively degraded into smaller and smaller scales of turbulence, but it is not possible to predict the properties of the large scale process by observing the smaller scales.

The many problems associated with the scaling up of models were discussed at length in a recent symposium of the British Ecological Society held jointly with the American Society for Limnology and Oceanography (Giller *et al*., 1994). Although the problems were raised and discussed, no clear solutions emerged. Apparently, the standard application of predictive models that can adequately address scale, pattern, and hierarchies will not be available for some time. The latest ideas on this subject are explored in Pahl-Wostl (1993a, b). Hofmann (1991) Also has considered the generalisation of coastal models to the global scale.

From the point of view of developing the global scale estimates required by LOICZ, it is necessary to select appropriate geographic units for analysis as illustrated by the following three examples from the scientific literature.

Nixon *et al*. (in press) have used a budgetary approach to examine the fate of nitrogen and phosphorus at the land-sea margin of the entire the North Atlantic. They estimate that estuarine processes retain and remove 30-65% of the total nitrogen and 10-55% of the total phosphorus that would otherwise pass into the coastal ocean. The major process removing nitrogen is denitrification and the amount lost appears to be proportional to the residence time of water. This study is a good example of the kind of methodology that might be used to scaling-up from local to regional summaries. It is hoped that this analysis for the North Atlantic can be refined with compilation and inclusion of additional regional information and that the application of this kind of approach to other oceans of the world for inter-comparison can be used in arriving at global models.

Ver *et al.* (1994) have developed a global biogeochemical model which has been used to evaluate coupled CNP cycles in the coastal zone and how they can be affected by terrestrial processes. Model results show that the coastal zone is extremely sensitive to changes in the dissolved and particulate organic matter loadings from the land delivered by rivers. In a global warming scenario with enhanced terrestrial denitrification, the coastal zone is predicted to become more autotrophic relative to its current heterotrophic state. In a cooling scenario, with decreased terrestrial denitrification, the coastal zone becomes more heterotrophic. Model output clearly indicates that the trophic status of the coastal zone is governed principally by the flux of organic matter from the land and that the coastal zone must be viewed as a separate entity in considerations of global change.

Smith and Hollibaugh (1993) have examined the role of the coastal ocean in the global oceanic carbon budget. Analysis of data from various sources on long-term rates of river loading of organic carbon, organic burial, chemical reactivity of land-derived organic matter and rates of community metabolism led them to conclude that the ocean as a whole is a net source of CO_2 release to the atmosphere. Their analysis suggests that about 30% of this net oceanic oxidation takes place in the coastal zone despite its relatively small area. Oxidation in the coastal zone takes on particular importance in the context of LOICZ and the IGBP because input rates are likely to be altered by human activities on land.

8. ACKNOWLEDGEMENTS

The authors wish to thank the large number of people who contributed ideas, support and encouragement to the development of this document. In particular, the authors wish to thank Dr. P. Ruardij, Dr. S. Ibarra-Obando, and Dr. K. Webb, as well as the participants of the SARCS/WOTRO/LOICZ Workshop on Biogeochemical Modelling, for their comments and suggestions during the development of these guidelines. The major portion of writting was conducted during the Canadian workshop in September 1995 which was ably assisted by Ms. Kora Pfinder, Ms. Lousie Foley and Ms. Heather Gordon. Throughout the development of these guidelines, the Core Project Office of LOICZ provided leadership, administrative support and financial resources. Additionally, Dr. John C. Pernetta, Core Project Director, has kindly provided editorial assistance. The authors would like to acknowledge their use of unpublished manuscripts by Haidvogel and Beckmann (submitted) and Nixon *et al.* (in press). The case studies on Tomales Bay have used data collected by the National Science Foundation-Land Margins Ecosystem Research Program.

9. REFERENCES

Anderson, L.A. 1995. On the hydrogen and oxygen content of marine phytoplankton. *Deep Sea Research*. **43**: 1675-1680.

