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IMO /FAO/UNESCO/WMO/WHO/IAEA/UN/UNEP
JOINT GROUP OF EXPERTS ON THE SCIENTIFIC ASPECTS
OF MARINE POLLUTION
- GESAMP -

REPORTS AND STUDIES

No.43

COASTAL MODELLING

INTERNATIONAL ATOMIC ENERGY AGENCY

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INTERNATIONAL ATOMIC ENERGY AGENCY
VIENNA, 1991

NOTES

1. GESAMP is an advisory body consisting of specialized experts nominated by the Sponsoring Agencies (IMO, FAO, UNESCO, WMO, WHO, IAEA, UN, UNEP). Its principal task is to provide scientific advice on marine pollution problems to the Sponsoring Agencies and to the Intergovernmental Oceanographic Commission (IOC).

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Definition of Marine Pollution by GESAMP

"POLLUTION MEANS THE INTRODUCTION BY MAN, DIRECTLY OR INDIRECTLY, OF SUBSTANCES OR ENERGY INTO THE MARINE ENVIRONMENT (INCLUDING ESTUARIES) RESULTING IN SUCH DELETERIOUS EFFECTS AS HARM TO LIVING RESOURCES, HAZARDS TO HUMAN HEALTH, HINDRANCE TO MARINE ACTIVITIES INCLUDING FISHING, IMPAIRMENT OF QUALITY FOR USE OF SEA WATER AND REDUCTION OF AMENITIES."

* * *

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FOREWORD

Limited quantities of potentially harmful substances have been and are being released into the coastal marine environment, usually under the control of national or international regulatory bodies. Guidance is needed on the levels at which materials may be disposed of in this environment such that no significant human or environmental health risks will result. At these levels the materials may be considered for dumping within a general permit under the London Dumping Convention. A necessary first step in this process is the identification of appropriate modelling techniques for predicting the behaviour of materials released in coastal environments. IAEA requested the fifteenth session of GESAMP in March 1985 to establish a Working Group to assist in the development of international guidance on low level waste disposal in coastal waters.

GESAMP subsequently agreed to establish a Working Group on "Coastal Modelling" with the following terms of reference:

(i) to evaluate the state-of-the-art of coastal (including continental shelf) modelling relevant to waste inputs by sea dumping or land-based discharges in such areas;

(ii) to determine what model parameters are site and source specific and what parameters are generic to different coastal situations and contaminants; and

(iii) to make recommendations as to the types of models appropriate for specific coastal situations.

The IAEA, as lead agency, has provided administrative and technical support for the work of the group, which has also received support from IMO, UNESCO, and UNEP. The Working Group met first in January, 1986 under the chairmanship of Professor J. Blanton and subsequently seven more times before presenting its report to the twentieth session of GESAMP in May 1990.

DEDICATION

Sadly, on November 16th 1990, a scant six months after the completion and adoption of this report by GESAMP, Dr. Bruno M. Jamart, a member of the Working Group since its inception, died at the early age of 41.

Bruno obtained his first degree in physics and oceanography from the University of Liège in 1972 and 1973 respectively. He then obtained M.Sc and Ph.D degrees from the University of Washington, the latter in 1980. After working for 3 years at the University of California at Santa Barbara, in 1983 he took up a position within the North Sea Mathematical Modelling Unit in Liège which was later moved to Brussels. He continued in this position until his death. During his career, Dr. Jamart authored or coauthored some 25 scientific and technical papers and coedited three scientific volumes.

Throughout this study, the Working group came to rely on Bruno Jamart's insightful, penetrating and analytical approach to marine environmental issues and his thorough understanding of mathematical modelling. Furthermore, all the members of the Working Group came to enjoy, and benefit from, Bruno's wit and unique sense of humour and to respect the gentleness, decency and humanism that endeavoured him to all those with whom he came into contact. It is profoundly unfortunate that these attributes and Bruno's outstanding ability in mathematical and biological science have been lost to the marine scientific community at such an early age. Accordingly, the Working Group wishes to dedicate this report to the memory of its late member:

Bruno M. Jamart

CONTENTS

EXECUTIVE SUMMARY

This report discusses approaches to modelling transport processes in coastal areas for marine environmental management applications. Its purpose is to provide guidance on the ways in which assessments of the transport and fate of contaminants introduced to coastal areas might be made for environmental and human health protection. This study is confined to the transport of materials in the coastal zone and excludes attention to exposure pathways. This results in the report being somewhat more general and wide-ranging than would have been the case if specific exposure pathways for animals, amenities, and humans, had been specified as critical to the study. However, case studies are included that show specific models may be designed.

TERMS OF REFERENCE

The terms of reference for this study were:

1. To evaluate the state-of-the-art of coastal (including continental shelf) modelling relevant to waste inputs by sea dumping or land-based discharges in such areas;

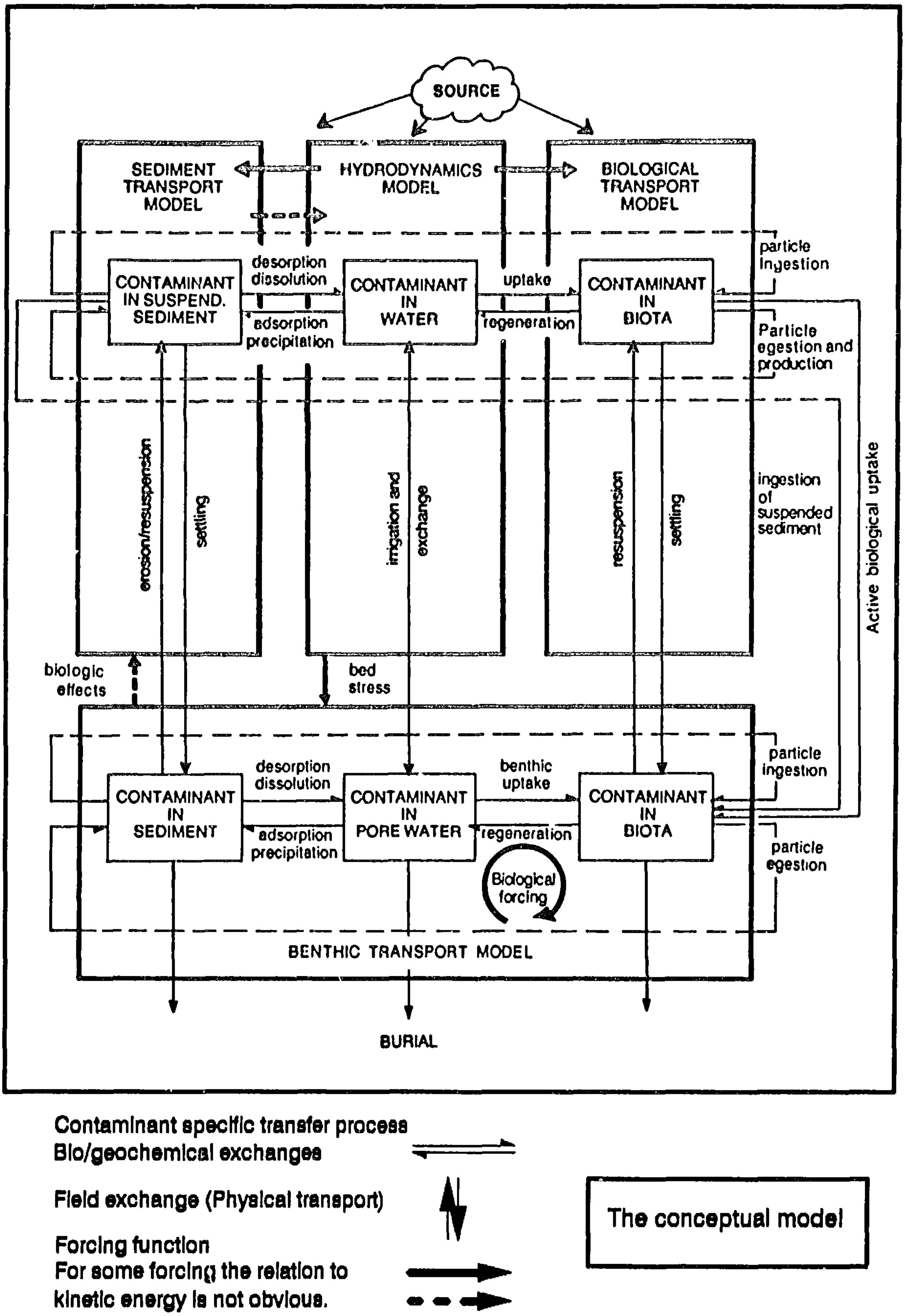
2. To determine which model parameters are site and source specific and which parameters are generic to different coastal situations and contaminants;

3. To recommend the types of model appropriate for specific coastal situations.

CONTENT OF THE REPORT

The report comprises seven chapters and two annexes. The introductory chapter contains a definition of the coastal zone for the purposes of the study and outlines potential applications of modelling to coastal waste management and marine environmental protection.

Chapter 2 defines modelling and the criteria which constrain the types of model that are suitable for a variety of management questions. This chapter also presents a conceptual model of the coastal marine environment, the kinds of processes that require consideration in the



The conceptual model

development of practical models, and the manner in which the various disciplinary components can be assembled and coupled together. Chapters 3 and 4 discuss respectively the ways in which models can be constructed and processes can be parameterized for representation in models. These chapters constitute the heart of the report.

Chapter 5 presents seven real or hypothetical case studies. Each case study presents a model that has been or could be constructed to respond to a specific management question. Collectively, these case studies provide some appreciation of the range, from simple to complex, of approaches to dealing with real and potential waste management issues. Chapter 6 discusses quality assurance procedures that are essential for ensuring the reliability of the results or answers obtained from modelling studies. Chapter 7 contains the summary and conclusions of the study.

The two annexes contain detailed specification of different coastal regimes and additional materials on parameterization.

THE CONCEPTUAL MODEL AND LINKAGES

The report is structured around a hypothetical model that covers all the features required to calculate concentrations of a contaminant in water, sediments, and biota over an appropriate space and time scale (figure opposite). This conceptual model does not directly depict all physical, geochemical and biological processes, but only those which influence the dispersion of contaminants. We know of very few models that cover more than a small portion of this total picture.

CONCLUSIONS

Recommendations on types of model

There are two major reasons for developing numerical models. The first is to gain insight (hopefully some fundamental understanding) of the processes governing the movements of material in the sea. The second is to produce answers of management questions with adequately quantified confidence limits.

The management question is often imprecise and we make a plea to carefully analyze just what questions are to be answered by a model. Relevant model inputs and outputs must be determined. In some circumstances, simple calculations (e.g. a mass balance) can indicate whether or not there is likely to be a problem associated with a proposed waste disposal activity, i.e. whether any limits on exposure are likely to be approached.

No single model is appropriate for all purposes, and a range of models is usually required. Successful models can frequently only be developed from a sound knowledge of the processes in the region of interest. This may require a well-conceived observational program prior to the modelling work to determine scales of motions, sediment sizes and types, and other parameters. Any field program should be designed to subsequently provide validation for the model.

Despite claims to the contrary, the art of modelling has not reached a stage where expert systems can be blindly relied upon. Only in exceptional circumstances can complex models developed by one group be turned over to another. All models and their solutions have limitations which need to be understood, and this requires that a minimum of expertise to be transferred with the models.

Site specific versus generic model parameters

While it is very difficult to produce generic models, coastal processes themselves can be considered as generic. The parameterization procedures that are relevant to one situation may be equally applicable to other coastal regions. It is usually the combination of processes and their relative importance that will distinguish one coastal model from that applied to a different coastal region. Parameter values themselves are often site-specific, particularly those that integrate information in time and/or space and those meant to be used to represent effects on aggregated biological populations. In general, the values of most parameters in a model have to be selected on the basis of data obtained at the site.

Evaluation of the state-of-the-art

Water circulation models and related advection/diffusion models are the most advanced. These are suitable for contaminants whose transport, dispersion and fate are primarily governed by water motion with the possible addition of simple decay processes. Sediment transport models have largely been approached from an engineering rather than a theoretical perspective because of the need to deal with practical problems in a shallow nearshore environment. There are few, if any, models which cover the movement of fine cohesive sediments across the entire continental shelf. Most biological transport models are based on the conservation of mass and contaminant within the coastal system. Complicated models of the "complete" marine ecosystem (if one can be defined), usually have many parameters whose values are not well determined. It will probably be several years before these complicated models become useful solutions to waste disposal problems. Most benthic transport models are one-dimensional in the vertical and very few consider horizontal variations in the seabed.

1. INTRODUCTION

1.1 Background

Sponsoring agencies of the GESAMP Working Group have expressed the need for advice on the state of the art of modelling in coastal environments, in relation to understanding the transport, dispersion and fate of contaminants disposed of in the coastal marine environment, including continental shelves. One application of modelling would be in defining which materials, containing radioactive substances, may be disposed of without requiring the full application of the entire system of radiological dose limitation and, thus, may be considered as non-radioactive for the purposes of dumping under the Convention for the Prevention of Marine Pollution by Dumping of Wastes and Other Matter (The London Dumping Convention). In this regard, the IAEA has defined the criteria for the exemption of materials from consideration as radioactive for both land-based, and marine disposal (IAEA, 1988a). These criteria are based, among other things, on values of individual and collective dose that may be regarded as sufficiently insignificant that the practice or source may be considered exempt from regulatory control. The recommendations in this report are intended to provide guidance to decision makers on the use and construction of mathematical models that would help to examine marine options for the disposal of potentially hazardous substances entering the marine environment. In this context, mathematical models are one of the important elements of strategies required to properly manage and protect coastal environments.

Advances in the knowledge of the processes of advection and mixing in oceanic waters, combined with improvements in the availability and speed of computers, has permitted increased mathematical simulation of environmental impacts of discharges. Such simulations are becoming increasingly sophisticated and include hydrodynamic, biological, geochemical, sediment transport and diagenetic processes. These types of mathematical simulation, hereafter called models, coupled with oceanographic data, are useful tools for use by scientists and environmental managers for estimating the transport, dispersion, and fate of contaminants discharged into coastal zones including continental shelves and marginal seas. It must be emphasized that models produce estimates whose accuracy is a function of the quality of the environmental data used to calibrate and validate the model. Furthermore, they depend upon how well the model simulates known processes such as turbulent dissipation of kinetic energy.

The overall purpose of this report is to recommend modelling techniques that could be used to determine the transport, dispersion and fate of materials discharged or dumped into coastal environments. In order to fulfill this purpose, this report will

- evaluate the state of the art of coastal (including continental shelf) modelling relevant to waste inputs by sea dumping or land-based discharges in such areas;
- determine which model parameters are site and source specific and which parameters are generic to different coastal situations and contaminants;
- recommend the types of model appropriate for specific coastal situations.

1.2 Definition of the coastal zone

For the purposes of this report, the coastal zone is bounded by the terrigenous environment and the continental shelf break (Fig.1.1). The terrigenous boundary of the environment is normally the coast. The location of the inshore boundary in the case of rivers and estuaries needs

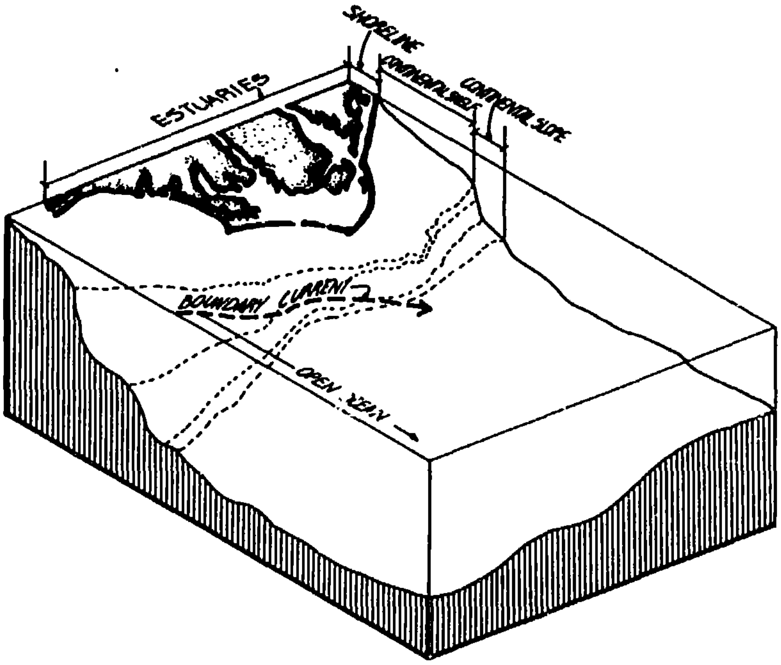


Figure 1.1. Schematic diagram of a coastal regime.

to be defined. For consistency with definitions advanced by other GESAMP Working Groups, particularly Working Group No. 22 on Land to Sea Transport of Pollutants (GESAMP, 1987), the river/coastal zone boundary should correspond to the riverine cross-section at which unidirectional downstream flow always occurs irrespective of tidal or flow conditions. This can be a section that is considerably upstream of the estuary and it may be necessary to recognize other boundaries for specific applications (see the Report of GESAMP Working Group No. 22 (GESAMP, 1987) for such alternative boundary definitions). The general offshore boundary is the continental shelf break. While this may be a rather distant boundary for many modelling situations, it nevertheless serves as an extreme limit to the coastal zone for the purposes of this report.

Within the coastal zone, there is a variety of sub-regimes. These include the downstream sections of rivers, different types of estuary, marginal sea basins, and both broad and narrow continental shelves subject to local, and/or the extensions of deep oceanic, circulation. The heterogeneity of conditions in the coastal zone, as well as the diversity of problems that need to be addressed, complicate the development of universally-applicable models. The hydrological and physical oceanographic conditions range from those of river flow to extensions of the open ocean circulation onto the continental shelf. Mixing conditions range from intense, such as in well-mixed estuaries, to weak in stratified fjords and well-stratified offshore areas. The nature of the biological system varies from riverine, through nearshore and estuarine to near-pelagic. In addition to salinity gradients, the diversity of redox conditions in some waters (e.g., fjords) and in marine sediments plays an important role in chemical reactions. The concentration, character and size distribution of suspended particulates in the coastal zone are also extremely diverse even aside from the production and decay of biogenic particles. This diversity has to be taken into account when studying the behaviour of particle-associative chemicals including many contaminants. The characteristics of a variety of coastal regimes are described in Annex 1.

1.3 Modelling for Marine Pollution Studies

Because biological, chemical, geological, and physical processes can all affect the transport, dispersion and fate of marine contaminants, the quantification of the important processes in a given marine environment often requires multidisciplinary study. However, such studies are often either too costly, or of insufficient duration, resolution and breadth, to adequately characterize the receiving system. Thus, compromises are required.

The mathematical modelling approach can be used to understand and trace the fate and transport of contaminants through a marine system. A model can be a useful tool for extending limited data sets to predictions of future conditions. However, it should be remembered that a model is an idealized and simplified representation of the environment. Although a model is not an exact representation, it can still be useful if it is designed so as to embody the important features and processes of the original system. The extent to which a model must reproduce conditions in the original system is dictated inter alia by the management questions and the resources available for model development and implementation. In general, the development of a mathematical model for any environmental system serves to organize information and data for the system; investigate linkages and further understanding of interactions among ecosystem components; interpret and understand field observations; provide a means for comparison with other systems; and identify areas for future research.

The development of a model for marine pollution investigations involves several steps. The first step is to analyse the management questions in relation to the time and length scales for which resolution is required. At the simplest level, the choice of model is determined by whether near-field or far-field contaminant distributions are required to answer the questions posed. If the interest is only in determining upper and lower bounds on contaminant concentrations, a model for which analytical solutions can be obtained may yield sufficient information. However, if the interest is in obtaining details of contaminant dispersal, contaminant transfer through the marine ecosystem, or obtaining predictions of far-field distributions, then a complex circulation model coupled to a biological and/or a chemical model may be required.

The second step is to determine the processes to be included in the contaminant transport model. All the processes that govern contaminant transport on short or long time and length scales need to be identified, in relation to their relevance to the question posed. Dispersive processes (i.e., turbulence) can be important on short length and time scales, whereas, detached eddies or river plumes may be the dominant transport processes on longer scales. For coastal environments, the important physical processes are typically specific to the region of interest. The chemical and biological interactions which transform or concentrate a particular contaminant may also need to be included in the model. These interactions usually include the scavenging of a contaminant by suspended and deposited particulate material and the accumulation of the contaminant within marine biota. Processes that contribute to the exchange of a contaminant between ecosystem components need to be identified. An example is the accumulation of a contaminant in benthic organisms by the ingestion of fine sediment particles with which the contaminant is associated.

After the important processes are determined, the third step is to parameterize the processes. At the outset, we emphasise the difference between generic and site-specific processes. Processes, such as bottom generated turbulence, wind-generated upwelling and primary production are generic. The parameterizations of these processes may also be generic. However, the parameter values adopted in a particular model are usually selected according to site-specific judgements based on data (hopefully) or a knowledge of the environment to which the model will be applied. Thus, parameter value selections tend to be site-specific.

The final steps in model development comprise model verification, sensitivity analysis (including calibration), and validation. Verification involves testing of the model to ensure that there are no errors in the computer coding and the numerical solution. The calibration procedure requires field and laboratory data sufficient to parameterize model processes. Model validation requires an independent data set against which model output can be tested. If there exists an agreement between simulated and observed distributions, within the uncertainty limits allowed by the management questions asked, the model can be used to conduct numerical experiments for various scenarios.

This report provides expanded discussions of each of the above steps in the development of mathematical models for marine pollution studies. Chapter 2 provides an overview of modelling contaminant transport processes in coastal marine environments. This chapter also presents a conceptual contaminant transport model. The methods of construction of models for contaminant dispersion in coastal marine environments are described in Chapter 3. The physical, geological, chemical and biological processes that can be important in coastal environments are discussed within the context of the approaches that can be used to parameterize these processes for inclusion in contaminant transports models, which are given in Chapter 4 and Annex 2. Illustrations of model construction and application are provided by a series of case studies in Chapter 5. Chapter 6 discusses procedures for establishing model reliability. Finally, Chapter 7 contains a summary and conclusions.

2. MODELLING FRAMEWORK

2.1 Introduction

Waste management problems are usually posed in a way that requires the relationship between quantity of waste input and the effects of the disposal. The consequences of past disposals are often monitored through the collection and analysis of samples of water, sediment and biota. The time history of results from such a monitoring programme is frequently used to predict future concentrations of a contaminant as the quantity of waste input varies from year to year. Since this information is not always available, or environmental conditions change, past data may often be unsuitable. Under these circumstances a model is needed.

The term 'model' includes physical and numerical simulations. A physical, or scaled (hydraulic), model can give considerable insight into what is happening in the real environment. However, these models are more frequently used to investigate specific physical processes rather than waste disposal problems. They will not be considered in this report. A numerical (or mathematical) model is one in which the system is described in terms of a set of equations. These are solved to predict the consequences of the waste disposal. The complexity of any model depends on the question being asked and the accuracy with which the answers are required. Model complexity is dealt with in chapter 3.

In order to relate the amount of waste input into a coastal region to the consequences, it is necessary to be able to predict how the waste disperses in the marine environment and then how the resulting concentrations are related to effects, such as the exposure of man to contaminants from the consumption of fish.

Effects are functions of exposure to the contaminant and its toxicity, in the case of biological organisms including Man, or of exposure and some other contaminant property, in the case of interference with amenities or adverse effects on non-biological components of the environment. The dispersion and the effects models can be separated, provided that the interface between the two is well defined. Through this interface, the nature of the effects model imposes constraints on what must be predicted accurately and reliably by the marine dispersion model.

For example, an effects model can dictate the time and space scales on which the concentrations are required and can also impose further restrictions. Although a discussion of effects modelling is outside the scope of this report, it is worth saying a little about how it may influence the nature of the dispersion model.

A waste manager has to consider both individual-related assessments and source-related (collective exposure) assessments of potential harm from a disposal. The need for individual assessments is obvious; exposure to a contaminant must not exceed a certain limit for an individual, or group of individuals, if harm to that individual, or group is to be prevented. If the limits are exceeded, then remedial action needs to be taken to reduce the adverse effects (or the probability of damage) to an acceptable level for that individual, or group. Account must also be taken of the aggregate exposure of a population to a contaminant for which the probability of harm is a function of exposure. Such situations apply to the (stochastic) effects of radioactive contaminants and should be equally applicable to other contaminants giving rise to similar (stochastic) effects (e.g., carcinogenic substances). In these situations, it will be necessary not only to take account of exposures to the most exposed group of individuals (the critical group through the individual-related assessment) but also of the aggregate exposure of the entire exposed population (through the source-related assessment). Reducing the level of harm to the individual may have wider consequences for the rest of the population.

For example, the building of high chimneys may reduce harm to individuals living and working in the vicinity of a chimney but may increase the aggregate exposures of individuals situated further away.

This discussion of assessments has shown how the effects model can influence space and time resolution in the dispersion model. However, the types of effect arising from exposure to a contaminant also impose other constraints. With non-stochastic effects, which usually manifest themselves at high exposure levels, there is certainty that harm will occur, perhaps above some threshold level of exposure, and that the harm will be a monotonically increasing function of the exposure (see Figure 2.1a). In the near field, where concentrations are highest and variability is often greatest, such effects are likely to be more important. Stochastic effects are those in which there is always a probability of harm from any exposure to a contaminant, no matter how small. This situation is described by a dose-response relationship (see Figure 2.1b), and it is relevant to both the near field and the far field. Again, in the near field, peak concentrations are of interest but, in the far field, it is important to define the long-term exposures in order to estimate both the individual and collective exposure risks.

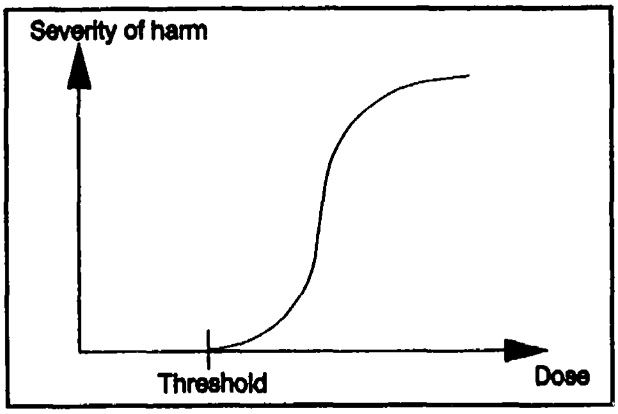


Figure 2.1a. Dose-effect relationship.