Atkinson, M.J. and S.V. Smith. 1983. C:N:P ratios of benthic marine plants. *Limnology and Oceanography* **28**: 568-574.

Baretta, J.W., W. Ebenhoh and P. Ruardij. 1995. The European Regional Seas Ecosystem Model, a complex marine ecosystem model. *Netherlands Journal of Sea Research* **33**: 233-246.

Bergström, S. and B. Carlsson. 1994. River runoff to the Baltic Sea: 1950-1990. *Ambio* **23**: 280-287.

Berner, R.A., M. R. Scott., and C. Thomlinson. 1970. Carbonate alkalinity in the pore waters of anoxic marine sediments. *Limnology and Oceanography* **15**: 544-549.

Blackford, J.C. and P.J. Radford. 1995. A structure and methodology for marine ecosystem modelling. *Netherlands Journal of Sea Research* **33**: 247- 260.

Brewer, P.G. and J.C. Goldman. 1976. Alkalinity changes generated by phytoplankton growth. *Limnology and Oceanography* **15**: 544-549.

Capone, D.G. 1983. Benthic nitrogen fixations. In E.J. Carpenter & D.G. Capone (eds.). *Nitrogen in the Marine Environment*. Academic, New York, 105-138 pp.

Carman, R. and F. Wulff. 1989. Adsorption capacity of phosphorus in Baltic Sea sediments. *Estuarine, Coastal and Shelf Science* **28**: 447-456.

Carpenter, E.J. and D.G. Capone (eds.). 1983. *Nitrogen in the Marine Environment*. Academic Press, 900 p.

Cassuli, V. and E. Cattani. 1993. Stability, accuracy and efficiency of a semi-implicit method for three dimensional shallow water flow. *Computers and Mathematics with Applications*. **27**: 99-112.

Cassuli, V. and R.T. Cheng. 1992. Semi-implicit finite difference methods for three-dimensional shallow water flow. *International Journal of Numerical Methods in Fluids* **15**: 629-648.

Chambers, R.M., J.T. Hollibaugh and S. Vink. 1994. Sulfate reduction and sediment metabolism in Tomales Bay, California. *Biogeochemistry* **25**: 1-18.

Christiansen, V., and D. Pauly (eds.). 1993. Trophic models of aquatic ecosystems. *ICLARM Conf. Proc. 26*. ICLARM. Manila, 390 p.

Cole, B.E. 1989. Temporal and spatial patterns of phytoplankton production in Tomales Bay, California. *Estuarine Coastal and Shelf Science* **28**: 103-115.

Dugdale, R.C. and J.J. Goering. 1967. Uptake of new and regenerated forms of nitrogen in primary productivity. *Limnology and Oceanography* **12**: 196-206.

Dyer, K.R., W.K. Gong and J.E. Ong. 1992. The cross sectional salt balance in a tropical estuary during a lunar tide and a discharge event. *Estuarine and Coastal Shelf Science* **34**: 579-591.

Eppley, R.W. and B.J. Peterson. 1979. Particulate organic matter flux and planktonic new production in the deep ocean. *Nature* **282**: 677-680.

Fasham, M.J.R., H.W. Ducklow and S.M. McKelvie. 1990. A nitrogen-based model of phytoplankton dynamics in the oceanic mixed layer. *J. Mar. Res*. **48**: 591-639.

Froelich, P.N. 1988. Kinetic controls of dissolved phosphate in natural rivers and estuaries: a primer on the phosphate buffer mechanism. *Limnology and Oceanography* **33**: 649-668.

Gaines, A., and M.E.Q. Pilson. 1972. Anoxic water in the Pettaquamscutt River. *Limnology and Oceanography* **17**: 42-49.

Giller, P.S., A.G. Hildrew and D.G. Raffaelli (eds.). 1994. *Aquatic Ecology: Scale, Pattern and Process*. Blackwell Scientific Publications, 649 p.

Gong, W.K. and J.E. Ong. 1990. Plant biomass and nutrient flux in a managed mangrove forest in Malaysia. *Estuarine, Coastal and Shelf Science* **31**: 519-530.

Haidvogel, D.B. and A. Beckmann. submitted. Numerical modeling of the coastal ocean. *The Sea*.

Hartman, B. and D.E. Hammond. 1985. Gas exchange in San Francisco Bay. *Hydrobiologia* **129**: 59-68.

Hofmann,E.E. 1991. How do we generalise coastal models to global scale? In R.F.C. Mantoura, J.-M. Martin and R. Wollast (eds.) *Ocean Margin Processes in Global Change*. Wiley, pp. 401-408.

Hollibaugh, J.T. B.E. Cole, S.J. Dollar, S.W. Hagern, S.M. Vink, W.J. Kimmerer, S. Obrebski, S.V. Smith, M. Valentino and T.W. Walsh. 1988. Tomales Bay, California: a 'macrocosm' for examining biogeochemical coupling at the land-sea interface. *Eos* **69**: 843-845.

Holligan, P.M and H. de Boois (eds). 1993. Land-Ocean Interactions in the Coastal Zone (LOICZ) Science Plan. *IGBP Report No. 25*, 50 p.

Holling, C.S. (ed.). 1978. *Adaptive Environmental Assessment and Management*. Wiley. Chichester.

Imberger, J., T. Berman, R.R. Christian, E.B. Sherr, D.E. Whitney, L.R. Pomeroy, R.G. Wiegert and W.J. Wiebe. 1983. The influence of water motion on the distribution and transport of materials in a salt marsh estuary. *Limnology and Oceanography* **28**: 201-214.

Jarvis, P.G., C.V.M. Barton, P.M. Dougherty, R.O. Teskey and J.M. Massherder. 1990. MAESTRO. In: A.R. Kiester (Ed.) *Development and use of tree forest response models. Acidic Deposition: State of Science and Technology Report 17*, pp. 167-178. NAPP; Government Printing Office, Washington DC 20402-9325.

Joye, S.B. and H.W. Paerl. 1993. Nitrogen fixation and denitrification in the intertidal and subtidal environments of Tomales Bay, California.. In: R.S. Oremland (ed.) *The Biogeochemistry of Global Change: Radiatively Active Trace Gases*. Chapman and Hall, pp. 633-653.

Joye, S.B., S.V. Smith, J.T. Hollibaugh and H.W. Paerl. In press. Estimating denitrification rates in estuarine sediments: a comparison of stoichiometric and acetylene based methods. *Biogeochemistry*.

Kaul. L.W. and P.N. Froelich. 1984. Modeling estuarine nutrient geochemistry in a simple system. *Geochim. Cosmochim. Acta* **48**: 1417-1433.

Kjerfve, B., L.H. Stephenson, J.A. Proehl, T.H. Chrzanowski and W.M. Kitchens. 1981. Estimation of material fluxes in estuarine cross-section: a critical analysis of the spatial measurement density and errors. *Limnology and Oceanography* **26**:155-170.

Knudsen, M. 1900. Ein hydrographischer Lehrsats. *Ann der Hydrog. usw*. **28**: 316-320.

Koop, K., W.R. Boynton, F. Wulff and R. Carman. 1990. Sediment-water oxygen and nutrient exchanges along an environmental gradient in the Baltic Sea. *Mar. Ecol. Prog. Ser*. **63**:65-77.

Lee, T.N., L.P. Atkinson and R. Legeckis. 1981. Observation of a Gulf Stream frontal eddy on the Georgia continental shelf. *Cont. Shelf Res*. **28**: 347-378.

Lenhart, H.J., G. Radach, J.O. Backhaus and T. Pohlmann. 1995. Simulations of the North Sea circulation, its variability, and its implementation as hydrodynamical forcing in ERSEM. *Netherlands Journal of Sea Research* **33**: 271-299.

Loder, T.C. and R.P. Reichard 1981. The dynamics of conservative mixing in estuaries. *Estuaries* **4**: 64-69.