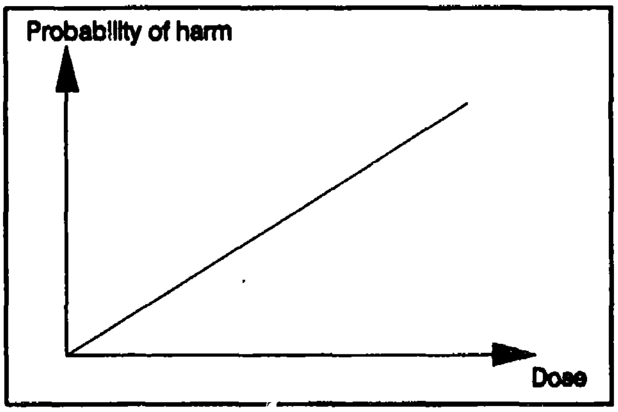


Figure 2.1b. Dose-response relationship.

Questions are usually posed on the assumption that the disposal site is already known. One way of selecting a site may be to set up a model of the region and evaluate the consequences of undertaking disposals at several potential sites and then choosing the 'best' in some sense. However, political, economic and social factors must also be weighed in the choice of disposal sites. These factors are not discussed in this report and so site selection will not be dealt with here, although most of the models discussed in this report can be applied to the scientific aspects of site selection procedures.

Without a knowledge of the relevant effects model for the waste disposal question under consideration, it is impossible to give clear recommendations on which dispersion model is appropriate to the question, the exposure pathway, and the specific coastal regime.

2.2 Questions to be answered

In a coastal region, where material has either been dumped by ship or discharged from a pipeline, the water disperses dissolved substances and can also stir up and transport seabed sediments and distribute the solid components of the waste. Close to the disposal point, concentration gradients of a contaminant are large, and fluctuations in water flow can give rise to large spatial variability. As the observer moves away from the point of disposal, mixing will cause the gradients to be smeared out and the variability reduced. This leads to the concepts of 'near field' and 'far field'. The near field is the region in which there are strong concentration gradients of the contaminant in time and space; the far field is characterized by smaller gradients. For example, if one watches from close proximity a patch of red dye being spread in the sea, then one can see red filaments in otherwise clear water; but when observed from far away, the patch appears pink. The near-field model would attempt to describe the movements of the red filaments whereas the far-field model would describe the spreading by a 'pinkness' parameter which captures the overall effect of the twisting filaments. Also, in the near field, the time scale of the variability is short, whereas, the far field usually involves longer time scales of the order of a year or the time to reach a steady state situation. The period of one year is frequently appropriate to regulatory applications. For example, there are annual limits for dose associated with exposures to radioactive material.

Processes in the sea occur on many different time and length scales but a model cannot hope to include all of them in extreme detail. Instead, a model will try to resolve all the processes above particular length and time scales and include the effect of smaller length and time scale processes, often called sub-grid processes, upon the resolved scale processes through a series of parameterizations (Chapter 4). If there are several processes involved in a model, the level of detail with which these processes are individually represented should reflect their relative contribution to the overall uncertainty of the results of the model.

Bearing in mind above discussion of space and time scales, and the constraints imposed by the appropriate effects models, the questions the marine dispersion models need to address can be summarised as follows:

a. The far field

What is the concentration in water, sediment and biota as a function of contaminant input, for periods of one year or to steady state?

b. The near field

What are the peak concentrations in water, sediment and biota and when and where do they occur?

The near-field question is framed so as to address regions where dose-effects are likely to be important, hence the reference to 'what, where and when do the peak concentrations occur?'. The far-field question is more suitable when a dose-response relationship is important.

2.3 Other model dependencies on the nature of the questions

2.3.1 Near-field models

Near-field models deal with the calculation of concentrations of contaminants in water, sediment and biota close to the disposal site for relatively short periods of time. This implies that the approach to modelling should ideally be 'stochastic' to reflect the variability in results related to the variability in the environment. For example, if the circulation in the region of the disposal site can be simulated as an eddying flow field, then the ensemble average of a number of simulations of the dispersion of the waste as a function of time gives the probable contaminant distribution and its envelope of variability.

Near-field contaminant distributions are influenced by the proximity of boundaries. A mid-water plume in deep water does not 'feel' the effect of the boundaries of the ocean until it has spread to occupy a significant fraction of the volume. However, near to a coast, close to the seabed or the sea surface, the shape of the plume is affected by boundaries.

Usually, the near field is spatially confined to an area immediately surrounding the discharge point or dumping site. However, in some cases, the near field can be spatially displaced from the disposal site as a result of natural reconcentration mechanisms in the environment. For example, if a liquid effluent, containing a substance which is highly adsorbed to fine particles, is discharged into a region with low suspended particulate matter concentrations and a sandy or gravelly sea bed, there will be a near field in the water as the effluent disperses and a secondary near field in the sediments if there is a depositional site for muddy material remote from the discharge site. The contaminant will be taken up by fine sedimentary particles and, if the initial effluent discharge subsides, the sedimentary mud patch can become a secondary source with its own near field.

As shorter time scales are involved in a near-field model, typically of the order of hours to months, some of the geochemical processes are not necessarily in equilibrium. However, the resulting contaminant distributions fall somewhere in the regime covered by performing calculations with an assumption of no geochemical effects and repeating them assuming the achievement of complete equilibrium. In most cases, this envelope of results will suffice to answer questions related to extrema in the contaminant distributions in the near field.

2.3.2 Far-field models

Far-field models tend towards a deterministic approach, thereby producing a 'best-estimate' solution to the problem. Until fairly recently, there has been no consistent method of estimating the errors in solutions arising from a) natural variability in the environment, and b) uncertainty in the observations that have been used to initialize and validate the model. A method of determining the variability in the results as a function of all possible variations in the values of the parameters, uncertainty analysis, can be used but it is frequently expensive in computer time, especially if the model is complicated.

A 'best-estimate' solution involves the parameterization of many short time and length scales. These parameterizations test the skill of the modeller, but they can be checked in many cases by comparing the results with those obtained from simulations with smaller length and time scales.

The spatial resolution of the model must be related to the concentration gradients involved, i.e. a high spatial resolution is required to resolve strong gradients and a lower resolution for more homogeneous areas. The distribution of biological species may also impose constraints on the spatial resolution of the model. Biological transport is important in the vertical, both in the water and in the seabed, and requires detailed attention in some instances, especially when there is strong vertical stratification.

2.4 Conceptual model of contaminant dispersion

The way in which a contaminant disperses in the marine environment depends upon many factors. In order to assist the reader to decide whether, when tackling a particular problem, all relevant processes have been included, a conceptual model has been designed. This is presented in Figure 2.2 and the remainder of Section 2.4 describes the components of this conceptual model and relates them to the coastal environment.

2.4.1 Description of water column processes

An unreactive dissolved (conservative) contaminant, i.e., one which does not react chemically or biologically in the receiving environment, moves with the water. Thus, the prediction of the rate and direction of transport of such a contaminant requires both a model of the water circulation (the hydrodynamic model) and a model of the advection and diffusion of the contaminant (the dispersion model). The hydrodynamic model can range from a simple well-mixed box, through average circulations derived from observations, to complex two- and three-dimensional numerical models. The choice among these model types depends on the accuracy needed for providing the answers to the management questions posed.

The contaminant transport model or dispersion model uses the hydrodynamic model as a foundation to derive the concentration field of the contaminant. These models are represented by the two central boxes in Figure 2.2.

Unfortunately, there are few contaminants which are simply passive and conservative. Many substances are sorbed by small particles in the water column and on the seabed. Particulate material is lifted from the seabed, carried with the water and settles under gravity. The amount moved depends upon the speed of the water flow and the turbulence intensity of that flow. Thus, to determine the distribution of sediment particles and consequently the distribution of a sorbed contaminant, a sediment transport model is also required. A hydrodynamic model is needed

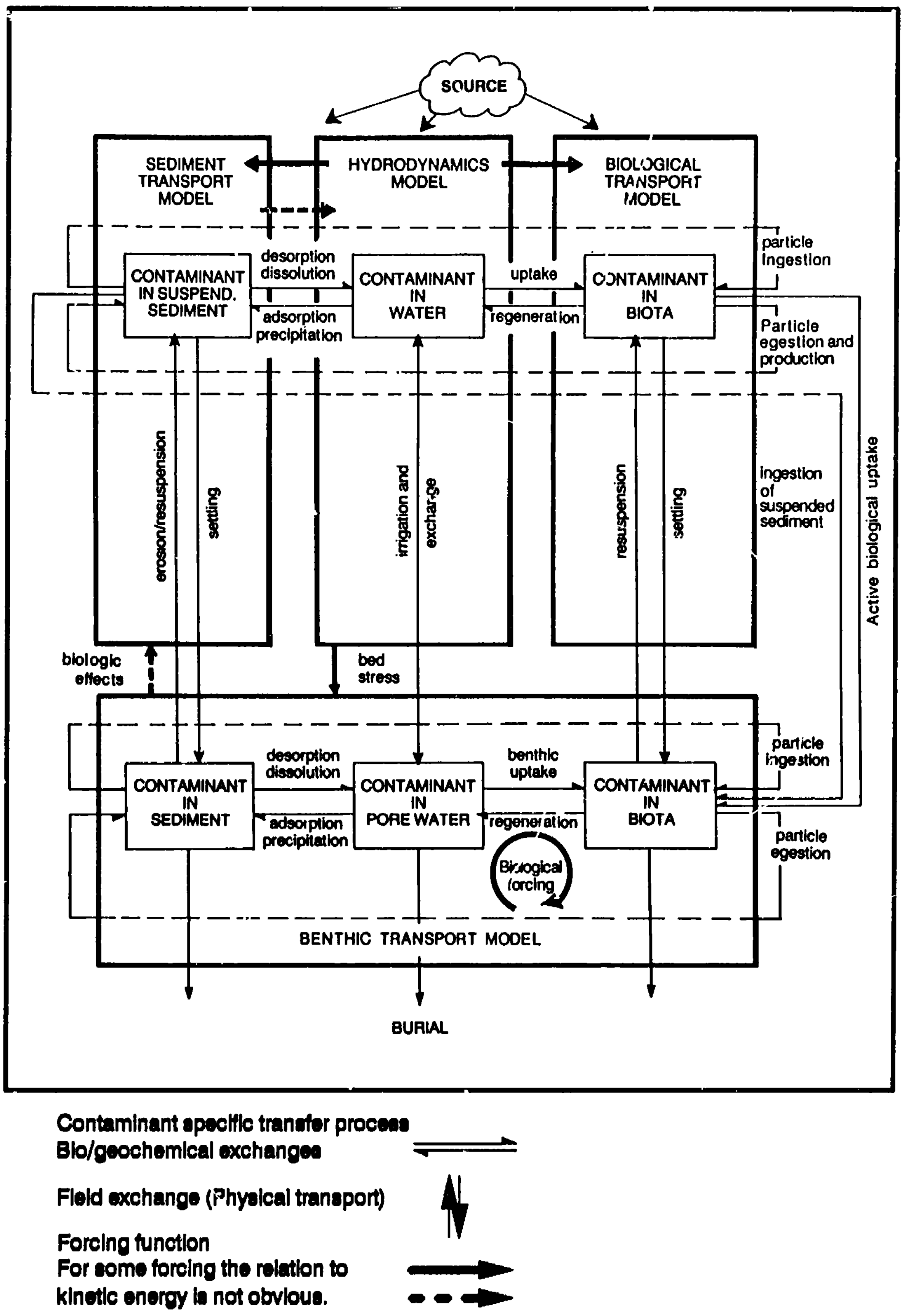


Figure 2.2. Conceptual Model.

to drive the sediment transport model and this coupling is represented by the heavy, horizontal arrow between the hydrodynamic model and the sediment transport model boxes in Figure 2.2. Usually, the amount of sediment moved by the water is low and it has a negligible effect on the water flow. However, when the concentration of sediment in motion is high, the turbulence intensity of the flow is modified and this influences water movements. This process is indicated by the dashed heavy arrow from the sediment transport to the hydrodynamic model box in Figure 2.2. From these discussions it should not be assumed that all sediment transport models are necessarily complicated. Under some circumstances, the model may assume a constant amount of particulate matter transported everywhere with the water.

Knowing where the sediment is and how the water moves is not enough to determine the concentration of the contaminant in water and on particles. Information is required on the rates at which the contaminant sorbs to, and desorbs, from particles. In Figure 2.2, the horizontal, half-headed arrows between the same two contaminant concentration boxes represent this process. If the rates of sorption and desorption are fast compared with the other processes in the model, the water concentration appears to be in equilibrium with the concentration on the sediment. In such cases, a rate-on/rate-off (kinetic) description may not be necessary, and one can use a simple equilibrium relationship for the concentration ratio between the two components.

Small biological particles (e.g., phytoplankton) sorb contaminants in the same manner as suspended inorganic particulate material. However, they reproduce, are grazed by zooplankton, and are an integral part of the coastal marine food web. Their behaviour is described by a biological transport model. It is similarly driven by the hydrodynamic model. The biological transport will have negligible influence on the water transport, which is reflected in Figure 2.2 by the appearance of a solid arrow leading only from the hydrodynamic model to the biological transport model.

If the contaminant is a plant nutrient, such as nitrate washed off farmland into rivers and then into the sea, it is taken up by the phytoplankton and is cycled in the marine biological system. In this case, determination of the concentration of the contaminant in the water and the biota requires a model of biological uptake and cycling. However, if the contaminant is scavenged by particles, inorganic and biogenic, both the rate of uptake on the biogenic particles and the rate of suspended particulate matter ingestion and egestion by biota, are required. These processes are represented in Figure 2.2 by the half-headed arrows linking concentrations in the biota box to the concentrations in both the water and suspended particles boxes.

Larger marine creatures are not moved with the water but swim freely consuming smaller biota. In this case, the biological transport model is not closely driven by the hydrodynamic model, and the concentration of the contaminant in the biota is more frequently determined by the transfer of the contaminant through a food web.

2.4.2 Description of the sea bed processes

The modelling of the movement of a contaminant within the seabed cannot be separated easily into models of the movement of water (hydrodynamic model), sediment and biota and models of the transport or dispersion of contaminant within these systems. Unlike the situation in the water column, hydrodynamics are neither always the dominant mechanism for the sediment transport model nor for the biological transport model. A benthic transport model is likely to be needed where there is a significant flux of contaminant into or out of the seabed. This usually occurs in regions of muddy sediments which sorb a greater amount of contaminants than the same volume of sandy sediments. In these areas the sediment and pore water mixing is frequently dominated by the movement of biota within the seabed. Nonbiologically dominated mixing can usually be dealt with as a part of the particulate transport model for the water column. As there is a much stronger coupling between the biology and the particulate and aqueous phases, processes in the sea bed tend to be modelled together and this is illustrated in Figure 2.2 by the inclusion of a single benthic (or seabed) transport model.

The seabed is not entirely separated from the overlying water column since sediment at the interface between the seabed and the water is periodically resuspended and deposited and contaminants are transferred by diffusion, pore water exchange with the overlying water and biological activity. The hydrodynamic model provides the forcing for some of these processes and this is represented in Figure 2.2 by the heavy vertical arrow between the respective models.

The benthic transport model comprises three components, namely the movement of sediment by biota, the movement of pore water, possibly enhanced by biological activity, and the mixing of the upper sediments by physical processes. All such processes can be included but frequently one dominates and it is often sufficient to include just a single process, its selection depending upon a knowledge of the conditions in the region of interest. The three boxes within the benthic transport model in Figure 2.2 represent the three types of contaminant concentration to be determined. There occurs an exchange of water and particles, both sedimentary and biogenic, as erosion and deposition of the seabed occurs. All three phases of the system (water, particles, biota) can carry contaminants between the seabed and the overlying water and these processes are represented in Figure 2.2 as vertical, full-headed arrows.

As in the case of the water column, contaminants in the pore water can be sorbed and desorbed from particles, sedimentary and biogenic, and biota ingest and egest particles. These processes are similarly represented by horizontal, half-headed arrows in Figure 2.2.

Certain types of benthic infauna are known to feed on suspended particulate material above the seabed and to defaecate in their burrows. This effectively transfers contaminants into the seabed. This is represented in Figure 2.2 by lines with half-headed arrows leading from both the suspended sediment and biota to the contaminant in biota box within the benthic transport model.

The benthos can also change the nature of the sea bed through bioturbation, for example, by increased irrigation through burrows or by altering the sediment characteristics so that it is more, or less, susceptible to erosion. These biological effects may, in the more extreme cases, need to be included in the sediment transport model; consequently, this linkage is shown by the dotted, heavy arrow from the benthic transport to the sediment transport models.

2.4.3 Sources and sinks

The description of Figure 2.2 above has implicitly assumed that the contaminant is both in the environment and partitioned between the various components without alteration of its chemical form. There has yet been no discussion of input and removal mechanisms.

Waste can be introduced to a coastal sea by dumping from a ship or barge in packaged or unpackaged form, by atmospheric deposition, by discharge from a pipeline, or through rivers and streams. This implies that it can enter the environment dissolved in water, attached to sediments, as the sediments themselves (e.g. fly ash), or as organic material. These diverse inputs are represented in Figure 2.2 by the cloud-like box marked 'source' with an arrow pointing towards the models, rather than by separate inputs to particular contaminant concentration boxes.

If there is net removal of a contaminant through the medium of sediment burial, the process of sediment accumulation will constitute a sink for the contaminant. This is represented by the arrow downwards from the bottom of the benthic transport model. It should, however, be stressed that the existence of such a sink depends upon the time scale being considered.

Changes in chemical form can also constitute inputs and outputs for a contaminant. For example, ^{241}Pu decays to ^{241}Am so that, when trying to predict the concentrations of the daughter nuclide ^{241}Am, it is necessary to know the inputs and distribution of ^{241}Pu. Similarly, mercury may enter the marine environment as an inorganic compound within a factory effluent but in the surficial sediments of the seabed it can be transformed to organic methyl mercury. It is not possible to represent such changes in the two dimensional diagram shown in Figure 2.2. If each related chemical form is to be treated as a separate contaminant, an additional dimension needs to be added to the representation of the conceptual model (Figure 2.3). Changes in chemical form can then be thought of as connections between individual two-dimensional conceptual models extending in the third dimension (like a series of sheets of paper, each with a Figure 2.2, connected by wires between the corresponding two-dimensional model representations to create the third dimension).

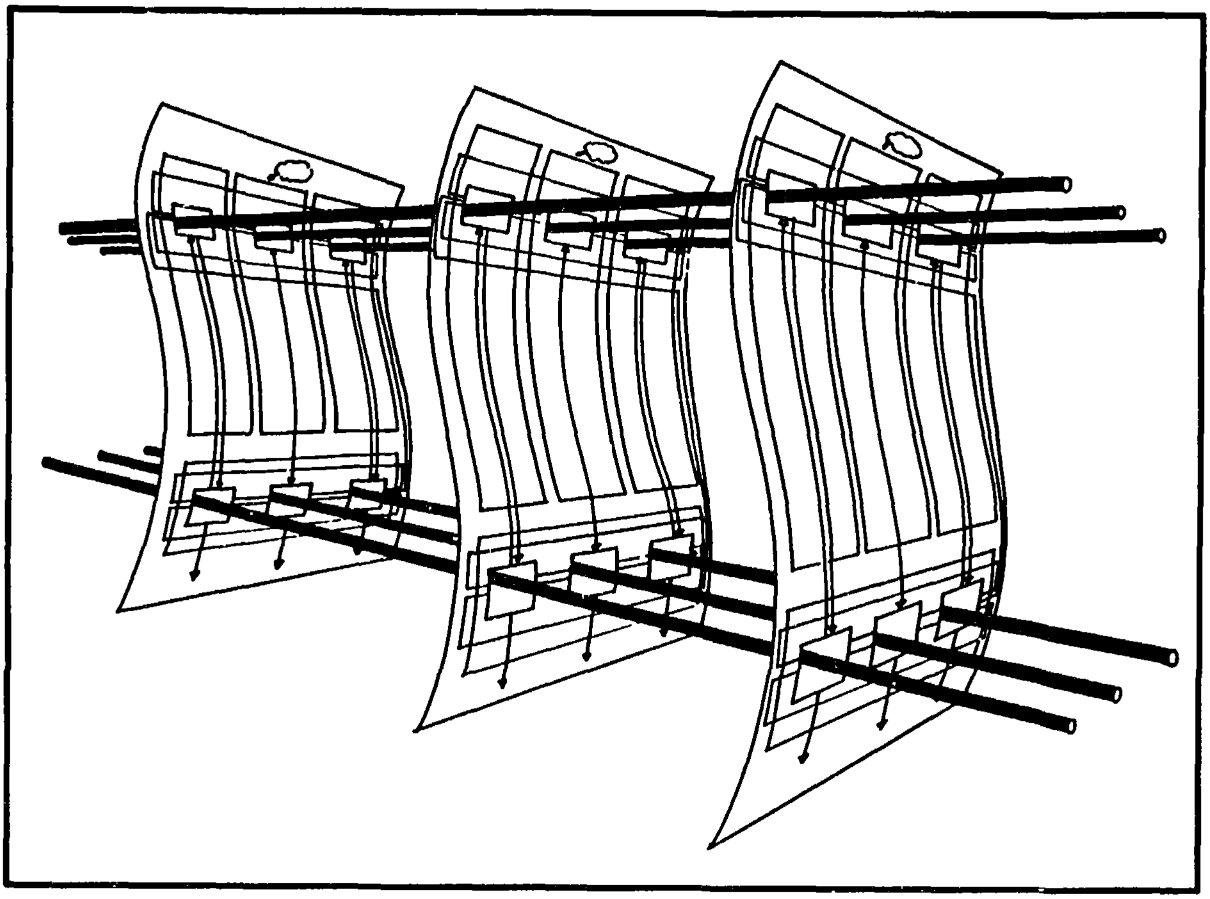


Figure 2.3. Three dimensional representation of conceptual model to take account of sources and sinks.

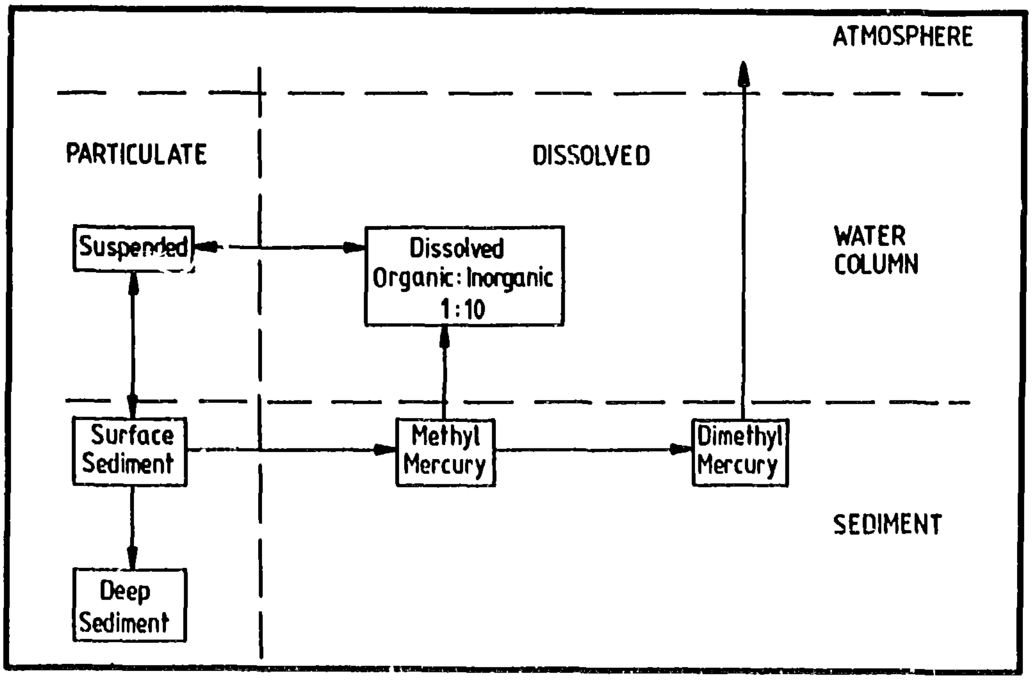


Figure 2.4. Model of mercury transport and transformation.

Thus, the removal of a contaminant from one model plane, by transformation to another contaminant form, constitutes a sink for the contaminant in one model and a source for a new contaminant in an adjacent model, reinforcing the initial concept that sources can appear in any compartment of the model.

Frequently, the full three-dimensional nature of the conceptual model is suppressed to simplify the graphics and different, but related, contaminant transports are drawn as components on a single sheet. This simplification of the graphics helps the presentation but may occasionally be somewhat confusing. Such a simplification can be used when not all transport model components in Figure 2.2 are present and/or when all contaminants being considered require the same type of transport model. Figure 2.4 shows how a model of the cycling of mercury in the environment from dumped contaminated sediments can also be represented in one simplified graphics form. Similarly, the cycling of nutrients through different trophic levels can be represented in this alternative form.

2.5 Selection of components of the conceptual model

The conceptual model described above, as depicted in Figures 2.2 and 2.3, allows for the inclusion of all possible processes that might require to be represented in a model constructed to determine contaminant concentrations in water, sediment and biota as a function of space and time. In many cases, not all processes and components need to be included in the same amount of detail when modelling the transport of a specific contaminant in a specific location. As has been indicated in Section 2.3, a passive (biologically and chemically unreactive) conservative tracer only requires a hydrodynamic model to describe its dispersion; contaminants adsorbed to, or scavenged by, particles require in addition a sediment transport and possibly a benthic transport model. The flow chart in Figure 2.5 gives a brief guide to setting up a model for a specific contaminant in a coastal area. It is not meant to be exhaustive nor does it tackle the problem of which model of each sort is appropriate. The latter is discussed in Chapter 3.