LOICZ. 1994. Focus 1: LOICZ Modelling. *LOICZ Meeting Report No. 5*, 36 p.

LOICZ. 1995a. The Dynamics of Global Change and the Coastal Zone. *LOICZ Meeting Report No. 9*, 108 p.

LOICZ. 1995b. LOICZ Workshop: Biogeochemical Modelling for Coastal Zone Research. *LOICZ Meeting Report No. 11*, 17 p.

LOICZ. 1995c. SARCS/WOTRO/LOICZ Workshop: Biogeochemical Modelling. *LOICZ Meeting Report No. 14*, 44 p.

LOICZ. 1995d. LOICZ Typology: Preliminary Version for Discussion. *LOICZ Report and Studies No. 3*, 48 p.

Mann, K.H. and J.R.N. Lazier. 1991. *Dynamics of Marine Ecosystems: Biological-Physical Interactions in the Oceans.* Blackwell Scientific Publications. Oxford, 466 p.

Mathäus, W. and H. Franck. 1992. Characteristics of major Baltic inflows--a statistical analysis. *Continent. Shelf Res*. **12**: 1375-1400.

Nixon, S.W., J. Ammerman, L. Atkinson, V. Berounsky, G. Billen, W. Boicourt, W. Boynton, T. Church, D. DiToro, R. Elmgren, J. Garber, A. Giblin, R. Janke, N. Owens, M.E.Q. Pilson and S. Seitzinger. In press. The fate of nitrogen and phosphorus at the land-sea margin of the Atlantic Ocean.

Odum, H.T. and E.P. Odum. 1955. Trophic structure and productivity of a windward coral reef community on Eniwetok Atoll. *Ecol. Monogr*. **25**: 291-320.

Officer, C.B. 1979. Discussion of the behaviors of nonconservative dissolved constituents in estuaries. *Est. Coast. Marine Sci*. **7**: 91-94.

Officer, C.B. 1980. Box models revisited. In: P. Hamilton and K.B. McDonald (eds.) *Estuarine and Wetland Processes*. Plenum, New York, pp. 65-114.

Officer, C.B. and D.R. Lynch. 1981. Dynamics of mixing in estuaries. *Est. Coast. Shelf Sci*. **12**: 525-533.

Ong, J.E. 1993. Mangroves - a carbon source and sink. *Chemosphere* **27**: 1097-1107.

Ong, J.E., W.K. Gong and B. Clough. in press. Structure and productivity of a 20 year-old stand of *Rhizophora apiculata* mangrove forest. *Global Ecology and Biogeography Letters*.

Ong, J.E., W.K. Gong and R.J. Uncles. 1993. Transverse structure of semidiurnal currents over a cross-section of the Merbok Estuary, Malaysia. *Estuarine, Coastal and Shelf Science* **38**: 283-290.

Ong, J.E., W.K. Gong, C.H. Wong, Hj. Din Zubir and B. Kjerfve. 1991. Characterization of a Malaysian mangrove estuary. *Estuaries* **14**: 38-48.

Pahl-Wostl, C. 1993a. Food webs and ecological networks across temporal and spatial scales. *Oikos* **67**: 415-432.

Pahl-Wostl, C. 1993b. The hierarchical organization of the aquatic ecosystem: An outline how holism and reductionism may be reconciled. *Ecol. Model.* **66**: 81-100.

Pernetta, J.C. and J.D. Milliman. (eds.). 1995. Land-Ocean Interactions in the Coastal Zone Implementation Plan. *IGBP Report No. 33*, Stockholm Sweden, 215 p.

Phang, D. 1994. A numerical model study into the hydrodynamics of the Sungai Merbok Estuary. B.Eng. (Hons.) Thesis, Faculty of Engineering, University of Western Australia, 131 p.

Platt, T., and K. Denman. 1978. The structure of pelagic marine ecosystems. *Rapport et Proces-Verbaux des Reunions du Conseil International pour l'Exploration de la Mer* **173**:60-65.