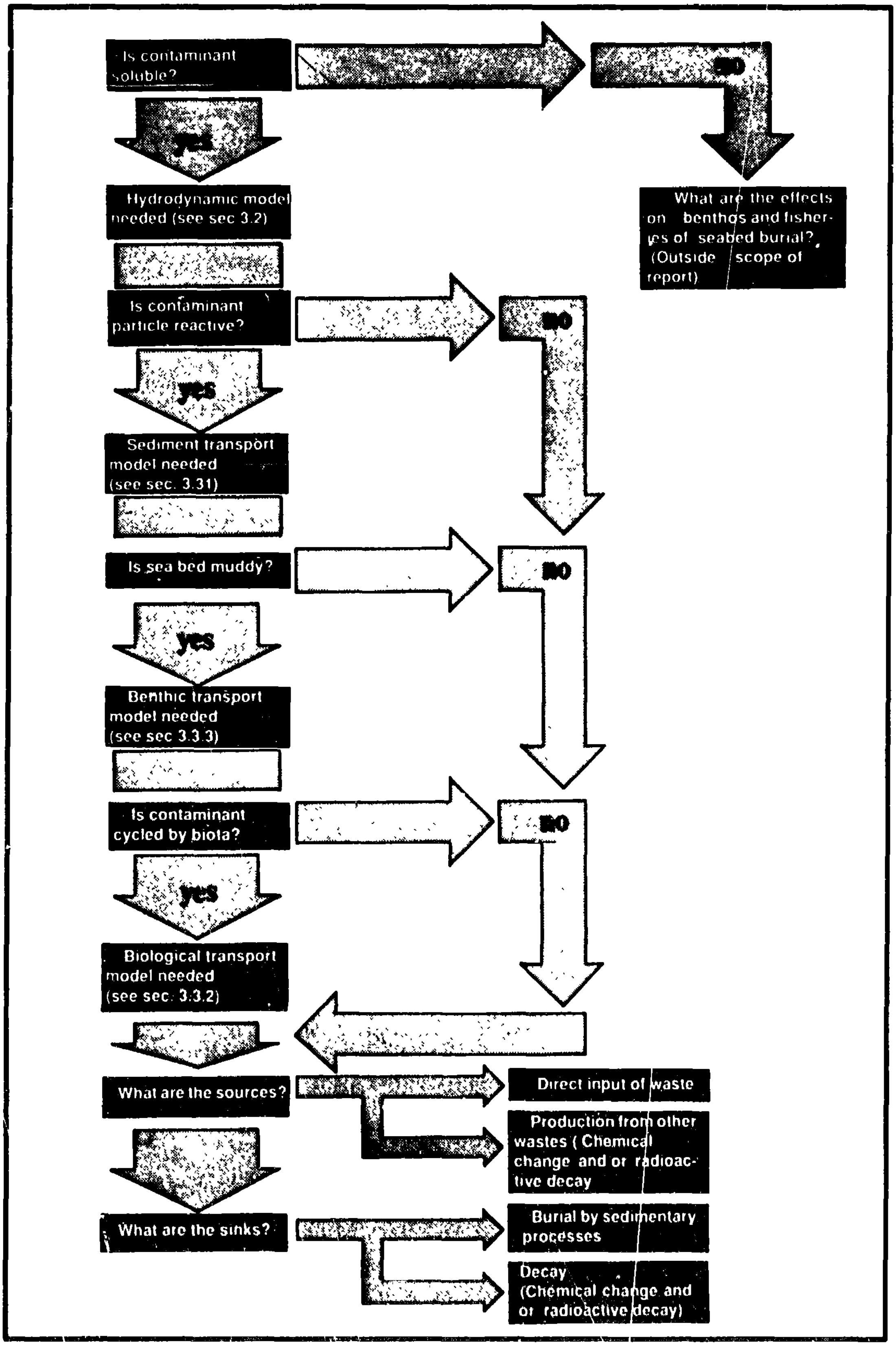


Figure 2.5. Flow chart to setting up a model for a specific contaminant in a coastal area.

3. MODEL CONSTRUCTION

3.1 Modelling approach

Simulation of coastal processes may require detailed treatment of inter alia irregular shorelines, estuarine and tidal effects, upwelling, sediment transport, chemical transformation, biological production, bioturbation, etc. (Figure 2.2). The translation of these complex processes into mathematical formulations is a nontrivial, if not an impossible, undertaking. Even if the problems to be addressed are limited to those of ocean dumping and land-based discharge of radionuclides, organic contaminants and heavy metals, the diversity of possible coastal situations is unlimited and a multitude of methodologies exist for developing models for each situation.

There are a number of fundamental principles that form the basis of models, of which the conservation laws of mass, momentum and energy (Simons, 1980), the chemical equilibrium equations and the population dynamics equations (Gray, 1986) are some examples. At the most basic level, the modeller uses the fundamental conservation principles to formulate the governing equations for the model that will be used to predict the concentration fields of interest. Once the model is formulated, there are a number of solution procedures such as, constantly-stirred-reactor box models (NEA, 1982), analytical methods (GESAMP, 1983), finite-difference (e.g. Simons, 1980) and finite-element schemes (Davies, 1982a) that can be used to obtain the concentration fields. However, the choice of the solution method depends on the complexity of the problem and on the accuracy to which the solution must be known.

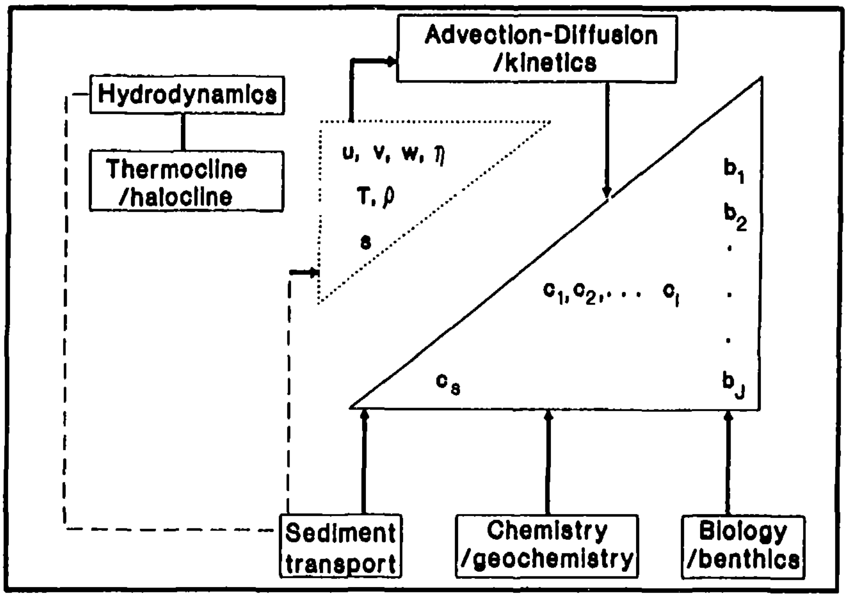
Typically modellers attempt to match the appropriate methodology to a given situation but, for the contaminant studies of interest here, the concern is to develop models that can be applied to specific situations or questions (e.g., GESAMP, 1983). The practical problems associated with coastal disposal can range from the choice of a dump site (McLaren and Bowles, 1985) to the estimation of possible damage to benthic fauna (IAEA, 1985a). These problems often require the prediction of the temporal and spatial changes in the concentration fields of suspended sediments, chemicals and biota. The concentration fields can, in turn, be used to assess the possible environmental effects of practices. While the attempt to design a general modelling package covering all possible applications remains rather idealistic (i.e., impractical), there is certainly a generalized approach to the development of models for contaminant transport studies. In this chapter, some aspects of model construction are examined and a general approach for developing models is presented.

3.1.1 Deterministic modelling approach

The majority of the existing models for coastal regimes were developed as research tools designed to provide a better understanding of individual processes. As such, they tend to specialize in one or two disciplines, e.g. hydrodynamics and sediment transport. In contrast, coastal disposal problems are multidisciplinary in nature and require the integration of several major model components. Depending on the nature of the problem, some components can be simplified and others cannot.

As depicted in Figure 3.1 there are essentially two major groups of model components. The first group consists of the hydrodynamic model, the thermocline/halocline model and (in principle) the sediment transport model. The second group is the chemical/geochemical and the biological/benthic models. These two groups are separated because the first group, while interacting among themselves, can be run independently of the second, but not vice versa. For example, the hydrodynamic model predicts the three-dimensional velocity components, u, v and w, and the surface elevation, η, which may influence the advection of the chemicals (c_1, $c_2,\ldots,c_I$) and/or biota (b_1, $b_2,\ldots b_J$); whereas, the chemical and biological components do not alter the flow field in any significant way. Similarly, the temperature, T, computed from the thermal stratification model, will definitely affect the primary production of phytoplankton but the heat resulting from chemical kinetics or radioactive decay is assumed to be too insignificant to disturb the thermal structure of the ocean. Increasing ionic strength will cause the precipitation of chemicals such as Fe but the chemical reactions are assumed not to contribute significantly to changes in ionic strength.

The sediment transport model predicts the horizontal and vertical movements of sediment particles in the water column and along the bed. Depending on the type and amounts of sediment available in the water column and on the bed, these movements may or may not affect the flow field. However, in most coastal disposal applications, morphological



Legends:

Physical Variables

u, v, w: velocities

η: water level (tide)

T: temperature

ρ: density

S: salinity

Transport Media

b_1, b_2 ....b_J: concentrations of biological (and benthic) species

c_s: concentration of suspended sediment (and seabed sediment)

(ρ): concentration of sea and pore water

Chemical contaminants

c_1, c_2,..., c_I: concentration of chemical in water (and pore water), biota (and benthics), and suspended sediment (and seabed sediment)

Figure 3.1. Construction of coastal models.

changes due to sediment transport are neglected; i.e., the interaction of the sediment transport on the flow is left out. This interaction is shown in Fig.3.1 by the dashed line that connects the hydrodynamic and sediment models, with the sediment transport model located in the second group.

In summary, there are two general stages of coastal modelling. In the first stage, the hydrodynamic quantities u, v, w, η, T, s and ρ are computed and archived for later use. In the second stage, the hydrodynamic quantities are obtained from the archived files and used in the advection-diffusion equations that describe changes in the concentration of c_s, c_1, c_2,...c_I and b_1, b_2,..., b_J (Fig. 3.1). The advection-diffusion equation for sediment concentration, c_s, is solved first using the information for u, v, w and η and the advection-diffusion-kinetics equations for c_1, $c_2,\ldots c_I$ and b_1, $b_2,\ldots b_J$ are solved as required. The final output of the model is time series of predicted c_s, c_1, $c_2,\ldots c_I$ and b_1, $b_2,\ldots b_J$ at selected grid points. Once available, these simulated time series can be used to make predictions for allowable time exposure to radioactivity/toxicity or establish acceptable levels for the bioaccumulation of radionuclides/toxic chemicals (Fagerstrom and Asell, 1973).

As shown in Fig. 3.1, the transport media for the chemical pollutants can be water, biota and/or sediment. In most cases, there are interactions among the chemical, the biota and the sediment. The model formulation of these processes is discussed in Chapter 4. Because of this interdependency, the model equations for these variables need to be solved together. In Chapter 5, case studies incorporating specific interactions among these variables are provided for answering different types of management questions.

3.1.2 Stochastic modelling

The above approach is intended to provide a general framework for the construction of deterministic models, i.e., models that describe the mechanistic processes with conservation equations. The alternative approach is to use statistical methods that relate a set of output variables to a set of input variables. For example, empirical models that are developed from statistical fits of data using simple or multiple linear regression analysis to predict the response of one variable to changes in one or more other variables are the simplest of this type of model.

Other statistical models use a stochastic approach in which the model inputs and results are given as a range of possible realizations, which accounts for the natural randomness that can characterize coastal processes. This type of model requires that a significant amount of reliable data be available so that acceptable confidence levels can be obtained for the model predictions. However, sufficient data are not always available, resulting in only a few coastal models that are statistically based (Murthy et al., 1986). These statistical models should really be regarded as a means of interpolation as they are most applicable within the range of the data available. However, when the knowledge of the underlying processes is too weak to allow the development of deterministic models, stochastic models provide a powerful modelling alternative (McLaren and Bowles, 1985).

3.2 Hydrodynamic model

3.2.1 From simple to complex models

The hydrodynamic model is the building block that is central to the conceptual model shown in Figure 2.2. In many problems (e.g., a passive contaminant discharged into the water column that does not react with the sediment or the biota, or undergo any chemical reaction) the hydrodynamic model (the output of which is the flow field) is all that is required to develop the contaminant transport model (whose output is the distribution field of the contaminant). If, however, the contaminant does react with sediment or biota, or undergoes chemical reactions, then further components must be added to the contaminant model. The range of hydrodynamic models that can be used in a contaminant transport study will be described within the context of a liquid waste discharged into an estuary.

3.2.1.1 Zero-dimensional model

If it is assumed that the estuary mixes instantaneously, that there is no exchange with the sea, that the contaminant is conservative and that the contaminant is released as a single pulse, then the far-field concentration in the estuary is readily determined from the mass of the contaminant and volume of the estuary. The near-field mass concentration, i.e., the concentration at the point of discharge, is simply the maximum concentration of the contaminant. If, however, the contaminant is released continuously, the maximum near-field concentration is the maximum concentration in the inflow and the far-field concentration will continue to increase with time, assuming there is no exchange of contaminant with the boundary or the region beyond the estuary and the volume is not changed.

If the estuary is stratified, either vertically or horizontally, and no exchange occurs across the interface between the regions, the same zero-dimensional model can be applied to each region separately. However, such a simplified idea cannot be applied when mixing is possible between the two layers. In such instances a one-, or higher-dimensional model will be required.

3.2.1.2 One-dimensional model

For a vertically-stratified estuary that can be regarded as a two-layer system, with each layer of common horizontal dimension, the simplest type of model is a two-box model in the vertical in which mixing can occur across the interface separating the two boxes, giving rise to differences in concentration above and below the interface. In each box the concentration of the contaminant is assumed to be uniform, but can vary from box to box, with contaminant exchange between boxes in the vertical being determined by an exchange coefficient (e.g., a diffusion coefficient). In the simplest model, a fixed value can be assumed for the diffusion coefficient. In practice, such an approach may be too simplistic (see Chapter 4 for a discussion of alternative parameterizations). Furthermore, the exchange of the contaminant through vertical advection may also need to be considered.

For some situations, higher vertical resolution may be needed. This can be accomplished by adding additional layers or boxes in the vertical. However, even when a multi-layer model is used to represent the time variation in contaminant concentration in the estuary, there still exists a range of techniques that are available for specifying diffusive processes. These techniques are described in Chapter 4.

In many cases, particularly in well-mixed estuaries, diffusion will occur very rapidly in the vertical but more slowly in the horizontal. A sequence of boxes in the horizontal will then be more appropriate than a sequence in the vertical. The contaminant concentration is again assumed to be uniform in each box with exchange between boxes represented by an exchange coefficient. This exchange can be assumed to be constant, or it can be computed from parameters such as current velocity, degree of stratification, and wind stress among others.

3.2.1.3 Two-dimensional models

In the previous section two one-dimensional models were described. The first, a point model in the vertical, is appropriate for conditions of strong vertical variation and uniformity in the horizontal; the second, a one dimensional model in the horizontal, covers the reverse situation of assumed homogeneity in the vertical. In many estuarine environments, there are significant variations in the vertical direction and along the axis of the estuary. To include those variations within the hydrodynamic model requires a two-dimensional, laterally-averaged, estuarine model (e.g.,Perrels and Karelse, 1981).

In other estuaries, cross-channel variations are larger than variations in the vertical. For example, wind-induced flow in an estuary often gives a circulation pattern with flow in the wind direction in the shallow regions and a return flow in the deeper areas. Modelling such a flow pattern, and the associated movement of the contaminant, requires at least a two-dimensional depth-averaged model in the horizontal.

3.2.1.4 Three-dimensional model

In situations where large variations occur in all three space dimensions, a full three-dimensional model must be used to account for the dispersion of the contaminant and to compute the current field advecting the contaminant.

3.2.2 Model complexity and predictability

With the progression from a zero-dimensional model to a full three-dimensional model, it is apparent that the computational cost associated with the model will increase dramatically. Also, the type and quantity of field data required to formulate, calibrate, and validate the model will increase. A zero-dimensional model requires only an estimate of the estuary volume and the amount of contaminant to be discharged. If exchange with an offshore marine region is to be considered, then an estimate of the magnitude of the exchange is also required. However, a three-dimensional model, requires significantly more observations and measurements e.g., a detailed description of topography, density field, flow across the offshore estuarine boundary and, in many cases, a temporal and spatial history of meteorological forcing.

Since no model is perfect, each solution will contain inherent uncertainty. The results of a zero-dimensional model will have a large uncertainty when predicting the concentration at a point in the estuary.

However, if the region is spatially uniform and sufficient time is allowed for the contaminant to diffuse throughout the region then, for this long time scale and large length scale problem, the concentration predicted from a zero-dimensional model may be sufficiently accurate for practical purposes (Figure 3.2). In general, the uncertainty in a prediction of maximum concentration will be greater than uncertainty in a prediction of a mean concentration.

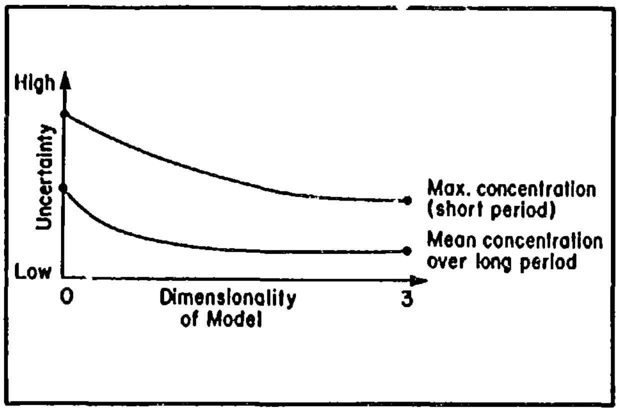


Figure 3.2. Schematic plot of uncertainty vs. physical dimensionality of the model.

Difficulties do, however, occur if the region is not spatially uniform and the peak concentration at a point is required. For example, if the peak contaminant concentration at a point (e.g., an oyster bed) in the estuary is desired, then the mean contaminant concentration obtained from the zero-dimensional model would be too low, particularly if the point in question was close to the source. In such a situation, a three-dimensional model would probably be required. The model should account for the details of the bottom topography of the estuary since this will influence flow paths. Information on the salinity and temperature fields in the estuary would also be required to determine the density field and associated density currents. Water exchange between the estuary and the offshore sea region in response to tidal and/or meteorological forcing would require adequate measurement or computations from a larger area model.

Accurate prediction of the peak concentration must take into account many factors. Near the discharge point, the contaminant is concentrated in a plume, which results in a large contaminant gradient between the plume and the surrounding water. The exact path followed by the plume is determined by the surrounding flow field and diffusion from the plume is related to turbulence. The model for this scenario would require high resolution in the region of the plume with adequate formulation of turbulence. Outside the plume, a lower model resolution is possible, but an accurate representation of the flow field, and the diffusion processes affecting the plume, would still be required.

Many of the processes that influence the magnitude of the diffusion coefficients for contaminants, salinity, temperature and momentum (eddy viscosity) are poorly known. However, these processes significantly influence the dispersion of the contaminant and the associated flow field. Possible means of parameterizing/representing these turbulent diffusion processes are covered in Chapter 4 and Annex 2. Whatever means are employed, the uncertainty in the answer derived from the model will be theoretically reduced (Figure 3.3), as the physical representation of these processes is improved. Using increasingly more sophisticated formulations of these processes, particularly formulations based on poorly-known physics with an associated high degree of uncertainty, does not in itself reduce the uncertainty in the final model. Increasing the complexity and resolution of the model significantly increases the computational cost (Figure 3.4, dashed line). For each process within a model there will be a curve of the form shown in Fig. 3.3. Consequently, the uncertainty in the entire model will be determined by the set of

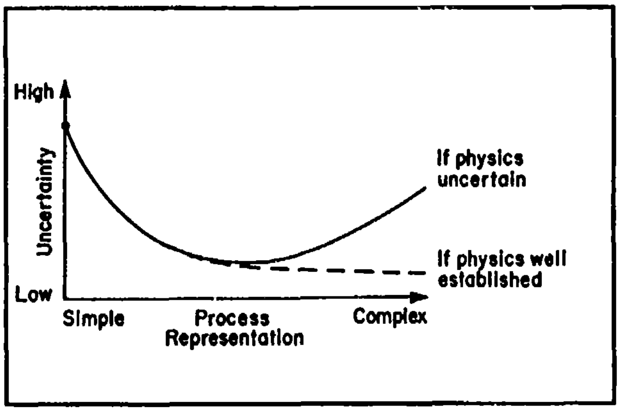


Figure 3.3. Schematic plot of uncertainty vs. physical knowledge of the process in the model.

curves shown in Fig. 3.4. The implication of these various uncertainty curves, for the accuracy of the model, is that there is little benefit in using a very complex model to represent one process if another process, which is crucial to the overall accuracy of the model, can only be modelled in a simple manner with correspondingly high uncertainties. Clearly, there should be consistency in the degree of complexity used in each stage of the overall model.

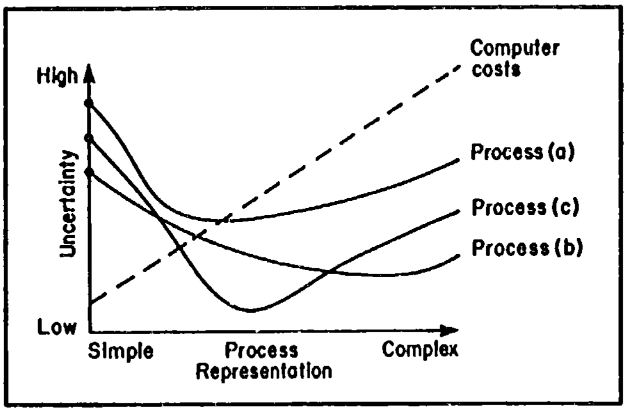


Figure 3.4. Schematic plot of range of uncertainty, depending upon various processes and their representation.

In this section, we have considered the problem of discharge into an estuary. However, in many situations, discharge occurs into a coastal region, into a marginal sea or onto a shelf. The complexity of the model in these circumstances will depend upon the question posed and the resolution required to answer it.

3.2.3 Dealing with the problem of open boundaries

In many models, the locations of open boundaries, the regions where exchanges occur, are selected on the basis of oceanographic property (i.e., temperature, nutrients) distributions. In cases where no such data are available, it is sometimes advantageous to choose open boundaries to coincide with natural changes in seabed topography (e.g., the shelf break) or changes in coastal configuration, which will minimize the spatial selection of extent of the open boundary. This latter point is advantageous in circumstances where data collection is needed to accurately specify the open boundary. Also choosing the open boundary to coincide with areas in which physical properties change uniformly will simplify data interpolation across the boundary.

Numerical models can be used to test which regions of an open boundary have the greatest influence upon the model solution (e.g., Davies, 1976). Such experiments provide a feedback with observations by indicating where field measurements need to be concentrated so as to provide information that is suitable for characterizing conditions at the selected model boundary.

In hydrodynamic models (or any model considering transport of material), the exchange of material across an open boundary can be specified in two ways. For the first, referred to as a clamped boundary condition, the concentration of the variable is specified at the boundary. For the second, referred to as radiative boundary conditions, disturbances are allowed to propagate out of the model region. The most common form of this latter condition is a point radiation condition in which it is assumed that a wave propagating out of the model domain is normal to the open boundary. For such a point radiation condition there are significant advantages in avoiding open boundaries along which bottom topography changes abruptly, causing waves to impinge at an angle to the open boundary.

3.3. Sub-models

3.3.1 Sediment transport model

In the previous section, it was assumed that the contaminant was passive and carried by the flow field. However, many contaminants are not passive and here we briefly consider, non-conservative, dissolved contaminants and contaminants entering the sea in particulate form.

If the contaminant adheres to the sediment, with some exchange between sediment and water, then a sediment transport model will be required together with the hydrodynamic model. The latter is used to determine the transport of the contaminant within the water and also to determine the bed stress which is used as a driving force for the sediment transport model.

In cases where high spatial resolution is needed, the hydrodynamic model will require an accurate representation of the near-bed region in order to be able to account for differences in sediment concentration within the water column and the diverse settling rates of different sediment types and sizes. A significant degree of parameterization, particularly of bed threshold stress and settling rates, will then be required. An extensive field survey may therefore be necessary to determine bed forms and types and the composition of the sediment below the surface layer. Equally, an assessment of the degree of vertical mixing (bioturbation) and compaction of the sediment may be required.

The sediment transport model will often impose a need for greater complexity on the hydrodynamic model than that required for describing water motion alone. The inclusion of additional parameterizations will normally increase uncertainties and lead to models that are not easily transportable. It will also impose requirements for an enhanced observational programme both to obtain data as input to the model and for calibration and validation purposes.

A first important decision to be made is whether the sediment is mainly transported as bed load or as suspended load. Bed load in rivers is often the dominant transport mechanism and appropriate parameterizations are discussed in Section 4.2.2. In most estuaries and coastal seas, however, sediment is mainly transported in suspension and an advection-diffusion equation has to be solved.

The question of dimensionality of the model then arises. The first constraint is that there must be dimensional compatibility between the sediment transport sub-model and the hydrodynamic model required to drive it. For an accurate representation of the bottom shear stresses, a three-dimensional model might seem to be the ultimate. However, the number of problems to be solved and processes to be parameterized do not generally justify the application of models that are still in a research stage of development. This does not mean that three-dimensional models should not be developed or applied to specific problems. Rather research should be continued on three-dimensional models for specific areas where all details of the flow field need to be represented and sufficient measurements are available to calibrate the parameters.

For many coastal problems, the output from a two-dimensional model averaged over depth (two-D, depth-averaged) is the appropriate input to the sediment transport model. For laterally constrained areas, such as shipping channels and harbours, a vertical plane, two-dimensional model might be useful. Furthermore, if winds are moderate to strong the influence of waves must be included. This would imply that for a semi-constrained area such as the North Sea, the following set of models would be appropriate:

- a wave prediction model, to predict the wave spectrum from meteorological data;
- a two-dimensional, depth-averaged flow model that takes into account the influence of tides, meteorological forcing, and, possibly, waves;
- a suspended-sediment transport model (an advection-diffusion model) with erosional and depositional functions for cohesive sediment; and
- a morphological model to compute the changes in the topography due to sedimentation and erosion.

These models must be coupled in real time if the morphological changes and the feedback of these on the flow are important. In general, however, these feedbacks are neglected, i.e., only the initial sedimentation and erosion is computed. By neglecting feedback from morphology to flow, the models can be separated and run sequentially. For some time, attempts have been made to calculate a so-called "residual flow", which is a long-term average current, and to use that flow to drive the sediment transport model. However, it has become clear that an accurate computation of the non-linear interactions between meteorology and flow, flow and morphology, and the various time and length scales in the flow itself, requires that the full non-linear equations be solved. Many examples of state-of-the-art sediment transport (sub-) models can be found in Wang et al.(1986).

3.3.2 Biological transport model

The objective of the biological transport model is to describe the concentration of the contaminant in the biota and/or the transfer of the contaminant through various biological (trophic) levels. The approach taken in constructing a biological transport model is dictated by the nature of the contaminant. Three broad categories can be used to classify the nature of the contaminant, and hence the biological transport model. These are:

1. The contaminant is a chemical, such as a nutrient, directly and naturally involved in biological cycling of matter and energy in the marine environment. The biological model is then one of the main tools used to describe the fate of the contaminant. It is also likely that the primary concern in such a case will be the response of the ecosystem itself;
2. The contaminant is a chemical which is passively transported by and through biota. In this case, biological transport is somewhat akin to the advection/diffusion processes moving the contaminant in water. The biota simply act as a carrier and may play only a minor role in determining the overall distribution of the contaminant. However, if the concentration of the contaminant in the biota is of concern, the processes of accumulation from food and water need to be represented in the model;
3. The contaminant is a chemical not normally present in the marine environment that influences living organisms to the extent that it can have a significant effect on the carriers themselves. In such a situation, the nature, characteristics and dynamics of the biological system need to be included in the model to allow for changes induced by the contaminant.

The level of sophistication required in the biological transport model in each of these three cases depends on the nature of the question(s) and on the degree of understanding of the biological system. In the first case, the main purpose of the biological model is to evaluate the biomass of various groups of organisms. In the second case (contaminant passively transported by biota), a detailed biological model may be necessary only in instances where the contaminant concentration field is significantly affected by the movement of the organisms. Otherwise, it is sufficient to apply partitioning between contaminant concentrations in different phases. In the third case, in which the contaminant effects the biological carriers, the interactions between the biota and contaminant need to be explicitly included in the biological transport model. This last case is likely to be important in the near field.

The starting point for the construction of a biological transport model is a set of advection-diffusion equations for the contaminant with terms describing the processes producing sources and sinks of the biota. These terms represent processes acting on individual biological components as well as interactions among biological components. Parameterization of biological processes often is difficult, as many of the important processes (e.g., mortality) cannot be directly measured in the environment. Consequently, biological models often contain poorly known coefficients to which the model solutions can be quite sensitive. Furthermore, biological interactions tend to be quite nonlinear, which requires attention when attempting to obtain numerical solutions for systems of biological equations. Some accepted parameterizations for biological processes are given in Annex 2.

The choice of the number of biological components to be included in the biological transport model depends to a large extent on the question being asked and on the knowledge of the system. If the transfer of a passive contaminant is of interest then bulk parameterization of ecosystem trophic levels may be appropriate, i.e., a single average phytoplankton or average zooplankton species. However, if details of the contaminant transfer are required, then individual species or life stages of specific species may need to be explicitly included. No general recommendation can be made on the number of biological components to be included in a biological transport model; the components that need to be included are question and site specific.

The specification of initial conditions for biological transport models can be difficult, especially if the spatial distribution of many variables (e.g., several life stages of a zooplankton species) is required. Field observations of biological distributions are rarely sufficient for this purpose. Typically biological models are initialized with average distributions and then integrated in time until the simulated biological distributions reach a steady distribution, i.e., the life cycle of an organism repeats in a regular manner. When such solutions are obtained, it is assumed that the processes included in the biological transport model are in equilibrium. Therefore, any departures from this equilibrium solution are due to the effects of the contaminant and are not the result of transient adjustments of the biological processes. The effect of the contaminant of the biota can then be quantified by calculating the percent difference in the simulated biological distributions obtained with and without the contaminant processes included in the model.

Depending on the questions being asked, biological transport models may need to encompass a wide range of space and time scales. For example, seasonal variations in biological distributions and abundance may be of interest for some contaminants; whereas, shorter time scale processes may be of concern for others. In either case, the dominant time scales inherent in the biological processes must be matched with those in the hydrodynamic model that is used to transport the biological material, or to any other model used in conjunction with the biological transport model. Similarly, it may be desirable to represent biological distributions in one, two, or three spatial dimensions. Again, the scales of the biological transport model must be matched with those inherent in associated hydrodynamic models and in the observations used to verify the simulated biological distributions. This may at times be difficult to realize because the questions of interest to biological and physical oceanographers, for example, often encompass differing scales.

3.3.3 Benthic transport model

The first stage in the construction of a benthic transport model is to determine the importance of the seabed in the uptake and recycling of the contaminant. If, for example, the seabed is a sink for the contaminant, with little or no return to the water column, then the bottom sediments act as a 'sticky mat'. A simple parameterization for such a case is to assume decay of the amount of contaminant in the overlying water, similar to that used for radioactive decay. If, however, the contaminant can be recycled into the water or chemical changes in the nature of the contaminant occur in the sediments, a more complicated seabed model will be required.

One representation of this increasing complexity can be to assume that the seabed is represented by a well-mixed box that exchanges contaminant with the overlying water. This type of benthic transport model accounts for the amount of contaminant held in the seabed, permits the seabed contaminant to become a source for the water if contaminant concentrations in the water decrease, and allows for contaminant uptake by the seabed to be reversible. This model requires that rates of contaminant removal to the seabed and contaminant remobilization be known. The latter depends inter alia upon the rate of overturning of the seabed, usually by biota, and the volume of the seabed which is mixed. The removal rate to the seabed depends upon the nature of the sediment (fine sediment scavenges contaminants to a greater extent than coarse sediment) and the rate of resuspension and deposition of surficial sediment. Different rates can be applied over different seabed boxes to represent the changing nature of the seabed and exchanges with the overlying water.

An introduction of several vertical levels, with mixing between the levels represents the next level of complexity in benthic transport models. The mixing rates between the layers can be derived from natural radionuclide concentration profiles within sediment cores. Separate exchange rates for sediment and pore water movement can also be included, if necessary. Exchanges represent generic processes but because of the heterogeneous nature of the seabed, the parameters involved in describing these processes are site specific.

So far, it has been generally assumed that the seabed is oxic. In some coastal environments the seabed comes anoxic below a certain depth; this redox boundary is often defined as a layer boundary in the model structure. The exchange rates across this boundary will be strongly affected by changes in the chemistry of the contaminant and may be represented by appropriate diffusion rates. More complicated or detailed models may be needed to parameterize these processes as exchange rates.

Not all biological mixing processes in the sediments can be represented by a simple bio-diffusion coefficient i.e., the diffusional parameterization is no longer valid. If it is important to know the depth distribution of the contaminant in the seabed, a one-dimensional model under each grid point of the overlying hydrodynamic model may be necessary following the ideas of Boudreau (1986a,b) and Robbins (1986). This could be computationally expensive and detailed data are needed on the behaviour of biota in different regions of the seabed. A less expensive approach would be to construct such a model separately and parameterize the integrated effects of the conveyor-belt feeders as exchange rates in a simpler seabed model (Chapter 4 and Annex 2).

In areas where there is major sediment movement, it may be necessary to have a three-dimensional, hydrodynamically-driven sediment transport model, which is considerably more complicated. For these systems, the exchange of contaminant with the seabed is related to the quantities of sediment lifted from the seabed and redeposited. If the seabed is sandy, there are likely to be fewer biota to mix the contaminant into the seabed than if the seabed is muddy. For a sandy seabed, mixing of the seabed will result more from the effects of ripples and sand waves. For a muddy seabed, where bioturbation is more important for contaminant transport, the cohesive nature of the sediment requires site-specific resuspension and deposition parameters to be added to the sediment transport model (Chapter 4 and Annex 2).

4. MODEL FORMULATION AND PARAMETERIZATION OF PROCESSES

4.1 Introduction

4.1.1 Philosophy

The oceanographic processes that determine the distribution of a contaminant are represented in the conceptual model discussed in Chapter 2, (Figure 2.2). In principle, such a model can be used to predict all spatial and temporal variations in the distribution of any given contaminant, provided all relevant processes and interactions between processes are formulated in precise mathematical terms and provided that these equations could be solved exactly. However, most processes and interactions between processes are not fully understood. Hence, resolving all spatial and temporal variations would not only require an almost infinitely large computational effort but it would also be meaningless. In practice, therefore, the processes that are taken into account, the interactions between these processes, and the length and time scales involved are tuned to the management questions that need to be answered. This results in a simplified version of the conceptual model that contains only a few of the different transport models and some or all of the interactions between them.

To build a mathematical model, the processes and the interactions between processes must first be expressed in mathematical terms, i.e., one writes down the 'governing equations' of the model. These equations are usually based on conservation principles.

Since an exact solution of the governing equations for all time and length scales is neither practical nor possible, it is necessary to decide upon spectral cutoffs below which scales of motion are not resolved. The influence of these unresolved processes on those having larger time and length scales must be expressed in terms of the resolved-scale processes. For example, the transport of a contaminant by detailed small-scale motion from molecular diffusion up to the chosen resolution of the model is often represented by a global diffusion process at the resolved scale. As will be discussed further in Section 4.2.1.1, the mathematical description of that global process involves a so-called dispersion coefficient (for a relationship between dispersion coefficient and scale size, see Okubo, 1971).

Similar expressions are used to take into account the effect of short period fluctuations on the resolved temporal scales. For example, the coefficient of eddy viscosity is used to represent the transfer of momentum by small-scale turbulence.

The process of parameterization, or simply parameterization, can be defined as the description of a specific process, or of the interaction between processes, in (approximate) mathematical terms.

If a small scale process has significant effect upon the larger scale, its parameterization and any uncertainty in the chosen form of parameteriza- tion is of critical importance. It is important to test the sensitivity of the model to this type of parameterization. This can give some insight into the confidence one can have in the model when it is used in a predictive sense (see Chapter 6 for discussion). Predictions of a model that are highly sensitive to a particular parameterization of sub-grid scale processes should be treated with caution.

4.1.2 Levels of parameterization

The objective of parameterization is to present formulations of processes and the interactions between processes that cannot be represented in complete detail in the mathematical model, either because we do not fully understand the nature of these processes or because not all time and length scales on which these processes are working are relevant to the management questions posed. The level of success in providing adequate parameterizations determines the applicability of the model to different conditions in the same area including extrema, or to different geographical areas.

If only a limited data set is available for model validation (see chapter 6), an accurate fit to these data can usually be obtained by simply adjusting some of the parameters (i.e., 'tuning' the model). In practice, when only a limited quantity of data is available for model validation, there is little merit in using complex parameterizations. Simple parameterization, guided by insight into the processes involved, is probably best and simplifies the 'tuning' problem.

In theory, a model with more refined descriptions of the processes involved and more sophisticated parameterizations should provide more accurate results and be more applicable to different situations and/or geographical areas. This philosophy reflects a conviction that a more detailed formulation provides a better description of the processes than a simple one. In practice, this concept breaks down in many cases, for the following reasons:

- it is sometimes questionable whether a 'true' description exists (e.g. for some biological processes);
- too many processes are included which have to be parameterized; or
- our knowledge of the unresolved processes upon which the parameterizations are based is very poor.

In such circumstances, a complex model can be of little value, since no more fundamental knowledge is being incorporated into the model, only more and more parameterizations of poorly-understood processes.

We now introduce the terms 'tuned', 'transportable' and 'robust' as applied to models. While there are no universal definitions for these terms, we choose to define them here because they allow us to explain more easily what is meant by a 'good' model.

We refer to a 'tuned model' as one in which the parameterizations and parameter selections have been adjusted to reproduce, as accurately as possible, given data sets in a specific region. In general, the more adjustable parameters there are in a model, the more difficult it is to tune the model, the more data are required, and the more site-specific the model becomes. In a 'highly-tuned' model, there are generally a large number of parameters that have been adjusted to reproduce the observations in a somewhat better manner than one might expect on the basis of the resolution of the model or the extent to which processes are represented. A tuned model can prove particularly useful in a given region for one specific range of physical conditions even though it may be neither 'transportable' nor 'robust'.

A model is 'transportable' if the parameterizations within the model are sufficiently comprehensive and representative of all relevant processes that, once calibrated and validated in one geographical area, the model can be used in any area containing the same generic processes. This does not imply that the specific parameter values that have been chosen for one area should remain invariant when the model is transported. However, a transportable model should yield similar levels of accuracy in different geographical areas once it has been properly calibrated.

A model is 'robust' when it can provide similar degrees of accuracy over wide variations in forcing functions. For example, storm-surge models are normally validated against observations during major wind events. Nevertheless, they are expected to reproduce conditions at comparable levels of accuracy for even more extreme events (e.g., the one-in-fifty-year storm) for which no direct validation is usually possible.

Some care needs to be taken over the definition of a 'good model'. A commonly-accepted definition, drawn from many examples in the literature, is that a good model accurately reproduces a given set of field observations. However, if this has been accomplished by tuning the model, so that it essentially fits a narrow set of conditions, then the model is no longer 'good' since it may not accurately predict different events in the same area, the same kinds of event in another geographical area, or provide any insight into the nature of the underlying processes. A model with little predictive capacity, but based upon established knowledge of the processes and with little or no parameterization, can be a 'good model' in the sense that it is a valuable tool for obtaining a better understanding of relevant processes. It can also be a valuable aid in determining the relative importance of different processes.

A range of models from the simple to the complex is obviously required to cover the range of problems and degrees of confidence required to predict complex events or conditions. One may then think of a 'good' model as one that retains a conceptual representation of the processes known to be important; uses parameterizations consistent with our knowledge of those processes; does not use parameterizations that are so complex that the model requires to be highly tuned; yet can reproduce/and predict phenomena over a range of geographical locations and differing conditions.

4.2 Parameterization in transport models

It is not possible to discuss the parameterization of all processes in this report. We have adopted the following method of presentation. Some detailed examples are provided in Annex 2. This section contains a general description of the formulation of the transport models and the important processes that may affect such a formulation. The emphasis is placed on the transport models for dissolved pollutants, suspended sediment and biological species within the water column, which are all affected by the water movement. Thus, the transport medium or transporter is sea water. It is beyond the scope of this report to derive the mathematical formulation of the hydrodynamical equations. In Section 4.3, the interactions of water with biota and sediment are further discussed. In these two cases, the transporters of the contaminant are no longer the water. The biological species are considered as the transporter and the pollutants ingested or bioaccumulated by the species are the materials being transported. Similarly, the sediment particles become the transporter for the adsorbed chemicals.

4.2.1 Hydrodynamical model

In hydrodynamics, a comprehensive set of equations (the Navier Stokes equations) for the flow is known to apply and few parameterizations seem to be required. In practice, however, the parameterization of subgrid-scale processes is always a pre-requisite, as discussed above. Also, for many practical situations, the gradients in the flow field are not of the same magnitude in all spatial directions. It is then sometimes useful to reduce the complexity of the model by reducing the number of spatial dimensions taken into consideration. Integrating the Navier Stokes equations over one, two, or all three dimensions leads to two-, one-, and zero-dimensional models. The integration procedure may result in new terms which must be expressed in terms of the integrated averaged quantities (e.g., the bottom stress term which arises when the 3-D equations are integrated over the vertical).

In a three-dimensional model, the vertical diffusion of momentum through the water column and the energy dissipation at the sea bed are the main processes that need to be parameterized. In general, both processes are related to the local horizontal velocity field or its gradient. In a shallow sea, for example, Bowden et al. (1959) suggest that the eddy viscosity in the vertical, A_z, can be parameterized by

$$A_z = \alpha\ h\ u$$

where α is a coefficient of proportionality to be tuned in the calibration procedure, h is the total water depth and u is the local horizontal speed of the flow (more details are given in Annex 2).

From a computational point of view, the simplest parameterization is preferable in order to reduce computer time. However, the simplest parameterization often means assigning a specific value to some coefficient and such an assignment, and its subsequent adjustment to give the best fit to a data set, may lead to a tuned model that is not appropriate to other regions or other conditions. Simple parameterizations in which subgrid-scale processes are related to the larger-scale velocity field (e.g., wind-dependent drag coefficients, flow-dependent viscosities, bed stresses related to the flow field), although requiring a slight increase in computational effort, may be preferred since they provide more transportable and robust models. Parameterization at the turbulent energy level (e.g., Mellor and Yamada, 1982) requires an even larger computational effort; however, it is aimed at improving the representation of the physics within the model and, hence, it approximates more realistically the full set of equations. We might thus expect such a model to be even more transportable and robust.

Besides parameterizing the mechanism whereby vertical diffusion takes place, it is also necessary to consider the parameterization of kinetic energy sources (e.g., wind stress on the sea surface) and sinks (e.g., shear stress at the sea bed) since these are responsible for driving and retarding the flow. At the sea surface, the complex physical processes, whereby wind energy is transmitted to the water, is represented by a frictional quadratic law involving the square of the wind speed and a drag coefficient the value of which often increases with wind speed. A quadratic frictional law is also employed at the seabed, with bed stress usually related empirically to the depth-mean current. A constant drag coefficient is often assumed, although there are parameterization schemes that use a variable drag coefficient. For a depth-averaged model the energy dissipation at the sea bed must be related to the depth-averaged velocities. This parameterization is more difficult than in three dimensions since a process occurring at a specific location, the sea bed, must be related to global quantities, the depth-averaged velocities. Obviously, this scheme is more susceptible to uncertainties and, thus, to error.

4.2.2 Pollutant transport model: advection-diffusion equation

The transport of dissolved contaminants by the water can be dealt with by the advection-diffusion equation. This equation is also integrated over the time and length scales below the spectral cut-off point. The concept of parameterizing subgrid scale processes can be explained with the simple one-dimensional mass conservation equation:

$$\frac{\partial c}{\partial x} + \frac{\partial}{\partial y}(uc) = 0 \qquad (4.1)$$

where c=c(x,t) is the instantaneous concentration of a pollutant observed at time t and distance x. The velocity u=u(x,t) is also an instantaneous quantity, i.e., u must be given for all t and x. In practice, it is impossible to describe such a flow field in the ocean, as u changes very rapidly in time and space. Therefore, an averaging process over a certain length scale l (e.g., Csanady, 1973) is often used in order to separate the velocity u into a mean component $\bar{u}$ and and a random component u', i.e., $u=\bar{u}+u'$. If we use the same averaging process for c, i.e., $\bar{c}=c+c'$, the mass conservation equation becomes

$$\frac{\partial}{\partial t}(\bar{c}+c') + \frac{\partial}{\partial x}[(\bar{u}+u')(\bar{c}+c')] = 0 \qquad (4.2)$$

Applying the averaging process on this equation, terms like c', u' $\bar{c}$ and $\bar{u}$ c' will average out. The equation becomes (Csanady, 1973)

$$\frac{\partial \bar{c}}{\partial t} + \frac{\partial(\bar{u}\bar{c})}{\partial x} + \frac{\partial(\overline{u'c'})}{\partial x} = 0 \qquad (4.3)$$

The first two terms in this equation refer to the mean concentration $\bar{c}$ and mean current $\bar{u}$ for the length scale l, and are therefore easier to describe than the instantaneous u and c. Indeed, many studies on ocean diffusion (Okubo, 1971) show that for a sufficiently large l, the mean flow can become quite smooth, i.e., it has small fluctuations over time and space. Such a threshold of length scale is often derived by statistical or spectral techniques and hence it is called the spectral cut off point in the length scale.

The term containing u' c' still retains the random properties. To circumvent the difficulty of dealing with randomness directly, this term is often related to the mean quantity by assuming that

$$\overline{u'c'} = - K_x \frac{\partial \bar{c}}{\partial x} \qquad (4.4)$$

The parameter K_x is called the turbulent eddy diffusivity or dispersion coefficient and it has a dimension of L^2T^{-1}. Thus, omitting the bar notation for simplicity, the mass conservation equation becomes

$$\frac{\partial c}{\partial t} + \frac{\partial (uc)}{\partial x} = \frac{\partial}{\partial x} (K_x \frac{\partial c}{\partial x}) \qquad (4.5)$$

This equation is called the advection-diffusion equation and is based on mean quantities averaged over the length scale, l. It predicts the mean concentration if the mean advective current, u, is given and the eddy diffusivity, K_x, is properly chosen. This eddy diffusivity is several orders of magnitude greater than the molecular diffusion which is ignored in the transport model. When needed, a source or sink term has to be added to the right-hand side of the equation. For example, adding a source term S, a similar derivation gives the two dimensional advection-diffusion equation 4.6:

$$\frac{\partial c}{\partial t} + \frac{\partial}{\partial x} (uc) + \frac{\partial}{\partial y} (vc) = \frac{\partial}{\partial x} (K_{xx} \frac{\partial c}{\partial x}) + \frac{\partial}{\partial y} (K_{yy} \frac{\partial c}{\partial y}) + \frac{\partial}{\partial x} (K_{xy} \frac{\partial c}{\partial y}) + \frac{\partial}{\partial y} (K_{yx} \frac{\partial c}{\partial x}) + S \qquad (4.6)$$

Usually only K_{xx} and K_{yy} are considered important, particularly if the mean flow is in the x or y direction, and are called the horizontal turbubent diffusivities (K_x, K_y, for simplicity). Similarly, the three-dimensional case gives rise to K_z, the vertical turbulent diffusivity.

In the near field, where concentration gradients are high, turbulent diffusion is very important. A fine-mesh model is required to resolve such gradients and when these change with time, a method must be used which follows them. Examples of models using this method include estuarine plume models (Garvine, 1984; Royer & Emery, 1985) and models of density currents at continental slopes (e.g., Griffiths, 1986).

The use of a constant diffusion coefficient in the near-field is probably inappropriate because it fails to reproduce the streakiness or patchiness often experienced in near-field situations. An alternative method is to use a stochastic approach whereby the subgrid-scale motion is represented in terms of random small-scale perturbations of a large number of particles (of order of 1000) intended to represent the contaminant. A good recent review of the method has been presented by Van Dam (1982). Applications of this latter approach for simulating the turbulent dispersion of a contaminant patch have recently been published (Dyke and Robertson, 1985; Jenkins, 1985; Chatwin and Allen., 1985). Examples of the use of stochastic models, with particular reference to the influence of assumptions about turbulence upon patch dispersion, are provided by Maier-Reimer (See Van Dam, 1982, and references therein).

The concentration gradient of a contaminant in the far field is significantly lower than that in the near field. In such cases, subgrid-scale turbulent diffusion can be parameterized using a constant diffusion coefficient or one that depends upon the flow field. Some indication of the magnitude of this parameter as a function of the length scale is given by Okubo (1971). Okubo (1971) found that with a grid scale of the order of 100 m the horizontal diffusion coefficient is of the order of 10^2 cm^2s^{-1}, whereas with a 10 km grid a coefficient of the order of 10^5 cm^2s^{-1} may be more appropriate. In a two-dimensional, vertically-integrated model, it is not possible to model explicitly horizontal dispersion by vertical shear/diffusion and this process must also be parameterized. One method of doing this is to relate the horizontal diffusion coefficient to the magnitude of the horizontal current velocity.

With both deterministic and stochastic methods, it is difficult to account for the influence of shallow-sea fronts that can significantly influence the dispersion of a contaminant. The means whereby 'frontal blocking' can be specifically included within a model (by using a fine-resolution model within a coarser one or by some form of parameterization) remains a research topic.

4.2.3 Sediment transport models

Many different, and often not fully understood, processes are involved in sediment transport. There are two modes of sediment transport. Particles can be moved either suspended in the water column (suspended load) or as sliding, rolling, and saltating grains along the bottom (bed load). Bed load is mainly confined to non-cohesive sediments (i.e. sand and gravel), but small amounts of organic material can be included. Suspended sediment comprises both cohesive and non-cohesive material. Sediment transport is predominantly influenced by the flow and the hydraulic characteristics of the area. Morphology and flow are coupled so there are direct feed-backs between flow and the sediment transport, sediment transport and morphology, and morphology and flow. Such feed-backs are ignored in this report. Only sedimentation and erosion are considered.

The conservation equation for the total volume of sediment available for transport is given by :

$$\frac{\partial z_b}{\partial t} + \frac{\partial}{\partial x}(q_b + q_s) + \frac{\partial}{\partial y}(q_b + q_s) = S \qquad (4.7)$$

where z_b is the thickness of the bed layer of sediment, q_b and q_s are the transport fluxes for bed and suspended load respectively and S represents the net effect of source and sink terms. S includes the rate of change of sediment stored in suspension.

The sediment transport flux due to bed load, q_b, is related to the shear stress exerted by the flow on the sediment grains on the seabed. Below a certain shear stress, the grains remain at rest and no bed load transport occurs. The paramerization of this process must obviously take into account the local flow characteristics and the bed composition. In general, this parameterization is strictly site specific and many field measurements are required to tune the parameters involved. A classical formulation relating the bed load to the bed shear stress is given by :

$$q_b = \alpha \tau_b (\tau_b - \tau_{cr}) \qquad (4.8)$$

where α is a coefficient of proportionality, τ_b is the bed shear stress and τ_{cr} is a critical bed shear stress derived from measurements. Recently published bed load transport formulae are more refined but also more complex (van Rijn, 1984).

Suspended sediment transport is described by an advection/diffusion equation taking into account a large variety of processes. The main processes that must be parameterized are diffusion in the vertical, flocculation, gravitational settling, resuspension and erosion. In nearshore areas, breaking waves are important and for muddy seabeds consolidation might need to be taken into account. The difference between the treatment of cohesive and non-cohesive sediments, in addition to the formulation of specific processes, is found in a different boundary condition for the advection/diffusion equation at the bottom. Many of these processes depend on the grain-size distribution of the sediment. Clearly, the values of the parameters will be highly site specific though several of the formulae used for the parameterizations can be used in a generic sense (i.e., confidence is growing that these formulae can be applied to processes in different geographical areas). The most relevant processes and their parameterization are discussed in Annex 2 in greater detail.