Platt, T., K.H. Mann and R.E. Ulanowicz (eds.). 1981. *Mathematical Models In Biological Oceanography.* The UNESCO Press, 156 p.

Pritchard, D.W. 1969. Dispersion and flushing of pollutants in estuaries. Am. Soc. Civil Engineers, J. Hydraulics Div. 95: HY1, 115-124.

Radford, P.J. 1990. Ecological modelling on personal computers. Paper presented at the Natural Environment Research Council and Institute of Mathematics and Its Applications Conference on "Computer Modelling in the Environmental Sciences. 10-11 April 1990, Nottingham, England.

Redfield, A.C. 1934. On the proportions of organic derivatives in sea water and their relation to the composition of plankton. *James Johnstone Memorial Volume*, Liverpool, pp. 177-192.

Richards, F.A. 1965. Anoxic basins and fjords. In J.P. Riley and G. Skirrow (eds.) *Chemical Oceanography*, Academic Press, pp. 611-645.

Ruardij, P., J.W. Baretta and J.G. Baretta-Bekker. 1995. SESAME, a software environment for simulation and analysis of marine ecosystems. *Netherlands Journal of Sea Research*. **33**: 261-270.

Sarmiento, J. L., R.D. Slater, M.J.R. Fasham, H.W. Ducklow, J.R. Toggweiler and G.T. Evans. 1993. A seasonal three-dimensional ecosystem model of nitrogen cycling in the north Atlantic euphotic zone. *Global Biogeoch. Cycles* **7**: 417-450.

Seitzinger, S.P. 1988. Denitrification in freshwater and coastal marine ecosystems: ecological and geochemical significance. *Limnology and Oceanography* **33**: 702-724.

Silvert, W.L. 1981. Principles of ecosystem modelling. In: A.R. Longhurst (ed.). *Analysis of Marine Ecosystems*. Academic Press, pp. 651-676.

Silvert, W. and T. Platt. 1980. Dynamic energy-flow model of the particle size distribution in pelagic ecosystems. In W.C. Kerfoor, (ed.). *Evolution and EcologyoOf Zooplankton Communities*. University Press of New England, Hanover, New Hampshire, USA, pp. 754-763.

Simpson, J.H., Gong, W.K. and Ong, J.E. (in press) The determination of the net fluxes from a mangrove estuary system. *Estuaries*.

Skirrow, G. 1975. The dissolved gases--carbon dioxide. In: J.P. Riley and G. Skirrow (eds.). *Chemical Oceanography*, Academic Press, pp. 1-192.

Smith, S.V. 1985. Physical, chemical, and biological characteristics of CO_2 gas flux across the air-water interface. *Plant, Cell and Environment* **8**: 387-398.

Smith, S.V., and M.J. Atkinson. 1994. Mass balance of nutrient fluxes in coastal lagoons. In B.J. Kjerfve (ed.). *Coastal Lagoon Processes*, Elsevier, pp. 133-155.

Smith, S.V. and J.T. Hollibaugh. 1989. Carbon-controlled nitrogen cycling in a marine "macrocosm": an ecosystem-scale model for managing cultural eutrophication. *Marine Ecology Progress Series* **52**: 103-109.

Smith, S.V., and J.T. Hollibaugh. 1993. Coastal metabolism and the oceanic organic carbon balance. *Reviews of Geophysics* **31**: 75-89.

Smith, S.V., J.T. Hollibaugh, S.J. Dollar and S. Vink. 1991. Tomales Bay metabolism: C-N-P stoichiometry and ecosystem heterotrophy at the land-sea interface. *Estuarine, Coastal and Shelf Science* **33**: 223-257.

Smith, S.V. and K. Richardson. in preparation. A coupled N and P flux budget for the Kattegat.

Smith, S.V., and H.H. Veeh. 1989. Mass balance of biogeochemically active materials (C, N, P) in a hypersaline gulf. *Estuarine, Coastal and Shelf Science* **29**: 195-215.