4.2.4 Biological Transport Models

For the purposes of describing the distribution of a contaminant in, and/or the effects of a contaminant on, biological substances, the general form of the mathematical model describing the transporter is the three-dimensional advection/diffusion/reaction equation, i.e.

$$\frac{\partial B}{\partial t} + \frac{\partial}{\partial x}(uB) + \frac{\partial}{\partial y}(vB) + \frac{\partial}{\partial z}(wB) - \frac{\partial}{\partial x}\left(K_x\frac{\partial B}{\partial x}\right) - \frac{\partial}{\partial y}\left(K_y\frac{\partial B}{\partial y}\right) - \frac{\partial}{\partial z}\left(K_z\frac{\partial B}{\partial z}\right)$$

$$= \text{biological sources and sinks} \qquad (4.9)$$

where B is the biological substance of interest. The terms on the left hand side of this equation represent local time change, advective, and diffusive effects on B, respectively. The terms that comprise the right-hand side of the equation are those biological processes that produce sources (e.g., production and growth) or losses (e.g., death and consumption) of B. It is through these terms that contaminant effects on a biological substance can be introduced.

As discussed for hydrodynamic models, the entire representation above is not usually used; rather, only a portion or simplified version of the equation is employed. The relevant dynamics that must be included in a biological transport model are dictated by the length and time scales that are of interest for a particular problem and by the trophic pathways that are of concern. If short length and time scales are of interest, as might be the case for determining near-field contaminant distributions, then perhaps only the temporal effects, diffusive processes, and those biological processes that occur rapidly (e.g., doubling of phytoplankton populations) will be of interest. If far-field contaminant distributions are of relevance then advective effects and other biological processes, such as population dynamics and interactions, may become important.

For biological transport models, it is often only the time-dependent behaviour of the contaminant, as it moves through an ecosystem, that is of interest. In this case, the relevant portions of the equation that are retained are the time-dependent term and the biological source and sink terms. The general equation reduces then to an ordinary differential equation of the form

$$\frac{dB}{dt} = f\,(t,\,B,\ldots) \qquad (4.10)$$

where f(t, B...) represents the relevant biological source and/or sink terms. These terms often include mathematical representations of the interactions between various biological compartments (e.g., trophic relations), and they are then functions of several variables. A characteristic of biological models is that the right-hand side of the above equation is usually non-linear and can be strongly so. This type of equation is analogous to the zero-dimensional models discussed in the preceding section on circulation models. These time-dependent models do not always require complex numerical procedures or considerable computer resources to obtain solutions, but care must be taken to ensure that they are numerically correct (see Chapter 6 on Quality Assurance). Such models can be used to consider interactions that occur in multi-component ecosystems, e.g., to investigate the fate of a contaminant as it moves through the nutrient, phytoplankton, zooplankton and fish components of a marine ecosystem. In this case, the model for the biological transporters consists of a system of coupled ordinary differential equations which, while more complex, are not difficult to solve. These models provide information on the time scales over which biological adjustments to perturbations occur and also provide a mechanism for investigating biological interactions without the added complication of circulation effects.

Parameterization of the various terms in the general biological transport model always involves a diversity of measurements and data sources. Specification of the advective field (u,v,w) can be derived from a circulation model or from measurements. The former implies that a circulation model has been developed for the region of interest. The flow distributions obtained from the circulation model are then input to the biological transport model as variable coefficients that may depend upon space and time. If this choice is made for the circulation portion of the biological transport model, care must be taken to ensure that the space and time scales of the two models are compatible. The use of measurements to specify the advective field requires that the measurements be of sufficient duration and breadth to capture the scales of motion that are relevant to biological transport.

The turbulent diffusion coefficients, K_x, K_y, K_z, represent processes that occur on scales not resolved by the model, as discussed previously. These coefficiently may be specified from observations or from theoretical considerations. Techniques and approaches for obtaining values for these coefficients have been discussed in conjunction with the contaminant transport model.

The most difficult part of constructing the biological transport model is determining the correct forms for the source and sink terms because there is no general governing equation for biological interactions in marine ecosystems. Appropriately defined biological systems must, of course, obey the law of mass conservation. There are some other ecological principles, such as Liebig's Law of the Minimum for growth, that govern aspects of biological processes. However, these do not apply to all biological interactions.

Often, parameterization of biological processes is done by relating the biological process to an easily-measured environmental variable such as temperature, light, or the ambient concentration of a nutrient. This approach is correlative in nature, i.e., it is empirical and does not try to describe the precise details (e.g., physiological) of the cause and effect relationships. Most biological relationships are approximated using linear or exponential functions. For the first, it is assumed that increasing the availability of a quantity such as food, or available nutrient, gives an equivalent increase in a biological process. This may be an accurate representation for some processes, up to a point.

Typically, biological rates, especially physiological rates, reach a point at which increasing the amount of a beneficial substance gives little or no appreciable increase in rate. These are referred to as saturated systems and are usually modelled with hyperbolic (combinations of exponential) functions. For other biological processes, such as population growth in the absence of predation, or increases in metabolic rates with increases in temperature, simple exponential functions give adequate representations. However, again, these relationships are only valid over specified ranges of time and forcing functions. It is also possible to combine the various functional relationships to reflect more complex behaviour. Many biological processes can be adequately modelled by relating processes with a power law relationship to animal weight or body size. This is particularly true for catabolic processes, such as excretion and respiration. Again, this approach is empirical, but it does provide a convenient way of parameterizing a process in terms of a quantity that can be measured.

Contaminant effects are usually introduced in the biological terms as a factor that increases or decreases a particular process, such as plant or animal growth. The forms chosen to parameterize contaminant effects range from simple linear relationships to complex non-linear formulations. In either case, laboratory or field measurements of the response of the biological process to the presence of the contaminant should be used as the basis for the parameterization.

Examples of some parameterizations that are used for modelling biological processes are found in Annex 2. These are not all-inclusive; rather, these parameterizations represent some of the more accepted ways of modelling certain biological processes. It should be stressed that there is no 'right' way to model a given biological process. The particular approach chosen is often dictated by the available measurements, or the level of understanding, relating to a particular process. For example, mortality terms are usually modelled as a linear decrease that proceeds at a constant rate and depends on the local biomass concentration. This is recognized to be an inadequate representation of the processes that produce population losses in marine ecosystems but, given the difficulty of measuring <u>in situ</u> mortality rates of marine organisms, this is the best that can be done with the available information. Whatever approach is chosen for modelling biological processes, care should be taken to adequately confirm the chosen formulation with data from field or laboratory measurements. Including complex formulations without adequate justification does not improve a biological transport model; it merely obscures the real issue. When faced with including a process (such as mortality) for which inadequate data exist, the best policy is to use the simplest formulation possible.

4.3 Contaminant transport model: couplings between transport models

As indicated in Figure 2.2, a contaminant within the water column can be associated with any one of three transporting media: water, sediment, or biota. The transport of the contaminant by water, i.e., the distribution of the dissolved phase, has been dealt with to some extent in Section 4.2.2 where the mechanical (or hydrodynamical) aspects of transport are discussed. The source and sink terms are mentioned without a description of possible parameterizations and the discussion of those parameterizations is postponed because the non-conservative aspects of the behavior of a contaminant are either the result of interactions between the various phases or, referring to Figure 2.3, linked to (geo)chemical reactions. The interactions or couplings between transporting media are considered hereafter. Section 4.4 addresses the topic of decay and production.

4.3.1 Biota-water interactions

Biological interactions with substances in solution include processes that are actually chemical in nature. The major interactions that often require to be represented in coastal zone models are:

- biological uptake and incorporation of substances into biological materials; and
- the subsequent release of incorporated substances to solution through excretion and during decay of marine organisms after death (regeneration).

It appears that passive uptake of metals by both living and dead phytoplankton is similar and these can be represented by Freundlich adsorption isotherms (Fisher et al., 1983, 1984; Fisher 1985). Therefore, we can frequently make an equilibrium partitioning assumption for the exchanges between biological organisms and water similar to those between inorganic particulate matter and water. In this sense a 'biological concentration factor' becomes analogous to a partition coefficient (see

4.3.3) but applied to the relationship between the concentration of the substance in organisms (or a particular type or organ of the organism) and the dissolved concentration of the substance in the surrounding water.

The use of such 'biological concentration factors' to represent the contaminant concentrations in living organisms implicitly assumes not only equilibrium conditions between the organisms and water but also between the organisms and any other transitional phases through which the contaminant moves towards its association with the organisms. This will often therefore include an implicit assumption of equilibrium between water, particles, colloids and the biota.

Active uptake of 'contaminant' from the solution by the biota also occurs for those substances that are metabolically essential. Thus, the incorporation of carbon, nitrogen, phosphorus and other essential dissolved elements occurs by way of active uptake by organisms. The parameterization of this process has been discussed in 4.2.4, and further details can be found in Annex 2. It should, however, be noted that for organisms other than autotrophs, particulate ingestion may be the dominant pathway for the incorporation of those essential elements and compounds that are relatively impoverished in solution.

The regeneration, or dissolution, of substances from decaying biological material is largely a passive chemical process. The amounts of organic and inorganic biogenic material that are regenerated will depend heavily on factors such as the depth of the water column and the settling rate of the particles. Parameterization of regeneration or dissolution is usually accomplished by the use of a time-dependent first-order rate function analogous to radioactive decay (see 4.4). In some circumstances, however, it may be necessary to characterize the regeneration of biogenically-incorporated substances separately for each major component of biogenic material, namely organic matter and calcareous, chitinous and silicious shell material. Concentration factors for substances appropriate for each component must then be known.

4.3.2 Biota-particle interactions

Interactions also take place between biota and other particulate material. In most instances the uptake of particles by biota is an active process and this is discussed in Annex 2 together with methods of parameterizing these interactions. Biota also generate particulate material by defecation and decay and the ways in which these processes may be parameterized is also discussed in Annex 2.

4.3.3 Particle-water interactions

An adequate parameterization of the complex adsorption/desorption processes of contaminants between water and particles is essential for dealing with contaminant behaviour in natural water-rock systems such as the coastal zone. It is generally assumed that adsorption/desorption reactions are reversible and can be represented by first-order kinetics of the form

$$C_d \underset{K_2}{\overset{K_1}{\rightleftarrows}} C_p$$

where

C_d is the dissolved concentration of the substance;
C_p is the particulate concentration of the substance;
K_1 is the reaction rate constant for adsorption;
K_2 is the reaction rate constant for desorption.

For nearly all substances in the coastal zone, excepting those that are undergoing changes in their dissolved and particulate concentrations due to chemical precipitation or dissolution, such as Fe, Mn, I and As, or those subject to radioactive decay, it can be assumed that adsorption/desorption proceeds rapidly to equilibrium. From the steady state balance

$$\frac{dC_p}{dt} = 0 = K_1 C_d - K_2 C_p \tag{4.11}$$

the thermodynamic equilibrium constant, or partition coefficient, denoted K_d, is found to be

$$K_d = \frac{C_p}{C_d} = \frac{K_1}{K_2}$$

For radioactive species no (formal) steady state exists, but the ratio of the concentrations can be used to define a quasi-equilibrum partition coefficient, (see Annex 2).

For elements for which equilibrium can be assumed throughout the marine environment, of which there are many, a partition coefficient (K_d) can be defined and estimated on the basis of the residence time (see Annex 2). This provides the possibility of being able, not only to rationalize effective partition coefficients for well-studied elements, but also to determine effective K_d values for poorly-understood elements. This has a great deal of utility in modelling of particle-solute interaction processes in the coastal zone. It is concluded that, in general, an assumption of equilibrium conditions for the interactions between particles and solutes can be made for most coastal zone areas and constituents. Even in cases where it is known that the equilibration takes considerable time, as for example with beryllium, manganese, cobalt, iodine, iron and arsenic, it may still be possible to make equilibrium assumptions while ensuring that the partition coefficient is appropriate to the specific environment in which it is to be applied (see Annex 2).

It should be emphasized that all that has been said with regard to particle-water exchanges applies only to the exchangeable phase of substances on particles. The lattice constituents of rock mineral matrices are not generally involved in exchanges within the marine environment at all. Furthermore, it also means that the only particles of interest in respect to particle-water exchanges are the silts and clays since larger particles have very small exchange capacities or specific surface areas for adsorption.

The transfer of sedimentary constituents into the water column during erosional conditions can be parameterized by a mass transport term and a representation of the composition of surficial sediment particles and pore water. The compositional term would have to be suitably modified in cases where significant vertical gradients occur in the distribution of a substance such as the cases of oxygen and organic matter in oxidized sediments. The migration of substances under depositional conditions can often be represented by diffusion equations in which sedimentary constituents are free to diffuse (vertically) in the sediment column and into the overlying water. For such constituents, whose vertical distribution is controlled by oxidation-reduction reactions (e.g. Mn^{2+} and MnO_2), the vertical gradient in redox potential will need to be coupled with a representation, in chemical terms, of the particle-water interactions.

4.4 Decay and production

So far Chapter 4 has dealt with changes between compartments of the conceptual model shown schematically in Figure 2.2. However, as was explained in Section 2.4.3, there is an additional dimension representing decay and production of contaminants. Figure 2.3 illustrates this concept. The simplest decay and production is that of a contaminant which decays at a constant rate to produce a second contaminant. This is parameterised as follows:

$$\frac{\partial C_1}{\partial t} = - \lambda C_1 + \text{decay} \qquad (4.12a)$$

$$\frac{\partial C_2}{dt} = + \lambda C_1 + \text{production} \qquad (4.12b)$$

where C_1 and C_2 are the concentrations of contaminants 1 and 2, respectively, and contaminant 1 is decaying into contaminant 2 at a rate λ. The most common example of this is radioactive decay where the decay constant is inversely proportional to the half life of the radionuclide. However, the same parameterization can be used if the decay rate is not constant. In a biological system, for example, the decay can be a rate of mineralisation and may be a function of such variables as temperature and light. The form of the equations stays the same but there will need to be an expression for the dependence of the decay rate on relevant quantities.

So far, the emphasis has been on the unidirectional decay of one contaminant to another. The methylation of inorganic mercury proceeds at a rate depending on a number of factors including concentration of sulphides present in the surficial seabed sediment. However, under altered conditions the net reaction will be reversed. Therefore, the parameterization for these processes can be written

$$\frac{\partial C_1}{\partial t} = - \underset{\substack{\text{decay} \\ \text{(methylation)}}}{\lambda_d C_1} + \underset{\substack{\text{production} \\ \text{(demethylation)}}}{\lambda_p C_2} + \text{other terms}$$

$$\frac{\partial C_2}{dt} = + \underset{\substack{\text{production} \\ \text{(methylation)}}}{\lambda_d C_1} - \underset{\substack{\text{decay} \\ \text{(demethylation)}}}{\lambda_p C_2} + \text{other terms}$$

where λ_d is the rate of methylation of inorganic mercury, λ_p is the rate of demethylation of the methyl mercury to inorganic mercury, and C_1 and C_2 are the concentrations of inorganic mercury and methyl mercury, respectively. Here, λ_d and λ_p are functions of the environmental conditions.

4.5 Parameterization in transport models for the sea bed

The discussions in 4.2 and 4.3 pertain to transport mechanisms in the water column. Ideally, the parameterization of sea bed processes should be organized and discussed in a similar way. However, the present knowledge of sea bed processes is insufficient to deal individually with each of the transporter types, i.e. pore water, biota and sediment, as presented in 4.2. The difficulty is compounded by the fact that each transporter may be transported by the others in the sea bed. For example, some biological organisms can move the sediment and pore water in the benthic layer via the conveyor belt mechanism, whereas in the water column movements of water and suspended sediments by biological organisms seldom occur. Thus, contaminants in pore water and sediment are affected by movements of the organisms in the benthic layer.

Some transport models have been developed for the individual transporters, e.g. the random walk model for the movement of the benthic organisms. By and large, many benthic contaminant transport models combine the modelling of the transport media with the modelling of contaminants (see Figure 2.2 and section 2.4.2). For example, one approach to modelling bioturbation is to use a large effective vertical diffusion coefficient in the upper few centimetres of the sediments. This combines many unknown (and perhaps unquantifiable) processes into a single parameter. The value used for the effective diffusion coefficient can be chosen empirically by fitting the profile predicted from a one-dimensional model to observed sediment profiles, particularly those of short-lived radio-isotopes (e.g., ^{7}Be). Another approach might involve counting the number of organisms in a given area and making assumptions about their behaviour. There can be significant, active vertical transport by in-fauna that consume and defaecate material at different discrete levels in the sediment. These organisms are referred to as 'conveyor-belt feeders' (see Annex 2 for the parameterization of that process).

Below a certain depth, oxygen can be depleted in the sediment. This results in the inhibition of bioturbation and a number of chemical reactions take place. For instance, manganese is redissolved under anoxic conditions. It may therefore be necessary to represent the sea bed by a number of layers depending on the chemical conditions which need to be represented. A term to represent non-conservative processes, such as biogeochemical reactions and radioactive decay, should be included in the equation. The exchange of a contaminant between the sea bed and the overlying water column may be enhanced by the presence of burrows. This process again is parameterized by an enhanced vertical diffusion in the sea bed (Aller and Yingst, 1985). More examples of parameterization of sea bed processes are given in Annex 2.

4.6 Characterizing source terms

The method of coastal zone disposal is an important consideration in the construction of models. Whether it is a large bulk dumping operation over a short span of time, or whether it is a coastal discharge through a submerged diffuser, the problem exists of parameterizing the input conditions, i.e., the source term in the mathematical model. Parameterizing the source term requires a knowledge of:

- the form and composition of the material entering the coastal zone;
- the disposal procedure; and
- the dimensions of the source.

If the contaminant is introduced in a free form, modelling of its behaviour can be carried out on the basis of representations of the various controlling processes (physical, chemical and biological). However, in most situations, the contaminant will be a constituent of some other host material when it enters the marine environment. In these instances it is necessary to include representations of the manner in which the contaminants of interest are retained in the host material and the extent to which they are transformed and released to become associated with other phases in the receiving environment.

The bulk forms that a material, intended for disposal into the coastal zone, may take are liquid and solid or a mixture of these. The solids can range from massive bulk forms to fine particulates, each of which will clearly have differing behaviour in the receiving environment. Dissolved contaminants may be in the aqueous phase or in other miscible or non-miscible liquids (e.g., oil-based wastes).

The disposal procedure, i.e., the timing of the releases of material to the receiving system, also needs to be characterized. Releases can be essentially constant, fluctuating or discontinuous. Constant releases are the simplest type to represent in models although fluctuating releases do not usually provide much greater complexity in modelling. Discontinuous releases, of either the single event or separated event form, where the release time is short compared with the intervals between releases, are the most difficult to accommodate in analytical models. Frequent discontinuous releases can sometimes be characterized as fluctuating releases if the time of release is long compared with the interval between releases and the flushing time of the receiving system.

The third aspect concerns the dimensions of the source. This can either be a point source, a line source or a diffuse (widespread) source. Examples of the latter case would be widespread dumping throughout the receiving environment or diffuse runoff that enters the system from a number of diverse line or point sources (GESAMP, 1987). The dimensions of the source would need to be considered in order to faithfully reflect transport of material from the source(s).

Aside from the characterization of deliberate contaminant introductions, through discharge or dumping, to the coastal zone there may be a need to include other inputs of these same contaminants. This will often be necessary to ensure that all sources of the contaminant are considered and to provide a rational basis for comparing model predictions with conditions in the real environment. A particularly important input of this type is atmospheric deposition. A simple approach to the aggregate deposition of atmospheric constituents is to express these as the product of atmospheric air concentrations and deposition velocities. In many cases, such a simplification will be adequate. Under most circumstances, transport of substances from the coastal zone water surface to the atmosphere can be neglected. However, there may be significantly volatile substances that are transported from sea to air thus representing a loss from the coastal ocean environment. Processes causing sea-to-air transport and their parameterizations are described in GESAMP (1989).

5. CASE STUDIES

5.1 Introduction

The heterogeniety of coastal seas precludes the existence of a single model capable of resolving all space and time scales in coastal environments and, thus, all possible situations. Also, as was stressed in chapter 2, the type of model to be used depends critically upon the management question being asked. Most management questions will require an exposure model/dose-effects model which itself has implications for the dispersion model that relates the contaminant inputs to the contaminent distribution in the environment. It is this latter model that is the subject of this report. There is little point in a manager initiating work on a sophisticated model designed to answer a research question, if that model either cannot answer the management question, or is so expensive to run that all scenarios of interest cannot be tested.

Dispersion models essentially describe the conservation of the contaminant in the environment. As was seen in chapter 3, such dispersion models can frequently be described mathematically by the advection/diffusion equation. As was also discussed in chapter 3, simple models tend to have simple representations of the processes involved and usually have low spatial or temporal resolution. The more sophisticated models normally result from more complex representations of the way in which the contaminant partitions between various parts of the environment and have higher (in relative terms) spatial and temporal resolution. The choice of which type of model to use depends on the accuracy needed to answer the management questions.

In selecting the case studies given in this chapter, the members of the Working Group have drawn on their own experiences. A range of problems has been selected to demonstrate how to choose the level of model complexity required to answer a particular question. The key to the constuction of the appropriate model is the clear definition of the management question and hence of the pathway of concern by which the effects of concentrations of contaminant or pollutant in the environment are delivered. This chapter presents a series of case studies as a means of illustrating how models may be used to answer specific management questions. Particular emphasis is placed on defining real, or hypothetical, management questions that specify the nature of the exposure or effects pathway before any attempt is made to construct the model.

5.2 Cadmium in an estuary

5.2.1 Statement of the management problem

A river flows into the head of a salt wedge estuary (see Annex 1) in which there are three mollusc fisheries (Figure 5.1): one in the downstream portion of the estuary where the bottom waters have salinities of 25-28; one near the estuarine null-zone in the salinity range 1-5; and one just beyond the estuary on the mud flats that are exposed to the mixed surface water leaving the estuary.

There are plans to build a factory that will discharge an effluent containing cadmium (Cd^{2+}) into the river. At what level can this discharge be allowed to proceed so that the molluscs are not exposed to cadmium concentrations that would make them unfit for human consumption and thus, require closure of the thriving fishery?

5.2.2 Model construction

The receiving environment is a laterally homogeneous salt wedge estuary with freshwater input from a single river into which the intended effluent is to be discharged. The longitudinal salinity distribution in the estuary is shown in Fig. 5.1. The mean salinity entering the bottom

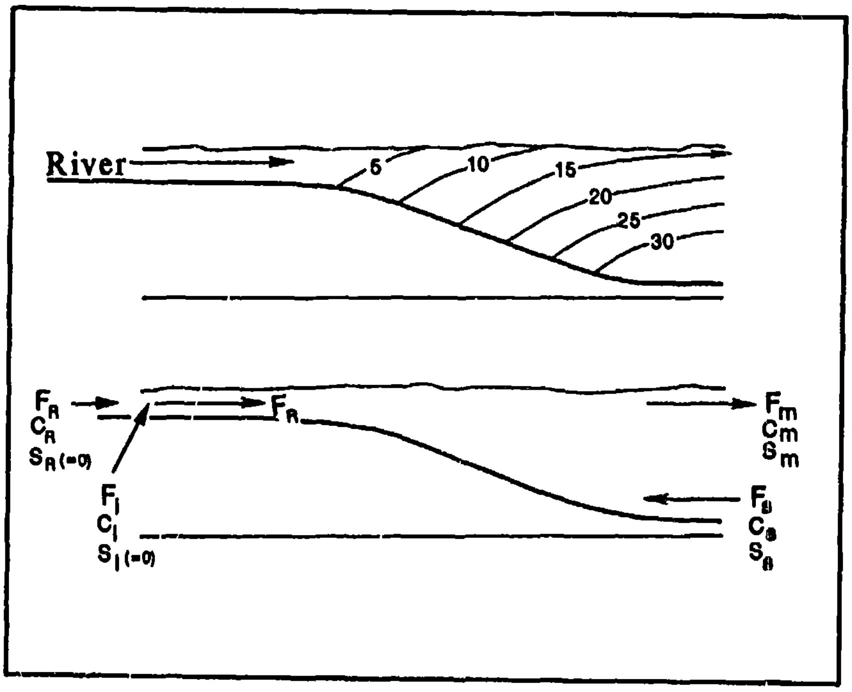


Figure: 5.1. Salinity distribution in the estuary and schematic representation of model variables.

layer of the estuary through its downstream limit is S_s. The rate of river water discharge, F_R, is constant with time and contains an average natural cadmium concentration of C_R. The circulation of the estuary is driven by runoff, and tidal effects are assumed to be insignificant. The cadmium is discharged at a rate C_iF_i, where C_i and F_i represent the input cadmium concentration and the carrier wastewater discharge rate, respectively.

If the existing concentration of cadmium in the river is C_R, that in the saline inflow is C_s, and that in the mixed outflow is C_m, and if a continuous discharge of new cadmium from the industrial source is assumed, then the following conservation equations can be written, after steady-state conditions have been achieved:

Mass conservation of water (assuming negligible density variations)

$$F_R + F_i + F_s = F_m \qquad (5.1)$$

where F_s is the rate of water input to the estuary at its downstream limit and F_m is the rate of production of mixed water.

Mass conservation of salt

$$F_s S_s = F_m S_m \qquad (5.2)$$

where S_m is the mean salinity concentration in the mixed water. If cadmium is conserved in water (i.e., if the rate of cadmium removal to particles and biota is small compared with the rate of transport in the aqueous phase) we can also derive a mass conservation equation for cadmium

$$F_iC_i + F_RC_R + F_sC_s = F_mC_m \qquad (5.3)$$

The cadmium concentration in outflowing mixed water is

$$C_m = \frac{F_iC_i + F_RC_R + F_sC_s}{F_m} \qquad (5.4)$$

As cadmium and salinity are both conserved, the cadmium concentration, at any point in the estuary, C_e, will be linearly related to the salinity, at that point, S_e. Hence, in the range $0 < S < S_s$

$$C_e = \frac{C_s - C_F}{S_s} S_e + C_F \qquad (5.5)$$

where C_F, the concentration of cadmium in the aggregate freshwater inflow, is

$$C_F = \frac{F_i C_i + F_R C_R}{F_i + F_R} \qquad (5.6)$$

It is now a simple matter, given appropriate salinity values and one of the aggregate flows into or out of the estuary, to calculate the range of cadmium concentrations in the water to which each of the mollusc fisheries will be exposed.

5.2.3 Example calculations

The parameter values assumed to calculate exposure of mollusc beds to cadmium are given in Table 5.1. The values for volume fluxes and cadmium concentrations obtained using these parameters and the above equations are shown in Table 5.2, and Table 5.3 gives derived values for cadmium concentrations at certain points in the estuary.

Table 5.1. Assumed parameter values for the case study of cadmium discharge in an estuary.

Parameter	Value
C_R	50 ng l^{-1}
C_i	10^5 ng l^{-1}
C_s	30 ng l^{-1}
F_R	10^6 l s^{-1}
F_i	10^3 l s^{-1}
S_R	0
S_i	0
S_s	32
S_m	25

Table 5.2. Calculated values for the case study of cadmium discharge in an estuary.

Variable	Values	Equation
F_s	3.58×10^6 l s^{-1}	6.1, 6.2
F_m	4.58×10^6 l s^{-1}	-"-
C_m	56.2 ng l^{-1}	6.4
C_F	150 ng l^{-1}	6.6

Table 5.3. Derived cadmium concentrations for different salinities using equation 5.5.

S_e	C_e (ng l^{-1})
0	150
3	139
7	124
18	82.5
22	67.5
25	56.2
32	30.0

Assuming the proposed level of discharge cadmium concentration, C_i, of 10^5 ng l^{-1}, the mollusc beds at the landward end of the estuary will be exposed to water containing cadmium at a concentration of between 124 and 139 ng l^{-1}, those in the middle estuary to concentrations of 82.5 to 67.5 ng l^{-1}, and those exposed to the estuarine outflow to concentrations of 56.2 ng l^{-1}.

Now assume that the human health tolerance for cadmium in molluscs for human consumption has been set at 2.0 mg kg^{-1} wet weight and that the biological concentration factor for molluscs has been established to be 2×10^4 (IAEA, 1985b). Thus, molluscs for human consumption should not be exposed to cadmium concentrations in water exceeding 100 ng l^{-1}. Since the molluscs at the head of the estuary will be exposed to cadmium concentrations that will exceed this level, and a very small margin of safety exists for the molluscs in the middle estuary, the planned release should probably not be permitted. The extent of reduction of cadmium in the industrial plant discharge required for the modified discharge to be acceptable will depend on the degree of safety required by the particular jurisdiction within which the application for a discharge license is being considered.

It should be noted, however, that it is likely that even molluscs exposed to natural levels of cadmium in seawater of between 10 and 30 ng l^{-1} will accumulate cadmium in concentrations exceeding 10% of the limit for human consumption. The adoption of safety factors exceeding a factor of 10 are therefore untenable. The discharge concentration must be less than 5×10^4 ng l^{-1} to meet the upper limit of 100 ng l^{-1} stated above.

5.2.4 Additional comments

The approach discussed above will often suffice for contaminants that have relatively low K_ds and are discharged into temperate systems. There will be instances in highly turbid systems where the partitioning between water and particles will result in perturbations to the dissolved concentration field but these, for low-K_d contaminants discharged in the aqueous phase, should arise infrequently.

For contaminants with very high K_ds, the approach outlined above will more frequently be unsuitable because the processes of exchange between dissolved and particulate phases will have a significant effect on reducing the aqueous concentrations below those assumed on the basis of conservation in water being made. A good example of this situation is iron discharged into an oxygenated estuarine environment in the form of dissolved Fe^{2+}. The very rapid oxidation of iron and repartitioning of iron between the dissolved and particulate phases will have a very pronounced effect on the dissolved iron distribution and will disallow assumptions of conservation of mass. Indeed, it is often difficult to set up equations for overall mass conservation with unambiguous definitions of the rate and character of sediment accumulation within similar estuarine systems. However, such complications should only arise in the cases of highly turbid coastal systems or for relatively high-K_d contaminants.

5.3 Monazite sand dregded from an estuary

5.3.1 Statement of the management problem

An estuary has a sandy bed which contains layers of monazite sands (Read, 1970; Pentreath, 1985) and quantites of silt are washed into the estuary by the rivers that empty into the estuary. With the expansion of the industry at a town part way up the estuary, larger ships need to have access to the town's port. It is proposed that the shipping channel be dredged and that the dredge spoils be dumped over the sandy gently sloping continental shelf 10 km offshore in waters with depths less than 30 m. The shoreline at the mouth of the estuary supports a lucrative tourist trade.

How much dredged spoil containing the thorium-bearing monazite sands, can be dumped so that sand from the disposal site does not wash up on the beach in sufficient quantites to cause unacceptable radiation doses to either to members of the public using the beaches for recreational purposes or workers involved in the tourist trade?

5.3.2 Model construction

For the purpose of model development, it is assumed that the monazite sand is dense, settles rapidly to the bottom, and that there is no environmentally significant concentration of thorium dissolved in sea water. Further assume that the critical pathway for radiation exposure to man is directly through beach contamination. The effects of monazite sands on fisheries and other economic resources are assumed to be unimportant.

From the above assumptions, it is clear that a model of sand movement, however simple, will be needed. In what follows, progressively more complicated models are described to show the level of sophistication needed to give increased spatial and temporal insight into the predictions.

A simple model of the transport of monazite sand out of the dumping area can be formulated by balancing the input of material with the loss from the dump site. If material is dumped at a rate of R ($m^3\ d^{-1}$) and a fraction k (d^{-1}) of the volume of monazite sand is lost each day, then the rate of change of the volume of monazite sands, V_s, at the dump site is

$$\frac{dV_s}{dt} = R - k\,V_s \qquad (5.7)$$

This equation can be written in terms of the fractional concentration of monazite sands, C_s, on the site by dividing each term by the volume of the site, Ad, where A is the area and d is the depth of mixed sand. Thus,

$$\frac{dC_s}{dt} = S - KC_s \qquad (5.8)$$

where S = R/(Ad). The thorium content is simply pC_s, where p is the fraction (by weight) of thorium in dumped sand. The fractional removal rate, k, encompasses a number of complex physical transport mechanisms such as propagating sand waves, bed load accompanying strong tidal and wind-generated currents near the sea bed, among others. The solution to equation 5.8 is:

$$C_s = \frac{S}{K} + [C_o - \frac{S}{K}]\, e^{-kt} \qquad (5.9)$$

where the integration constant (C_o) represents the initial concentration of monazite sand at time t = 0. After a long time C_s = S/k which is the steady-state concentration of monazite sand at the site, representing a balance between input and output of sand at the site. The product kt represents the fraction of sand moved out of the dump site in time t and the problem becomes one of determining suitable values of k.

5.3.3 Specific examples

The important variables for this problem are the mixing volume Ad, R, S and p. Two cases are presented to illustrate the character of the solution described by equation 5.9. The first represents a small operation in which 1000 $m^3\ d^{-1}$ of sand is dumped in a relatively small area. The second case represents a larger operation where about 20,000 $m^3\ d^{-1}$ is dumped over a larger area For both cases, the sands are mixed over a depth, d, of 1 m, with no monazite sand present prior to dumping (C_0=0) and with a thorium content of 10% by weight (i.e.,p=0.1) The remaining parameter values for these two cases are given in Table 5.4. Note that since the larger operation spreads the sand over a much larger area, the source strength, S, is only a factor of two greater than for the smaller disposal.

Table 5.4. Numerical data for monazite sand examples.

	Case 1	Case 2
Volume input rate, (m^3 d^{-1})	1000	20000
A (m^2)	1.0×10^6	10×10^6
Volume = A*d (m^3)	1.0×10^6	10×10^6
Source rate, S	1×10^{-3}	2×10^{-3}

The relationship between sand concentration, C_s per unit source strength, S, versus time for different values of k is shown in Fig. 5.2. A value of k = 0.1, probably an unrealistically high value, signifies that 10 per cent of the sand is transferred from the dumpsite each day, and

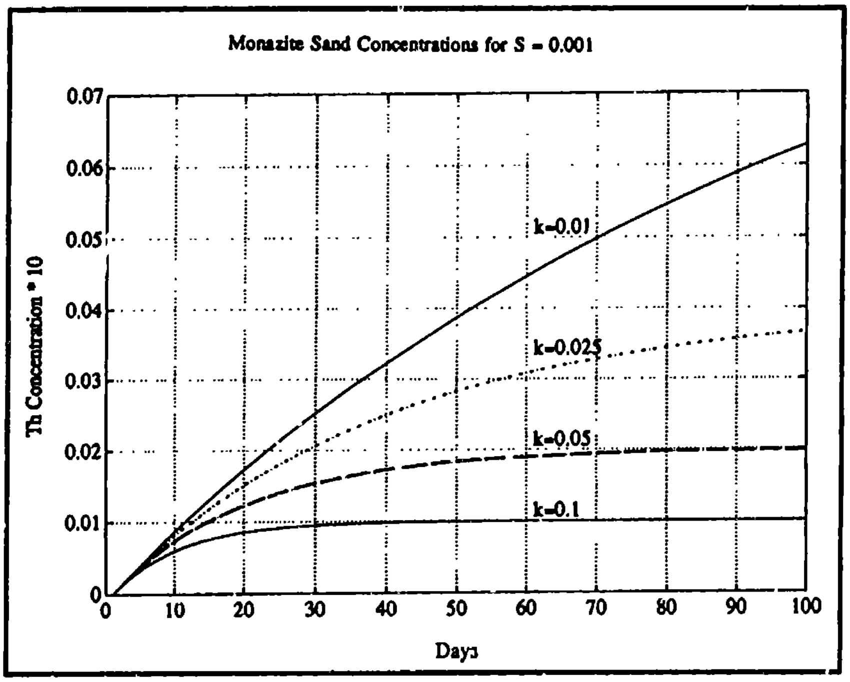


Figure: 5.2. Relationship between sand concentration per unit source strength and time for different values of k.

that a steady-state concentration is reached within 30 days (regardless of S). As the transfer rate decreases, longer times are required to reach steady state. When k = 0.01 (1 per cent is transferred per day), steady state is not achieved within 100 days. This examination of the possible variation in the value of k allows limits to be placed on solution of the model.

This simple model can be extended by linking a number of boxes to represent the transport in the along-shore and the cross-shore direction. The output, kC_s, from one box is used as the input source to an adjacent box. The sand transport through these boxes depends upon variables such as the depth of water, wave-tide interactions and the proximity to the coast line. The added complexity results in more complex parameterizations of k and may require an elaborate field programme at the site of interest. A grain-size analysis of existing seabed sediments in the area of the proposed dumpsite can provide two pieces of information: an indication of how the seabed is being moved by the long-term average water flows (McLaren and Bowles 1985) and data for calibrating and validating the model.

In order to answer the original question about shoreline exposure to members of the public, the monazite sand model must have a sufficient number of interconnected boxes to give a solution with the required accuracy and confidence. If thorium concentrations can be shown to be sufficiently low by placing realistic bounds on the values of k, then nothing further needs to be done than a simple linked box model. If this is not the case, more complex models are needed.

Obviously, if models already exist which are more complex than required, but still address the management question, then these models can be used because such an approach may be more cost effective than building a new model.

5.4 Impact of the disposal of titanium dioxide wastes into coastal waters

5.4.1 Statement of the management problem

The 1985 Report of the ICES Advisory Committee on Marine Pollution (ICES, 1985) provides an assessment of the impact of the coastal disposal of wastes from the titanium dioxide extraction industry on the North Sea.

The evaluation takes the form of a series of model calculations designed to determine waste concentrations in the environment for comparison with levels at which the wastes induce effects on marine organisms. The assessment considers the effects of an existing industry rather than predicting the impact of a planned industrial installation, and the nature of the simple assumptions and models used should be clear. Nevertheless, the model calculations provide an illustration of a crude, but effective, means of impact assessment that could be inverted to determine, rather conservatively, the capacity of a coastal system to assimilate planned wastes if adequate toxicological criteria for defining limiting contaminant exposures are available.

Concerns about the effects of titanium dioxide wastes dumped or discharged to European coastal waters became heightened in the early 1980s. The waste is derived from the extraction of titanium from the minerals illmenite and rutile using strong acid leaching procedures, and contains a wide variety of inorganic constituents. No synthetic organic compounds are involved and, in many aspects, the wastes are similar to those mobilized through natural weathering processes. In drawing this analogy, however, it should be stressed that the concentrations of metal ions and acids in the waste are considerably larger than those found under natural conditions and some of the ions may be in an unusually active form relative to those produced by natural weathering. Nevertheless, after large-scale dilution and some time in the marine environment, the products of neutralization, hydrolization, oxidation and precipitation will act on the titanium dioxide waste similarly to those that are discharged in natural runoff.

The methods of marine disposal of titanium dioxide wastes include both pipeline discharge into coastal waters and dumping from vessels into the North Sea. The North Sea has received more waste from titanium dioxide production than any other regional marine area, with five countries having contributed to such disposals. The input of Fe via titanium dioxide wastes is about the same as the aggregate iron discharge from the Rhine, Elbe, Schelt, Thames and Humber rivers. For the other constituents, with the possible exception of manganese, the input via titanium dioxide wastes is considerably smaller than the corresponding discharges from rivers.

It is evident that after large-scale dispersion (e.g., over basin-wide scales) the impact of titanium dioxide wastes is no more adverse than that caused by the discharge of natural weathering products from rivers. However, in the vicinity of the disposal sites, effects may be severe and there exist toxicological and environmental measurements to define both the threshold for adverse effects on marine organisms and the types of effects induced. The problem is to define the distance scales over which these wastes might have significant impact in the coastal zone.

5.4.2 Model construction

The model is a series of simple calculations performed to determine, on a conservative basis, the average concentrations of titanium dioxide waste, or its major constituent, Fe, in water and sediments of differently-sized receiving areas. These concentrations are then compared respectively with concentrations causing sub-lethal effects and to ambient levels of sedimentary Fe to determine the extent of likely impact of the wastes in the North Sea. The values used in the following calculations are given in Tables 5.5 and 5.6.

Table 5.5. Parameters assumed for North Sea in TiO_2 case study.

Volume	$5x10^{13}$ m^3
Area	$5.8x10^5$ km^2
Flushing time	2 a
Net alongshore velocity(1)	1.9 km d^{-1}
Iron content (by mass) of sediments	3%
Sublethal limit of TiO_2 on marine life(2)	22 ppm

(1) Net speed along coastal belt of Belgium, Netherlands and Federal Republic of Germany (Topping, 1978)

(2) Lowest TiO_2 concentration causing a detectable sub lethal effect on marine life (Kayser, 1969).

Table 5.6. Discharges/Dumping of Wastes from the TiO_2 Industry by Countries Bordering the North Sea.

Country of Origin	Rate of Waste Discharged/Dumped ($t\ d^{-1}$)	Iron Content %	Rate of Iron Discharged/Dumped $t\ d^{-1}$
Federal Republic of Germany	1,300	14	165
Netherlands	4,000	7	280
Belgium	600	2	12
			457
United Kingdom	22.7*	0.8	182*
Total~6000			639

* Assuming the wastes have a specific gravity of 1.0

5.4.3 Example calculations

5.4.3.1 The whole of the North Sea

If it is assumed that the waste discharged becomes uniformly distributed throughout the entire North Sea, then the volume of water available annually for waste dilution is the ratio of the volume of the North Sea to its flushing time. Thus, the effective concentration of titanium dioxide waste in the North Sea waters will be the annual discharge rate divided by this volume replacement rate. Taking the discharge rate as 30000 $t\ d^{-1}$ to be five times the total given in Table 5.6 to allow, conservatively, for all additional disposal of wastes from the titanium dioxide industry into the North Sea by countries other than The Netherlands, the Federal Republic of Germany and Belgium, yields an average titanium dioxide concentration of $4.4\ 10^{-7}\ t\ m^{-3}$.

The concentration derived from this calculation (0.44 p.p.m.) is a factor of 50 lower than the lowest concentration at which detectable sub-lethal effects on marine life occur (22 p.p.m.). Therefore, deleterious effects on marine life in the North Sea as a whole are most improbable.

5.4.3.2 The Coastal Zone of Belgium, the Federal Republic of Germany* and the Netherlands

If it is assumed that titanium dioxide wastes discharged or dumped by Belgium, the Netherlands and the Federal Republic of Germany are all retained within a 30 km-wide belt, with an average depth of 25 m, along the eastern coast of the North Sea, the daily volume of water available for diluting the wastes is the cross-sectional area of the coastal strip (0.75 km^2) multiplied by the mean water transport (1.9 km d^{-1}), that is 1.4 10^9 m^3 d^{-1}. As above, the concentration of wastes in this coastal belt is the dumping rate (6000 t d^{-1}) divided by this dilution rate, i.e., 4.3 x 10^{-6} t m^{-3}.

The concentration derived from this calculation (4.3 ppm) is only a factor of 5 lower than the lowest concentration at which detectable sub-lethal effects on marine organisms occur (22 ppm). Furthermore, this safety factor must be viewed against the probability that the coastal water flow may already be contaminated by wastes arising from industries situated 'upstream' of this flow, for example, in France. Clearly deleterious effects over scales comparable with that of such a coastal belt must be expected and are likely to be most evident in sub-areas of only slightly smaller dimensions. Any peaks in the discharge/rate may result in a significantly greater impact in the receiving areas but, based on the previous calculation, are unlikely to affect the North Sea as a whole.

5.4.3.3 Impact on North Sea sediments

If it is assumed that the wastes become uniformly distributed over North Sea sediments and that they become uniformly mixed throughout the upper 10 cm of sediments by bioturbation and physical mixing, then a similar calculation can be performed to estimate the sediment iron concentrations. Natural North Sea sediments contain about 3% by mass of iron, therefore, the top 10 cm of sediment contains approximately'3.48 x 10^9 t of iron, assuming a mean sediment density of 2 t m^{-3}.

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* This text was compiled before the recent reunification of Germany.

The quantity of additional iron provided to the sediments through the release of wastes from the titanium dioxide industry is 639 t d^{-1} (Table 5.6), which provides a 0.007% increase in iron incorporated into North Sea sediments annually. Even allowing for an additional 300 t d^{-1} of iron through disposal of titanium dioxide wastes by other countries, the proportional increase in the iron content of sediments is only 0.02% per year. This calculation does not account for dilution of the iron concentration by sedimenting particles. It is, therefore, clear that titanium dioxide disposal will not result in broad-scale modifications of the iron composition of North Sea sediments. It would take about 1000 years to double the present sediment iron content.

5.4.3.4 Impact on sediments in a Coastal Belt of the North Sea

Assuming the iron in the titanium dioxide wastes disposed of by Belgium (2 dump sites), the Netherlands (1 discharge point) and the Federal Republic of Germany (3 dump sites) is deposited close to each point of input within one day of release, then the area affected in each case is about 4 km^2, i.e., 1.9 km (the net movement of water in the eastern coastal strip each day) by about 2 km to represent dispersion across the flow. The total amount of iron already present in the top 0.1 m of the sediments in the six areas affected will be 1.44×10^8 kg, again assuming a sediment density of 2 t m^{-3}.

The amount of iron added per year to the six areas is 1.67×10^5 t (from Table 5.6) and so the percentage increase per annum is 116%. Since it is known that the inputs in the German Bight are never supposed to be dumped more than once in the same place and total deposition within one day is unlikely, the above represents a worst-case situation. Nevertheless, it does indicate that, in the area of input and downstream thereof, detectable increases in the iron content of the surficial sediments must be expected. Indeed, this is demonstrated in the German Bight.

5.4.4 Additional comments

These calculations demonstrate that measurable changes in sediment composition and sub-lethal biological effects can be expected to occur on small scales within the eastern North Sea adjacent to Belgium, the Netherlands and the Federal Republic of Germany. The horizontal spatial dimensions of affected areas will be of the order of 1 to 10 km. It is also demonstrated that similar disturbances on the scale of the entire North Sea will not occur as a consequence of titanium dioxide waste disposal.

5.5 Nutrient inputs to Osaka Bay

5.5.1 Statement of the management problem

Increased nutrient input into a coastal zone can result in enhanced biological production and, hence, a higher biological oxygen demand. If there is only limited flushing of the region, or strong stratification, then anoxic conditions may develop. This can result in catastrophic changes in the aquatic ecosystem. A typical question posed by environmental managers is:

> "What is the maximum rate (or amount) of nutrient discharge that can be maintained without producing anoxic conditions at all, or only in a specific area?"

This scenario requires that the oxygen concentration in the water be maintained above some threshold value for either all, or part, of the region of interest.

5.5.2 Model construction

A model was constructed (Nakamura and Nishimura, 1988) to consider the effect of discharging effluent from a sewage treatment plant into Osaka Bay, Japan. Osaka Bay is a semi-enclosed basin with one major inflow, the Yodo River. The circulation of the Bay is primarily tidal, and, the horizontal (residual) currents are significantly sheared in the vertical. The stratification of the Bay plays a major role in regulating the vertical transfer of oxygen. Observations have shown that when anoxic conditions occur; the extent of the affected area is limited in both the horizontal and the vertical directions.

Given the complexity of the circulation and biochemistry in Osaka Bay, a three-dimensional model is required to describe the processes contributing to anoxia in this system. Nakamura and Nishimura (1988) divided their study of Osaka Bay into three major steps:

1. calculation of the residual flow field;

2. estimation of the horizontal and vertical diffusion coefficients;

3. simulation of the major processes related to the development of anoxic conditions.

The specification of the circulation in the Bay was primarily derived from observations. The horizontal currents in Osaka Bay have been measured for a long time at two different depth levels at several closely spaced stations. Various assumptions on the vertical distribution of the current were then used to inter/extrapolate these current observations and the vertical velocities were calculated by assuming continuity. For these calculations, the horizontal grid spacing was 4 km x 4 km (see Figure 5.3) and the water column was divided into 5 layers with thickness of 2 m, 3 m , variable spacing, 3 m, and 2 m, respectively (see Figure 5.4).

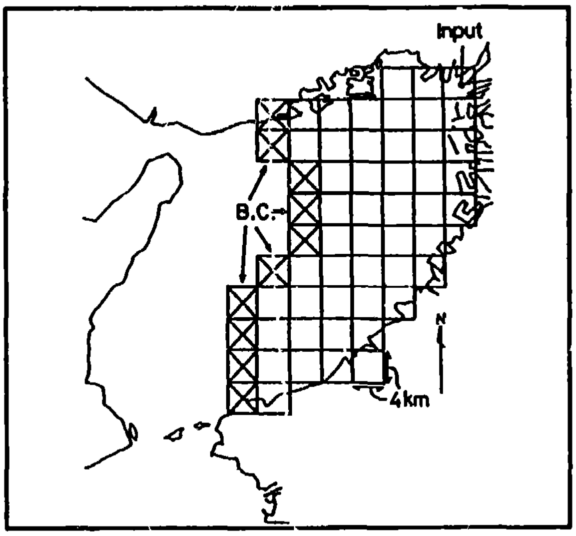


Figure 5.3. Horizontal structure of the model (Nakamura and Nishimura, 1988).

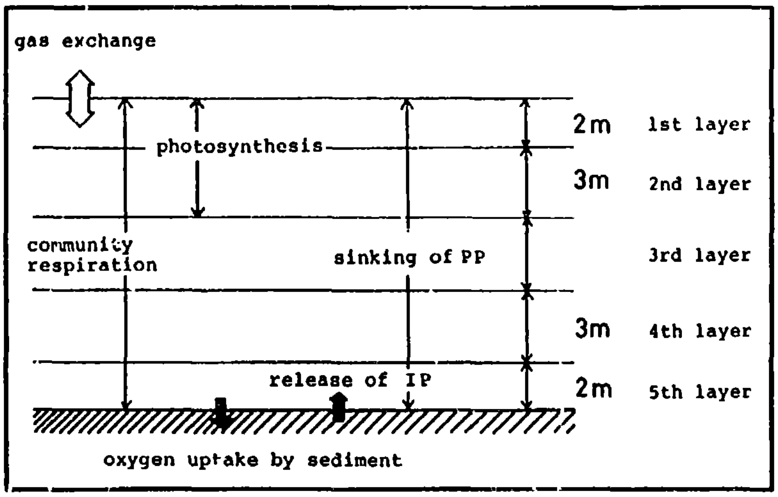


Figure 5.4. Vertical structure of the model (Nakamura and Nishimura, 1988).

The average horizontal and vertical eddy diffusivities for Osaka Bay were estimated from the simulation of observed salinity distributions in Osaka Bay. Two sets of salinity data, separated by one week, were available. The observed changes in the salinity distribution over one week were simulated using the flow field model mentioned above and estimates of the riverine freshwater input, which was also determined from field observations. Eddy diffusivities were obtained by adjusting model parameters so that the simulated salinity distributions matched the observed salinity distributions. The empirically-derived eddy diffusion coefficients were consistent with those calculated from observations by Nishimura and Nakamura (1987).

The main biological, chemical and physical processes contributing to the development of anoxic conditions are: photosynthetic production of oxygen; oxygen consumption by community respiration in water and sediment; supply of organic materials to the bottom and the oxygen demand imposed by them during decay; advection; diffusion; and exchange of oxygen at the air-sea interface. The biochemical model considered three state variables: dissolved O_2; particulate phosphorus (a measure of the phytoplankton biomass) and dissolved phosphorus (the limiting nutrient). The detailed mathematical formulations of the various processes are given in Nakamura and Nishimura (1988).

5.5.3 Example calculations

The Osaka Bay simulations were performed using a 4-hour time interval and a total simulation time of two weeks. Nutrient loads to the Bay were specified at the mouth of the Bay and from a river at the Bay centre as shown in Fig. 5.3. Phosphorus, as an inorganic nutrient, was the major concern because it is important in controlling the development of anoxic conditions in the water. The biochemical model parameter values were tuned to provide the best fit between simulated and observed dissolved oxygen distributions.

5.5.4 Additional comments

The model mentioned above allows for many numerical experiments that cover a range of possible scenarios that can produce or contribute to anoxic conditions including the one posed earlier. As an example, the simulated distributions showed that the area of anoxia in Osaka Bay could be decreased to less than one-third of the observed area when the nutrient loading was reduced by half. The Osaka Bay model was also used to determine which are the key processes in determining and controlling anoxia in the Bay, and therefore require further field measurements.

5.6 Sewage discharge near a beach

5.6.1 Statement of the management question

One of the main concerns with sewage effluent is the incidence of coliform bacteria on recreational beaches. For existing outfalls, monitoring the adjacent recreational areas becomes a necessity for public health protection. For the installation of new outfalls, it is essential to have reliable estimates of the probable mean concentration distribution of coliforms as a function of travel time or distance from the source outlet.