Stigebrandt, A. and F. Wulff. 1987. A model for the dynamics of nutrients and oxygen in the Baltic proper. *J. Mar. Res.* **45**: 729-759.

Stockenberg, A. and R. Johnstone. In press. Denitrification in the Gulf of Bothnia. *Aqua Fennica.*

Sverdrup, H.U., M.W. Johnson and R.H. Fleming. 1942. *The Oceans*. Prentice Hall, Englewood, N. J., 1087 p.

Turner, R.K. and W.N. Adger. 1996. Coastal zone resources assessment guidelines. *LOICZ Report and Studies No. 4.*

Ulanowicz, R.E. and T. Platt. 1985. Ecosystem theory for biological oceanography. *Can. Bull. Fish. Aquat. Sci.* **213**. 260 p.

Uncles, R.J., W.K. Gong and J.E. Ong. 1992. Intratidal fluctuations in stratification within a mangrove estuary. *Hydrobiologia* **247**: 163-171.

Uncles, R.J., J.E. Ong and W.K. Gong. 1990. Observations and analysis of a stratification-destratification event in a tropical estuary. *Estuarine and Coastal and Shelf Science*. **31**: 651-665.

Ver, L.M., F.T. Mackenzie and A. Lerman. 1994. Modelling pre-industrial C-N-P-S biogeochemical cycling in the land-coastal margin system. *Chemosphere*. **29**: 855-887.

Vollenweider, R.A. 1969. Possibilities and limits of elementary models concerning the budget of substances in lakes. *Arch. Hydrobiol.* **66**: 1-36.

Wattayakorn, G., E. Wolanski, and B. Kjerfve. 1990. Mixing, trapping and outwelling in the Klong Ngao mangrove swamp, Thailand. *Estuarine, Coastal and Shelf Science* **31**: 667-688.

Webb, K.L. 1981. Conceptual models and processes of nutrient cycling in estuaries. In: B.J. Neilson and L.E. Cronin (eds.). *Estuaries and Nutrients*. Humana Press, pp. 25-46.

Wolanski, E. and P. Ridd. 1986. Tidal mixing and trapping in mangrove swamps. *Estuarine, Coastal and Shelf Science* **23**: 759-771.

Wulff, F. and L. Rahm 1988. Long-term, seasonal and spatial variations of nitrogen, phosphorus and silicate in the Baltic. An overview. *Mar. Environ. Res.* **26**: 19-37.

Wulff, F., and L. Rahm 1993. Accumulation of chlorinated organic matter in the Baltic Sea from 50 years of use. A threat to the environment? *Marine Pollution Bulletin* **26**:272-275.

Wulff, F., and A. Stiegebrandt. 1989. A time-dependent budget model for nutrients in the Baltic Sea. *Global Biogeochem. Cycles* **3**: 63-78.

Wulff, F., J.G. Field and K.H. Mann (eds.). 1989. *Network analysis in marine ecology - methods and applications*. Coastal and Estuarine Studies. **32**. Springer-Verlag, 284 p.

Wulff, F., M. Pertillä and L. Rahm. 1994. Mass-balance calculations of nutrients and hydrochemical conditions in the Gulf of Bothnia, 1991. *Aqua Fennica* **24**: 121-140.

Wulff, F., L. Rahm, P. Jonsson, L. Brydsten, T. Ahl and A. Granmo. 1993. A mass balance of chlorinated organic matter in the Baltic Sea - A challenge for ecotoxicology. *Ambio* **22**:27-31.

Yanagi, T. (ed.) 1996. *Oceanographic study in the East China Sea and the Yellow Sea*. Dept. of civil and Ocean Engineering, Ehime University, 181 p.

Yanagi, T. 1989. *Coastal Oceanography*. Koseisha-Koseikaka, Tokyo, 187 p.

Yanagi, T. and S. Takahashi. 1993. Seasonal variation of circulations in the East China Sea and the Yellow Sea. *J. Oceanogr*. **49**: 503-520.