A number of questions arises: For example, under what tidal, wind or offshore current conditions would the effluent plume impact the beach, violating the water quality standard? How frequently could these conditions occur and how could they be remedied by controlling the discharge rate or by imposing chlorination? Where should the monitoring sampling sites be located? Where and how deep should the new outfall be installed? As discussed in Section 2.2, these questions dictate the choice and complexity of models required. While it is not possible to cover all questions, we can examine several methods used to construct models and focus on their potential merits and pitfalls in providing answers to some of the above questions.

5.6.2 Model construction

While there are known effects of temperature, dissolved organic carbon, detrital carbon and nutrients on bacterial activities in the ocean (Colwell and Morita, 1974), most coliform models use a simple, first order, biological decay (or growth) rate, λ, to simulate the net decay (or growth). The simplest model for coliform distributions in a 'closed' coastal region with volume V, outfall discharge rate Q and initial concentration C_o is

$$V \frac{dC}{dt} = Q - \lambda VC \qquad (5.10)$$

where λ is a simple, first order, net decay rate for coliform bacteria.

Solution of equation 5.10 gives an expression for the coliform concentration C, at time t, as

$$C = \frac{Q}{\lambda V} + [C_o - \frac{Q}{\lambda V}]\, e^{-\lambda t} \qquad (5.11)$$

Which at steady state (t=o) reduces to,

$$C = \frac{Q}{\lambda V} \qquad (5.12)$$

As a first approximation, equations 5.11, cf. 5.8 or 5.12 provide the mean concentration using a zero-dimensional approach. The far-field hydrodynamic model is a closed, homogenous box. It is certainly unrealistic and could not answer, for example, the question about where the outfall should be located. It assumes that the concentration is uniform, i.e., the concentration at the beach is the same as everywhere else. Therefore, equations 5.11 or 5.12 can only give a crude approximation of the concentration at the beach if the volume, V, is appropriately chosen. The equations represent, to a limited degree, the dependence of the coliform concentration on the outfall discharge rate, the decay rate and the volume of the coastal zone.

By increasing the dimensionality of the hydrodynamic model, one can obtain better spatial resolution. For example, one can simulate the straight plume formed by releasing an effluent from an outfall in a strong, along-shore current with velocity u in the x-direction by assuming a steady-state balance between advection, cross-flow diffusion (diffusivity of K_y in the y-direction) and the decay of coliform bacteria, so that

$$u \frac{\partial C}{\partial x} = \frac{\partial}{\partial y} [K_y \frac{\partial C}{\partial y}] - \lambda C \qquad (5.13)$$

Turbulent diffusion can be parameterized, for example, by a shear diffusion law (Lam et al., 1984)

$$K_y = q_y \sigma_y \tag{5.14}$$

where q_y is an empirical diffusion velocity and σ^2 is the variance of the concentration in the cross-flow direction y, (i.e., $\sigma_y = q_y x/u$). The steady-state concentration is then given by (Lam et al., 1984):

$$C(x,y) = \frac{C_o}{2} \left[\text{erf}\left(\frac{b-y}{\sqrt{2}\,\sigma_y}\right) + \text{erf}\left(\frac{b+y}{\sqrt{2}\,\sigma_y}\right)\right] e^{-\lambda x/u} \tag{5.15}$$

where erf is the error function, C_o is the initial concentration at the outfall and b is the width of the outfall.

In this case, the model provides more spatial details such as the plume shape and the linkage of the concentration to the outfall width. At least, then, the concentration at the beach is dependent on the location of the outfall. However, there are still major drawbacks, such as the beach boundary is undefined (the model assumes the domain to be a semi-infinite plane) and the flow and concentration fields are assumed to be homogeneous in the vertical direction. Nevertheless, the model (Equations 5.13-5.15) may provide approximate answers for questions that the zero-dimensional model (Equations 5.10-5.12) cannot answer. For example, what is the spatial distribution of the probable mean concentration under different flow speeds and directions?

5.6.3 Example calculations

Figures 5.5 and 5.6 show the mean dilution contours near an outfall in the coastal zone for two typical climatological episodes with strong and weak currents respectively. The contours are computed (Lam et al., 1984) by the two-dimensional (x,y) plume model (Equations 5.13-5.15) with $\lambda=0$, $K_y=1000\ \text{cm}^2\text{s}^{-1}$ and a layer thickness of 1 m, using hourly currents observed over a month in each episode. The dilution shown is derived from the average of the computed concentrations for these currents.

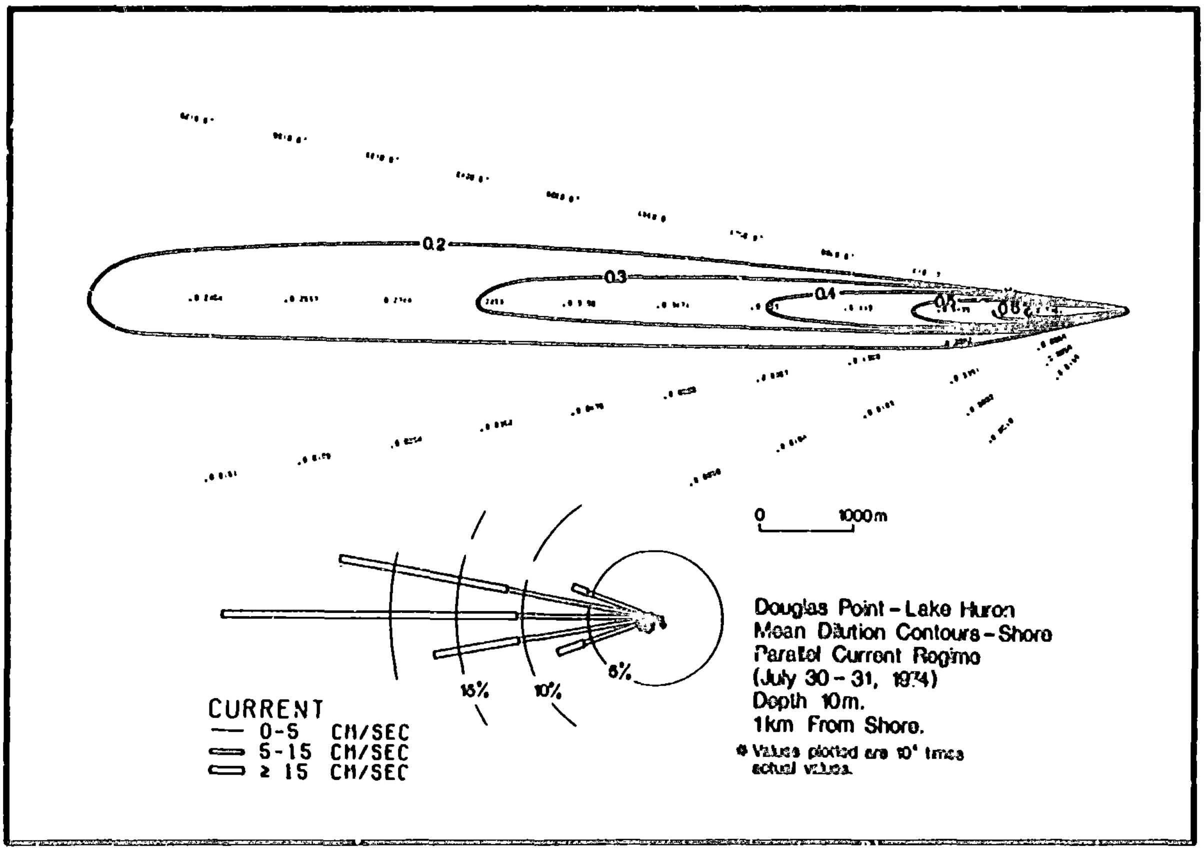


Figure 5.5. Simulated effluent concentration using an analytical model for a along-shore current regime, near Douglas Point, Lake Huron (Taken from Lam et al., 1984).

The freqency distribution of the current, in both direction and magnitude, is shown in the current rosette (Figures 5.5 and 5.6) These figures show clearly that, even at the same location, seasonal changes in the current field may distort the concentration field significantly. Thus, for proper construction of the model, accurate measurements of the current and the coliform decay rate and an appropriate choice of the parameterization (Equation 5.14) for the cross-flow turbulent diffusivity are required. These may require a set of physical and biological experiments.

A good example of incorporating these physical and biological measurements into the construction of a coliform model for a marine outfall is presented in Stewart et al. (1971). In their model, submerged

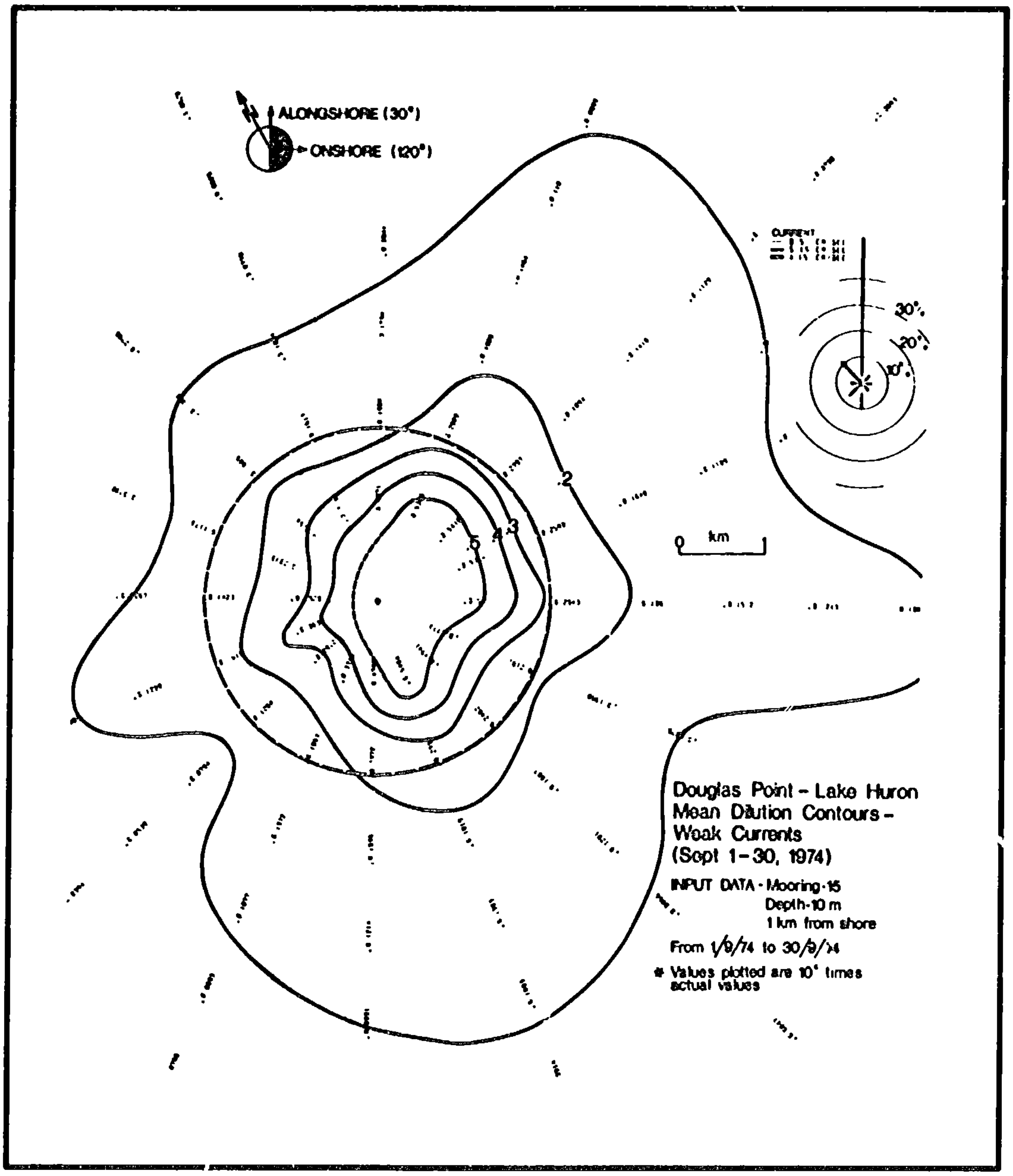


Figure 5.6. Simulated effluent concentrations using an analytical model for a weak current regime, near Douglas Point, Lake Huron (Taken from Lam et al., 1984).

outfalls were considered and therefore vertical diffusion (vertical diffusivity, K_z) was included in the model equation

$$u \frac{\partial C}{\partial x} = K_y \frac{\partial^2 C}{\partial y^2} + K_z \frac{\partial^2 C}{\partial z^2} - \lambda C \tag{5.16}$$

through a series of physical experiments on current and dye diffusion near the outfall. They found that the cross-flow standard deviations σ_y and σ_z follow some empirical power law in x of the form

$$\sigma_y = \sigma_{yo} (1 + \frac{x}{x_o})^m \tag{5.17a}$$

$$\sigma_z = \sigma_{zo} (1 + \frac{x}{x_o})^n \tag{5.17b}$$

where m and n are empirical constants and x_o is the distance of the displacement upstream from the virtual point source of strength Q. Here, σ_{yo} and σ_{zo} are standard deviations of the plume width where

$$K_y = \frac{u}{2} \frac{d\sigma^2_y}{dx} \quad \text{and} \quad K_z = \frac{u}{2} \frac{d\sigma^2_z}{dx} \tag{5.18}$$

Based on these empirical diffusion characteristics and the results of a parallel coliform study, die-off curves for coliform counts were constructed and the net coliform decay rate, λ, determined. These results lead to the analytical solution for Eq. (5.16) assuming the absence of boundaries:

$$C(x,y,z) = \frac{Q}{\pi u \sigma_y \sigma_z} \exp[- \frac{1}{2} \frac{\lambda x}{u} (\frac{y^2}{\sigma^2_y} + \frac{z^2}{\sigma^2_z})] \tag{5.19}$$

This model may be used to answer the question of how deep the submerged outfall should be placed in order to meet a given water quality standard for coliform counts in coastal waters. Of course, the use of equation 5.18 for vertical diffusivity is questionable but it is a necessary step to deal with questions relating to the depth of the outfall. By including more spatial resolution, however, the model requires more parameterization. For example, the empirical constants m and n are site-specific. There are also other shortcomings, namely:

(1) The model neglects the representation of a lateral boundary, e.g., a beach, which is of central importance in practical applications;

(2) In a shallow region, bottom topography will have a significant influence upon the solution, developed above, which is based on an assumption of an infinite medium;

(3) The solution is restricted to a homogeneous sea region. In some applications, for example, vertical stratification or the presence of a front, will modify the model, in particular, the parameterization of the diffusion coefficients;

(4) A unidirectional background velocity field is assumed. In a physically-realistic environment, horizontal and vertical circulation patterns are common;

(5) The model assumes a steady state situation; in many cases a time-varying solution will be required, for example, in dealing with spills; and

(6) A bottom boundary condition, reflecting the interactions between the coliform and the benthic biota.

An accurate model to cope with these detailed features requires the inclusion of more processes in the model equation and more complex boundary conditions. Generally, it is difficult to derive analytical solutions for these equations with physically-realistic lateral and vertical boundary conditions. Hence, at the beach, a range of numerical boundary conditions must be incorporated. The simplest of these is the assumption of a solid reflective wall at the beach. Other more complex dynamical boundary conditions, reflecting the movement of water across the beach, can be incorporated using a Lagrangian approach. Similarly, at the sea bed, a simple boundary condition on the flow field would involve the use of a drag coefficient to retard the flow or a more complex representation of energy loss through a turbulence energy model. For the coliforms, a boundary condition incorporating an appropriate source or sink term would also be necessary.

5.6.4 Additional comments

The solutions to these equations are generally approximations defined on a system of spatially discretized grid points or nodes, as opposed to a continuous concentration field as defined in the analytical models (e.g., eq. (5.19). As mentioned in Chapter 2, the hydrodynamic model needs to be constructed first. Then, depending on the choice of the biological and chemical/geochemical component, the contaminant transport model is contructed using the computed currents and, probably, though not always necessarily, the same model framework (i.e., model dimensions and numerical grid). In the present case, since the coliform kinetics are based on a simple net decay representation, the major portion of model development will be centered on the hydrodynamic component.

Section 3.2 has provided ample discussion on the choice of model dimensionality for the hydrodynamic model. After this choice is made, one may obtain the hydrodynamic information by either the diagnostic approach or the prognostic approach. Both methods require the support of observational data. In the diagnostic approach, observed current data must be obtained first, particularly for those sites near areas of interest, e.g., the outfall and the beach. These are interpolated over a chosen system of spatial grid points. The interpolated currents are then adjusted by minimizing a residual function requiring the currents to satisfy mass continuity, or momentum conservation, as well as the no-flow condition normal to the beach. By using the adjusted currents, the concentration can be calculated over the grid system, including the coastal area near the beach. For example, Lam and Durham (1984) used this approach to simulate a discrete release from an outfall to coastal waters. This method requires, however, continuous monitoring of currents at the chosen sites. To avoid such major dependence on observed currents, the diagnostic currents can be correlated with other observed data such as wind, tide and offshore currents. An example is the method by Murthy et al. (1986) in which the wind data are used as model inputs.

The prognostic approach is the most frequently used method. Instead of interpolating or correlating observed currents to generate the flow field, model equations governing the conservation of mass, momentum and energy are used to predict the flow field. Observed currents are required only for calibration of model parameters and validation of computed results. While the principles of conservation are the same in all hydrodynamic models, they differ in many aspects, such as dimensionality, parameterization, boundary treatment and numerical methods. For example, some use the finite difference method (Simons, 1980); and others the finite element method (Davies, 1982b). Typical model inputs include meteorological time series of quantities such as wind, solar heat, air temperature, pressure, and typical model outputs are water level, salinity, temperature and currents.

The water level is important in relation to tidal currents and the definition of the beach boundary. Water temperature and salinity are equally important for defining the position of the pycnocline, under which deeply submerged outfalls may be located. The water temperature is also an important influence on coliform growth and decay (Stewart et al., 1971). If a more accurate model on coliform kinetics is to be constructed, the decay rate, λ, should become a function of many factors including temperature, ultraviolet irradiation, detrital carbon concentration. One should also consider the use of a growth function embodying these and other factors (Colwell and Morita, 1974). Separation of the total coliform into different species, or the inclusion of other bacteria/viruses, would require even more substantial observational information for model construction. These complicated modelling attempts would probably enhance our scientific understanding of the microbial activities in the ocean, but their practical use for answering typical management questions is cost-prohibitive and would actually lead to greater uncertainty.

In summary, most coliform models use a simple decay rate function. Differences among them mainly lie in the choices of the hydrodynamic model and the means of parameterizing the turbulent diffusion. Similar models can be used for simple radionuclides such as tritium. Simple models are not necessarily useless; complicated ones not always useful. The choice is based, inter alia, on a balanced consideration of whether the model can provide a sufficiently accurate answer, whether the experimental effort required by the model is cost-effective, and whether there exists the expertise to develop and maintain the model.

5.7 Model for the Dutch North Sea water quality management plan

5.7.1 Statement of the management problem

In May 1982, the Dutch Government presented an official note to Parliament entitled "Harmonization of North Sea Policies". As a consequence, a study was commissioned to formulate a water quality management plan for the Dutch Portion of the North Sea (Figure 5.7), and

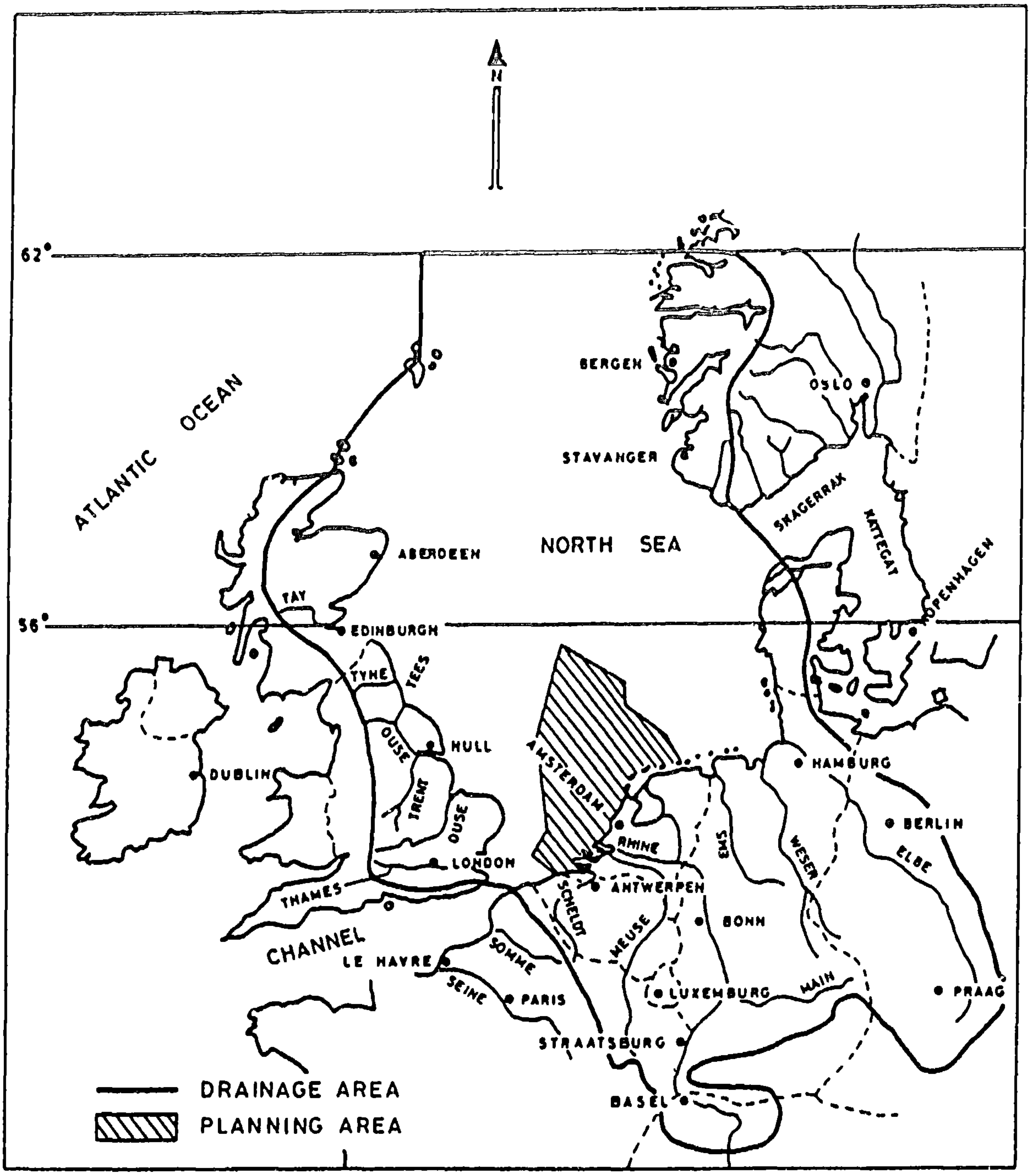


Figure 5.7. North Sea and Planning area Dutch Water Quality Management Plan.

the results of this study are presented in Delft Hydraulics (1985). The general objective of the Dutch North Sea water quality management plan is stated as:

> "To maintain or to obtain a water quality in the North Sea, which enables preservation of the ecological values, thereby taking into account societal demands for the production of goods and services from the North Sea."

Given the general objective and in view of observed effects on various biological species, particularly in the Dutch sector of the North Sea in recent decades, it was concluded that the analysis should mainly consider the problems of : (1) heavy metals in relation to concentration in both water column and in sediments, (2) euthrophication as a result of nutrient inputs, (3) and the resulting possible effects of both aspects on the species.

This case study concentrates on the input of cadmium, mercury, lead, copper, chronium, zinc, phosphorus, and nitrogen into the Dutch sector of the North Sea. Although these substances do occur in both dissolved and particulate forms, only total (dissolved + particulate) concentrations are considered. In this way, the complex interaction between dissolved and particulate forms due to physical, chemical, and biological processes do not need consideration. Particulate forms, however, can settle to the bottom, a process which is neglected in this analysis. A review of the Dutch North Sea model and comparisons of the results obtained with this model with those obtained from other models is given by Taylor (1987).

5.7.2 Model construction

The source of discharges are grouped as direct and combined sources. Direct sources include coastal outfalls, dumping of industrial wastes, sewer sludges and dredging spoil, burning of industrial wastes, and marine transport. Combined sources include river inputs, influx through the open sea boundaries, and influx from the atmosphere. For each of the sources estimates are made of the substances and quantities released, based on data available in literature. All estimates relate to the reference year 1980.

The major assumptions made in this study are:

- mass transport calculations are based on tidally-averaged residual flows,
- atmospheric deposition rates for the Dutch coastal zone are applied to the whole North Sea area,
- water from the English Channel and the Atlantic Ocean has a reference concentration (none, or very limited, human influences),
- river discharges and loads are assumed to be constant during the year,
- the contaminants are conserved in water
- stratification is neglected,
- only total concentrations in the water are taken into account.

An important consequence for the last assumption is that no sediment transport model is required, though the long term development of concentrations in bottom sediments was studied for a small part of the area using residual flow data and measurements. These assumptions call into question the suitability of the model, as originally designed, to answer these additional questions posed by management.

5.7.3 Example calculations

The discretized model grid for the portion of the North Sea considered in this study is shown in Figure 5.8. The grid dimensions were 10 km x 10 km. Up to 20 river inflows and water discharge locations are specified with a total discharge of 5.8×10^3 m^3 s^{-1}. Characteristic winter and summer situations were simulated, and the residual flow for winter conditions is given in Figure 5.9, as an example. The residual flow field is obtained from averaging the results of a time-dependent tidal flow model over a tidal period (Gerritsen, 1983).