Yanagi, T., and M. Shimizu. 1993. Sedimentation processes in Tokyo Bay, Japan. *La mer.* **31**:91-101.

Yurkovskis, A., F. Wulff, I.Rahm, A. Andrulewicz and M. Rodrigues-Medina. 1993. A nutrient budget for the Gulf of Riga, Baltic Sea. *Estuarine, Coastal and Shelf Science*. **37**:113-127.

ANNEX 1 REVIEW OF SELECTED MODELLING SOFTWARE PACKAGES

The following list of modelling software packages was prepared at the request of the LOICZ community. It is by no means exhaustive. The purpose is to merely provide an introduction to some of the software packages that are currently available. The focus is on general modelling packages that can be used to build system process models, not the models themselves. They are listed in alphabetical order.

BSIM

BSIM is a software package designed to help develop ecosystem models. It is based on the idea that it is relatively easy to translate scientific concepts into a computer simulation model if you don't have to worry about the technical details that programming entails. The BSIM package is intended to handle all of the hard parts of programming and let the users focus on translating their ideas into quantitative expressions that a computer can deal with. BSIM is available for virtually any computer which has a FORTRAN-77 compiler. It currently runs on microcomputers (both MS-DOS and Macintosh) as well as UNIX systems and mainframes. BSIM is copyrighted by the Government of Canada but is available free of charge. Further information and the software can be obtained from:

Dr. William Silvert
Department of Fisheries and Oceans
Bedford Institute of Oceanography
P.O. Box 1006
Dartmouth, N.S.
B2Y 4A2
CANADA E-Mail: silvert@biome.bio.ns.ca

ECOS Version 2

ECOS is a software package designed to run water quality simulations of estuaries on a PC which was developed at the Plymouth Marine Laboratory in consultation with the UK National Rivers Authority. Special features include rapid simulations, versatile process specification, particle-water partitioning, particulate transport, sediment transport, contaminant degradation, atmospheric exchange, multiple interacting contaminants, contaminant transformations, tidal or tidally-averaged simulations, enhanced graphics, enhanced function handling, on screen data comparisons and spread-sheet compatible output. Current price is 560 pounds Sterling (excluding VAT) but discounts are available for academic and multiple purchases. Site licenses and network versions are available. For further information or a free demonstration disk, contact:

Plymsolve
Plymouth Marine Laboratory
Prospect Place
Plymouth PL1 3DH
UNITED KINGDOM Phone: (01752)222772 Fax: (01752)670637

MATLAB

The name MATLAB stands for matrix laboratory. MATLAB is a technical computing environment for high-performance numeric computation and visualisation. It integrates numerical analysis, matrix computation, signal processing and graphics into an easy-to-use environment where problems and solutions are expressed just as they are written mathematically without traditional programming. It is an interactive system whose basic data element is a matrix that does not require dimensioning. MATLAB has evolved over a period of years with input from many users. Typical uses include general purpose numeric computation, algorithm prototyping and special purpose problem solving with matrix formulations that arise in disciplines such as automatic control theory, statistics and digital signal processing (time-series analysis). It also features a family of application-specific solutions called toolboxes which are available for signal processing, control systems design, dynamic systems simulation, systems identification and others.
For further information, contact: E-Mail: info@mathworks.com

ModelMaker

ModelMaker is a modelling software package developed for PC's running Windows. In-depth mathematical and programming skills are not necessary to assemble and analyse models. Models are constructed conceptually using a diagram which shows how the various elements are interrelated. The model diagram gives an overall view of the model and provides constant feedback about it. The model equations are instantly accessible so there is no need to search through computer code of find key relationships. For further information, contact:

Cherwell Scientific Publishing, Inc.
744 San Antonio Road
Suite 27A
Palo Alto, CA 94303
United States
E-Mail: modelmaker.usa@cherwell.com
http://www.cherwell.com/cherwell

Network Analysis Software

This software is designed to analyse the structure of marine foodwebs. Unlike the above software packages, it can not be used to developed simulation models. Full details are provided by Wulff *et al.* (1989). To obtain a diskette containing the software for these techniques (for IBM or compatible computers on a MS-DOS 360 KB diskette, for a Macintosh computer on a 3.5" diskette) send a money order or bank draft for US $10.00 payable to SCOR requesting the network analysis software to:

Executive Secretary, SCOR
Department of Earth and Planetary Sciences
John's Hopkins University
Baltimore, Maryland 21218
United States
E-mail: scor@jhu.edu

SENECA Version 1.2

SENECA is an ecological modelling package developed by the Dutch Delta Institute for Hydrobiological Research. Like BSIM, it is user friendly and is designed to perform most of the routine tasks automatically. Models built using SENECA can be easily manipulated, even by people without programming experience. Values of parameters and forcing functions can be adjusted in menus and source files of process formulations can be easily edited. Little learning time is required to work with SENECA. SENECA has been developed in FORTRAN 77 and runs on PC's with MS-DOS. It is available at the cost of Dfl 150 to users who are willing to share the modelling experience. The licence fee includes Version 1.2 and one update. For information and orders, contact:

Delta Institute for Hydrobiological Research
Department of Modelling and Statistics
Vierstraat 28
4401 EA Yerseke
The Netherlands

SESAME

SESAME stands for Software Environment for the Simulation and Analysis of Marine Ecosystems. It is an ecological modelling package developed and used by the European Regional Seas Ecological Modelling (ERSEM) Project. The software implementing the OpenSESAME Modelling Environment has been developed to run on most UNIX systems, either SYSTEM V or BSD compliant, and is written in (standard) C. The software enables the development of large and complex models in a modular way by a number of different researchers.

The user communicates with OpenSESAME through a graphical user interface based on Sun OpenWindows Version 3.x or through an ASCII interface if there are no graphics capabilities available. The graphical user interface allows the user to perform many actions by using the point-and-click method. Full details are provided in a recent publication Ruardij *et al.* (1995). For more information, contact:

Dr. P. Ruardij
Netherlands Institute for Sea Research
P.O. Box 59
1790 AB Den Burg , Texel
The Netherlands
Phone: (31) 0222 3 69300
E-Mail: rua@nioz.nl

STELLA

STELLA is a multi-level hierarchical environment for constructing and interacting with a model. It was originally developed for Macintosh computers but is now available for the Windows graphical environment as well. It is highly graphically oriented. The user usually starts by drawing a diagram of the system, using a simple symbol language describing state variables, processes and flows. One then continues to define the numerical values for rate constants, initial conditions, etc. The functional relationships that drive the model can be described either by mathematical equations or graphically by drawing curves. The differential equations that actually constitute the model in mathematical terms are generated by the software without the user having to write a single line of code. The user can also interact with the mathematics of the model, select integration methods, time steps etc. if desired. Although models can be built up hierarchically with submodels in different levels, STELLA is not meant for highly complex systems, particularly highly resolved 2D or 3D systems.

STELLA is an excellent teaching tool for systems thinking and for the development of models. The graphical environment helps the user to concentrate on model formulation. It is easy to learn and less intimidating to students that have limited experience in mathematics and programming. But it is also very useful for the professional scientist in developing models and should be an excellent tool for many of the models that have to be developed in the LOICZ context.

The Macintosh (System 7) version allows a flexible data exchange between the model (inputs or outputs) and other programs or files on the computer. A new version, STELLA 4, has just been released with the same features for both Macintosh and Windows computers. There is also a ‘Stella Research 4.0’ version available that makes it possible to use arrays for models of greater structural complexity than in earlier versions.

STELLA 4 is available for a price of approximately 500 US $ from:

High Performance Systems Inc.
43 Lyme Road, Suit 300
Hannover , NH 03755
United States
Phone: 603-643-9636 Fax 603-643-9502
E-Mail: support@hps-inc.com WWW Site: http://www.hps-inc.com