The calculated residual flows obtained from the hydrodynamic model were then used in, an advection-diffusion equation with source and sink terms to compute the spatial distribution of the concentrations of substances, the contribution of sources to the distribution of water masses and the concentration of substances, and the retention time or age functions of water masses. Thus, the model provides estimates of the spatial distributions of water masses for inflowing water from different sources and the age of a given water mass. All model results are stored

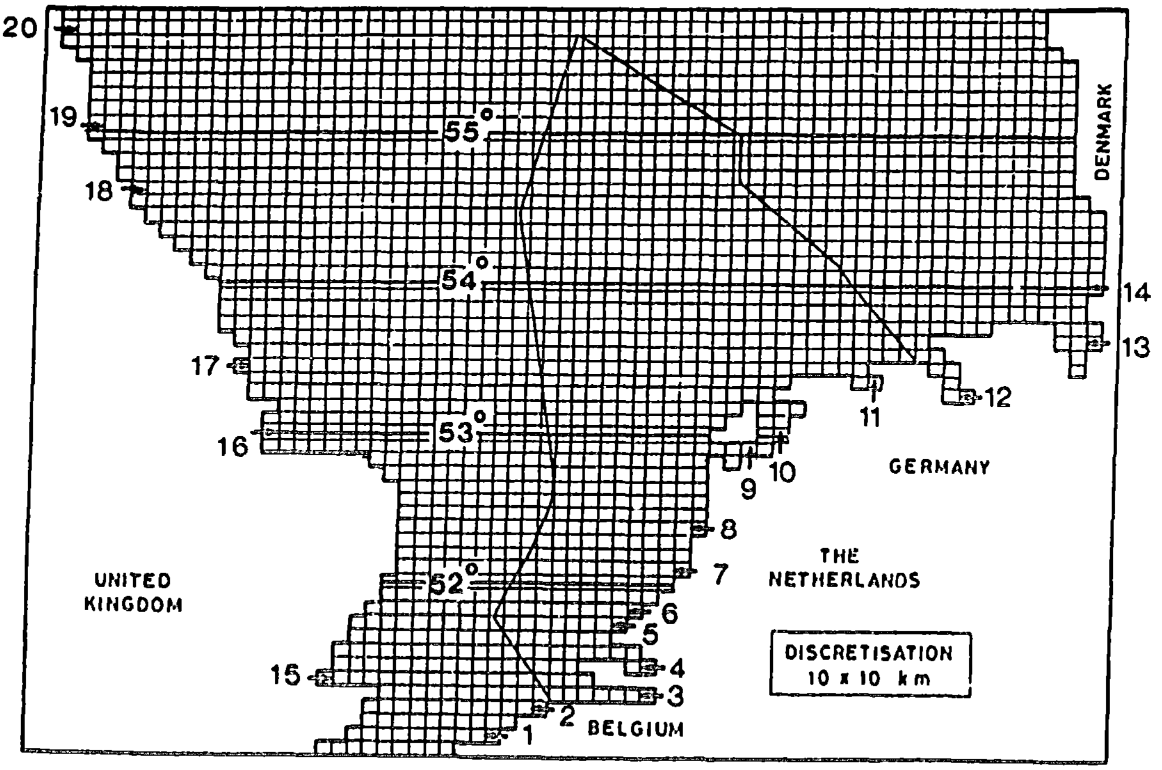
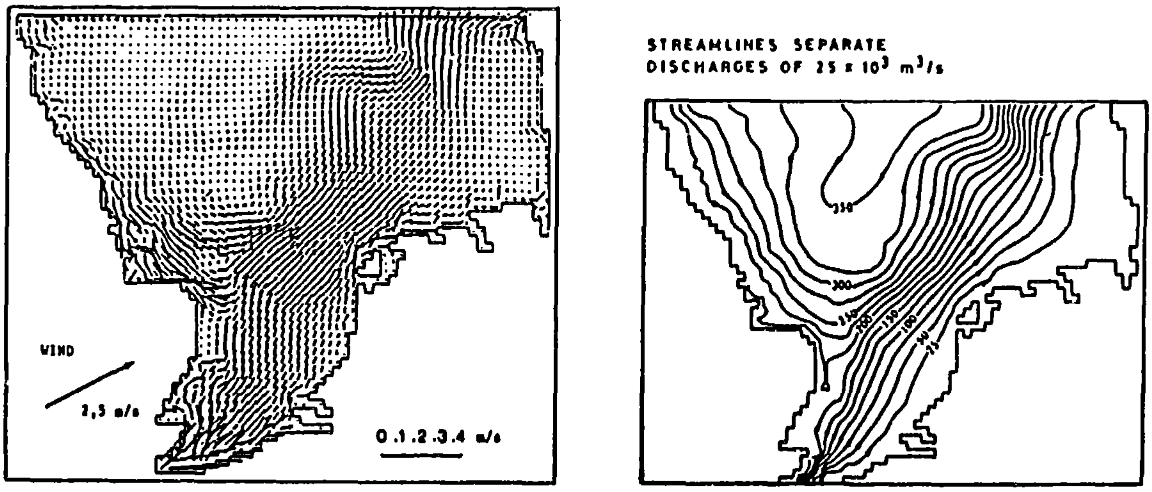


Figure 5.8. Model schematization ESTFLO-DELWAQ: grid and location of river inflows.

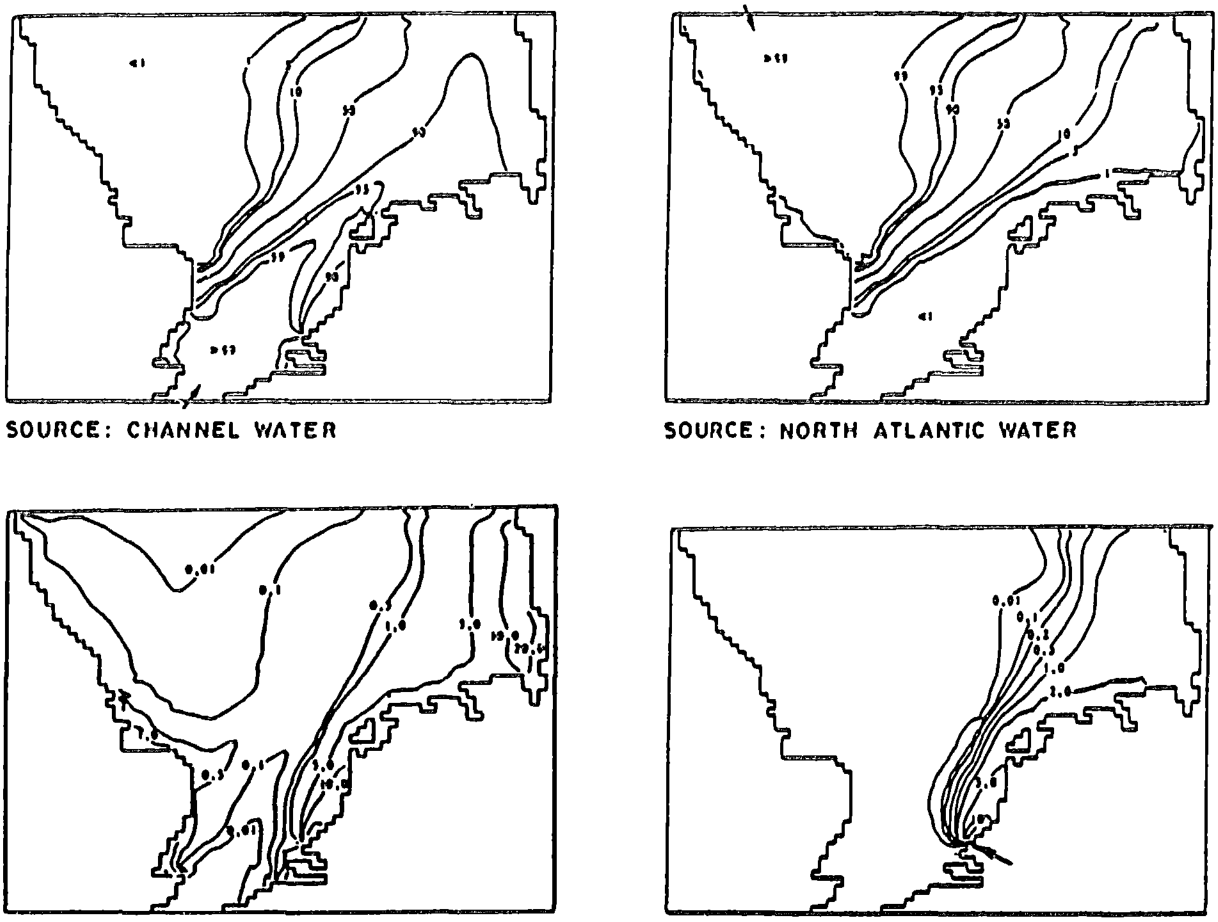


WATER TRANSPORT VELOCITIES OF RESIDUAL CURRENTS

RESIDUAL WATER FLOWS

Figure 5.9. Residual flow for winter conditions.

in a data base and the actual concentration of substances is subsequently determined by multiplying the actual fraction of a certain source of water with the source concentration. Figure 5.10 represents the spatial distribution for winter conditions for four sources of water.



SOURCE: CHANNEL WATER

SOURCE: NORTH ATLANTIC WATER

SOURCE: RIVER WATER

SOURCE: RHINE WATER

Observations:
- Calculations made for winter conditions
- numbers represent fraction in % of locally present water, originating from respective sources

Figure 5.10. Spatial distribution of water masses for inflowing water from different sources.

5.7.4 Additional comments

The biological cycling processes are modelled to evaluate the potential influence of increased nutrient concentration on primary production, phytoplankton biomass, and on species composition. A numerical model, SEAWAQ, is used, which describes the carbon and nutrient (Si, N, and P) cycles (Delft Hydraulics, 1984). The state variables simulated are: phytoplankton, suspended detritus, bottom detritus, and dissolved nutrients. Though interesting results are obtained concerning the relation between nutrient loadings of the North Sea, total biomass, and species differentiation it is difficult to assess the relevance of the results.

From the transport model simulations it is possible to estimate the various factors contributing to the total concentrations in the North Sea. The anthropogenic fractions of different substances can be inferred for winter and summer conditions. De Ruijter et al. (1987) have produced a transport atlas with graphical representations of the results that can be displayed on a personal computer. This enables the manager to change the magnitudes of specific sources and derive a visual presentation of the results.

Obviously, more refined modelling is required before all relevant processes in the North Sea can be modelled with the degree of confidence required for studying management scenarios. Nevertheless, this study has shown that some important questions can be answered with existing models.

5.8 Radioactive discharges from a nuclear reprocessing plant

5.8.1 Statement of the management problem

There are only a small number of nuclear reprocessing plants in the world, such as Sellafield in England and La Hague in France. A different mix of radionuclides are discharged from these reprocessing plants depending on the type of fuel being reprocessed. This section will deal with the discharges from the Sellafield nuclear reprocessing plant into the eastern Irish Sea that have been taking place, under authorization, for 30 years.

The Irish Sea is a semi-enclosed sea connected to the Atlantic Ocean via St George's Channel in the south and via the North Channel and the Malin Shelf in the north. The area is effectively divided into two regions to the east and west of the Isle of Man. The western portion consists of a deep channel (> 100 m) whereas depths in the eastern Irish Sea are generally less than 30 m. The sea bed is mainly sandy, but there are two mud patches, one off the English coast near the Sellafield outfall and one in the deep channel between the Isle of Man and Ireland. The residual flow through the Irish Sea tends to be from south to north. A more detailed description can be found elsewhere (Pentreath, 1985).

The management question is: what are the dose rates to members of the public from past and present discharges of radioactivity into the Irish Sea, both now and in the future?

5.8.2 Model construction

This question clearly identifies the exposure model which has been discussed in many documents by ICRP and IAEA. This requires that the dispersion model be able to predict the concentration of radioactivity in sea water, on sediments and in biota. The latter concentrations for fish and shellfish are normally calculated using a concentration factor approach which relates the radionuclide concentration in the fish or shellfish to that in filtered sea water. The model requires a hydrodynamic model, and, as many radionuclides are scavenged by suspended particulate material, a sediment transport model. The observations reveal that a large amount of the activity for the particle-reactive nuclides is incorporated into the muddy sea bed off the Sellafield pipeline, and that, as discharges have decreased, this may now be becoming an important secondary source of radionuclides (Woodhead, 1988).

Consequently, a benthic transport model is necessary, particularly for the particle-reactive radionuclides. The partitioning of activity between water and particles is normally described by an equilibrium partition coefficient (K_d) but some modellers have used first order kinetics (Howorth and Kirby, 1988). This is far more expensive in computer time but does not appear to produce significantly different results.

The other constraint the management question imposes on the model construction is that of timescales. Dose rates are calculated from annual exposures to radiation through different pathways, either internal exposure, such as that resulting from the consumption of fish and shellfish, or external exposure, such as from beach sediments. Thus, the model needs to predict integrated annual concentrations over periods of many years. Highly-sophisticated, high-resolution, three-dimensional hydrodynamic models, with sediment transport could probably do this but the cost of integrating such models forward for a century would be very high and the accuracy of the result would not necessarily be compatible with the data used in the exposure model. Simpler models will usually suffice.

The simplest models which can describe all the processes are box or budget models. In these, the Irish Sea is divided into one or several regions (boxes) and the amount of radioactivity entering and leaving each region (box) is calculated. In this way, inputs are balanced by losses by advection to other regions, radioactive decay and removal to the sea bed. In each box, this balance can be represented by equations such as:

$$\frac{d N_i}{dt} = \sum_{j \neq i} (k_{ji} N_j - k_{ij} N_i) - \lambda N_i + S_i \qquad (5.20)$$

rate of change in box i	inputs from neighbouring boxes	losses to neighbouring boxes	radioactive decay	external sources

where N_i is the number of atoms of the radionuclide in box i, k_{ij} is the fractional rate of transfer from box i to box j, λ is the radioactive decay rate and S_i are all external sources in box i whether from discharges or ingrowth from the parent radionuclide.

Assuming equilibrium partitioning between water and sediments, N_i is related to the water concentration C_w in box i by

$$C_w = \frac{N_i}{V_i(1 - f + K_d \rho f)} \qquad (5.21)$$

where V_i is the volume of the box, f is the volume fraction of particles in the box, K_d is the equilibrium partition coefficient (in units of volume per mass) and ρ is the dry density of the particulate material. These equations (5.20) can be solved for N_i by any number of standard methods. If, as frequently happens, the coefficients are such that the equations are 'stiff', that is, the solution has widely different time constants, then a suitable stiff equation solver (e.g. NAG, 1987) will be needed to save computer time.

The coefficients, k_{ij}, in equations 5.20 disguise many of the problems in setting up a model of this sort. If we ignore all sediment interactions, then the k_{ij} simply represent the advection and diffusion of radionuclide between the different regions.

To demonstrate how to construct k_{ij}, consider two boxes with a flow u $m\ s^{-1}$ from i to j through an interface area, A m^2, and an eddy mixing coefficient for the water, κ $m^2\ s^{-1}$. The number of atoms advected from i to j is

$$\frac{uA}{V_i} N_i$$

The number of atoms moved from i to j by water mixing is related to

$$- \kappa \frac{\partial C}{\partial x}$$

where $\frac{\partial C}{\partial x}$ is the concentration gradient, which can be

represented by $\left(\frac{N_i}{V_i} - \frac{N_j}{V_j}\right) / D$,

where D is a suitable distance over which to evaluate the gradient.

Thus the amount mixed from i to j is

$$\frac{\kappa N_i}{D\ V_i}$$

and from j to i is

$$\frac{\kappa N_j}{D\ V_j}$$

Hence the total loss from i to j is

$$\frac{uA}{V_i} N_i + \frac{\kappa N_i}{D V_i}$$

and so k_{ij} is

$$\left(\frac{uA}{V_i} + \frac{\kappa}{D V_i}\right)$$

and k_{ji} is

$$\frac{\kappa}{D V_j}$$

The values of u and κ need to be determined from observation and D and A are dependent on the box sizes and configuration. Such formulations for the coefficients k_{ij} can be extended to erosion of sediment from the sea bed and deposition on the sea bed, and mixing within the sea bed. One important consideration in all of this is that the mass of particles is conserved. This is especially important between two boxes which have widely differing particle concentrations such as the sea bed and the overlying water column. In this extreme case, a unit volume in the overlying water contains a large proportion of water and a small proportion of particles, whereas the sea bed has the reverse conditions. Typical expressions for the sea bed exchanges, ignoring pore-water exchanges, are from water to sea bed

$$\frac{r\ A}{V_i} \quad \frac{K_d}{(1 - f_i + K_d \rho f_i)}$$

and from the seabed to the water

$$\frac{eA}{V_j} \quad \frac{K_d}{(1 - f_j + K_d \rho f_j)}$$

where r is sediment deposition rate (kg m^{-2} s^{-1}), e is the sediment erosion rate (kg m^{-2} s^{-1}) and subscript i refers to the water box and j to the seabed box. These resuspension and deposition rates have to be determined by observations (Kershaw et al., 1988). Similar problems arise in the water column when the model uses non-uniform, but constant, in time, suspended concentrations. However, these can be overcome (Gurbutt and Kershaw, 1989).

5.8.3 Additional comments

There have been many box models of this type which have been used to describe dispersion of radionuclides from Sellafield (Camplin et al., 1982; Hallstadius et al., 1987), but most have only dealt with ^{137}Cs which is only slightly scavenged (low K_d) by suspended particles. It is not until one has to deal with the actinides which have high K_ds that a suitable sediment description is necessary.

The simplicity of the box model equations (5.20) is balanced by the difficulty in defining the exchange coefficients. The alternative to this is to solve the advection/diffusion equation, with some pre-defined water circulation pattern (Prandle, 1984; Hainbucher et al., 1987). In this way all the coefficients for water exchanges are easily determined from the flow data and all that one is left which is describing the sediment interactions. These can be included by adding a box model, using constant, but non-uniform, suspended sediment loads (Howorth and Kirby, 1988) or by solving the sediment transport equations with the hydrodynamic equations (Onishi and Thompson, 1984).

As is clear from chapter 4, the art of parameterizing sediment transport, especially if the sediments are cohesive, is still in its infancy and much work needs to be done in determining suitable response functions for sediment pick-up under bed stresses predicted by the hydrodynamic model. Also these more sophisticated models are more expensive to run than the box models, and it may be difficult to use them for long predictive simulations.

5.9 Overall observations

All the models described here have been presented in the context of specific management questions or objectives. Some of these management questions are based on hypothetical needs, others on real demands for answers to specific problems. It should be stressed that only where the management question has been posed in specific terms, and consequently the nature of the limits of exposure have been defined, can a clear understanding of the requirements of appropriate dispersion models be gained. This explains the difficulty of generalizing both the construction of models and the parameterization of processes that are discussed respectively in Chapters 3 and 4. As can be observed from the case studies presented here, models can often be conceptually simple and yet adequately meet the management demands even if some conservation has to be introduced to allow for uncertainty.

The case studies can be considered only as examples of model construction ranging the simple to the complex. Some of these are hypothetical, and some pertain to real management questions. Clearly, the extrapolation of these models to real circumstances depends crucially upon the compatibility between the questions attached to the case studies here and those posed for actual situations. The main reservation concerning these case studies is that few have been subjected to rigorous quality assurance procedures as discussed in the following chapter.

6. QUALITY ASSURANCE PROCEDURES

6.1 Introduction

A mathematical model is, at best, an approximate representation of the real world and, hence, its predictions are inherently uncertain. This uncertainty results from a lack of knowledge of the full set of equations and an inability to solve them; therefore, approximations have to be made that involve the use of parameterizations of the processes. Uncertainty also arises from errors in observational data used to derive input and parameter values, i.e., the initial state of the model and the boundary conditions. In addition, there may be problems with the accuracy of the computer code and the method of solving the numerical description of the mathematical model. All these need attention when determining the accuracy (error bars) of model predictions that is the subject of this section (for a more detailed discussion see IAEA, 1988b).

In this chapter we consider model verification (i.e., checking that the mathematical equations are being solved correctly), model sensitivity (i.e., understanding the model response to changes in input data, parameter values and parameterisations) and model validation (i.e., establishing the agreement between predictions and observations). The process of model calibration, interpreted as tuning the parameter values to a given data set, has been subsumed in the discussion of model sensitivity.

6.2 Verification

At an early stage in model development, it is necessary to check that the computer code is correct (i.e., "bug free" in computer terminology). Thisis not a trivial task in the case of a complex numerical model with many tens of thousands of lines of coding. Additional complications arise because solutions of the various partial differential equations in the model are solved wholly by numerical methods. The major task here is to ensure that the numerical method, developed to solve the partial differential equations, is sufficiently rigorous that it will provide an accurate solution of these equations under a range of physical/chemical/biological conditions. This can be particularly difficult since most numerical solutions are prone to error in regions where the gradient of the predicted property is strong. In some cases, the occurrence of such gradients can be anticipated, e.g., high velocity gradients in shear boundary layers and high concentration gradients close to the source of a contaminant discharge. However, in many cases, the occurrence of gradients cannot be anticipated and they may also evolve with time, e.g., front formation (and its tidal advection) and thermocline formation including their movement with internal waves, breakdown under wind events and their subsequent reforming at low wind speed and sustained solar heating. The development of numerical techniques and advanced supercomputing, which can provide an accurate solution of the coupled partial differential equations representing the processes in the model, is currently in its infancy.

Model verification is a particularly important first stage in model development. At this stage the model is tested to ensure that there are no errors in the computer coding and the numerical solution. Ideally, numerical solutions need to be compared with analytical solutions; however, for most complex problems no analytical solutions exist. Nevertheless, it is usually possible to test separate parts of the entire model against either analytical solutions or accurately-known numerical solutions. Only by this means can confidence be established in the accuracy (meaning the degree to which thenumerical solution approximates the true solution of the partial differential equations) of the model. Regrettably, this important stage in model development is frequently omitted in the construction and application of many numerical models. Once verified, the numerical model is deemed a proper representation of the mathematical formulation although, inevitably, the mathematical model is a gross approximation of the real system.

6.3 Sensitivity analysis

Having verified that the model can accurately compute the solution of the partial differential equations, the subsequent stage of model validation (that determines whether the model accurately reproduces conditions in the 'real world') can be considered. A significant part of model quality assurance, which also gives some insight into the predictive capability of the model, is a model sensitivity study. In essence, there are two distinct components of sensitivity analysis; the first deals with sensitivity to input data and conditions, and the second involves sensitivity to parameterizations.

The first is to accept the model as formulated (knowing that certain terms in the hydrodynamic equations have been approximated and other complex processes reduced to simple parameterizations) and test the sensitivity of model output to variations in the input data (usually based on variations in field observations). The range of variations in the input data can be determined from a knowledge of variations and estimated errors in the observed data. Such an exercise, often called uncertainty analysis (IAEA, 1988b), is particularly revealing both in terms of establishing the sensitivity of the model and in identifying crucial field observations. If the sensitivity study reveals that the model result is critically dependent upon the precision and accuracy of certain measurements, then effort must be made to reduce the error in these measurements. If, for example, the model shows that representation of processes and boundary conditions at one geographical location has a larger effect upon model output than at others, then an observational programme can be designed to sample more intensely in the critical area.

The second component of the sensitivity analysis involves the various assumptions which have been made in developing the model. The major difficulty here is related to the problem of the parameterization of small-scale processes (e.g., in particular, mixing processes in the hydrodynamic part of the model and comparable small-scale processes in the biological model) that cannot be resolved explicitly within the numerical model. Consider, for example, the parameterization of mixing processes in the hydrodynamic model. Physically, these processes are associated with turbulent motions in the fluid. The mechanisms producing this turbulence and its intensity are poorly understood; however, they are clearly related to larger-scale physical phenomena. In this context, bed roughness determines near-bed turbulence; shear across the thermocline/pycnocline enhances mixing; and wind/breaking wave activity at the surface is a major source of upper-ocean turbulence. The representation of such processes, and similar biological and geochemical processes, in a water quality model is particularly difficult. On the one hand, they can be parameterized by a single coefficient e.g., a diffusion coefficient; on the other hand, they can be represented in a hydrodynamic model by a complex system of turbulence energy equations. In any true sensitivity study, a range of formulations/parameterizations of these mixing processes must be considered. If such a sensitivity study shows that contaminant distributions are sensitive to the formulation of mixing parameters (this is usually the case), then a confidence limit can be placed upon the model based upon the accepted range of parameterizations of the mixing process. In the unlikely event that a sensitivity analysis reveals that the model is insensitive to the formulation of mixing, then only the simplest formulation of this process is required. (Naturally, similar conclusions hold in the biological and geochemical parts of the model.) However, in reality, the major problem arising in a sensitivity analysis of an 'all-encompassing' model is that, in certain circumstances, results may be insensitive to one part of the model. In other circumstances, the formulation of this same part of the model may be critical. Such a finding obviously leads to a conclusion that, in practice, a range of models are required. Each model needs only to embody those processes that are essential for providing accurate answers to the specific questions raised. In most applications, this conservative approach to modelling is to be preferred. By contrast, an 'all-encompassing' (and hence complex) model, designed to cover every conceivable situation, is rarely constructed because of the requirements for immense computer power, a large body supporting field data, and the problems imposed in conducting a comprehensive sensitivity analysis.

6.4 Validation

The ultimate test of a model's usefulness in a waste management application is its ability to accurately predict contaminant distributions at appropriate interfaces with the effects model. At first sight the ability of a model to reproduce a given data set would appear to be a good guide to its predictive capability. However, some care must be taken in reaching this conclusion. If a sensitivity analysis has revealed that the model is sensitive to variations of a poorly-known parameter, and a good fit between model and observations has been achieved by adjusting this parameter, then the model may then legitimately be regarded as a 'tuned', or highly-calibrated, model. Ideally, such a model should be able to produce similarly accurate results under similar conditions elsewhere; but in practice, such a model is probably neither transportable nor robust. The conditions under which the model may be applied, providing confidence in the answers, should then be stated.

Naturally, the user must be aware of how extensively a model has been validated before it can be used (Sonzogni, 1986). If the model can reproduce various observational data obtained under a large range of physical conditions without adjusting parameterizations, the model can be regarded as transportable. It may therefore be applied with confidence over a wider range of situations.

In general, data are required both for model operation and model validation. Data used for model operation include the initial and boundary conditions, the source terms and meteorological forcing functions. One of the most difficult aspects of coastal modelling is how to provide a description of an open boundary. In particular, data for defining conditions of the hydrodynamics and contaminant fluxes between the far field and the open ocean beyond are not always available. In the absence of appropriate data, the only recourse is to use simple assumptions, such as diffusion into an infinite field or periodic flow conditions at the boundary, in order to keep the model operational.

Ideally, model validation is achieved when the model output compares favourably with data sets independent of those used during model calibration. In the case of complex deterministic models this could be an imposing task. In theory, the predictions of the model should be compared at all appropriate levels with different data obtained from real systems. However, this is rarely done in practice. In some cases, all or part of the calibration data is used again in the validation step but this procedure does not constitute proper validation. Such a partial validation, using data from the same site, is called model confirmation. In the final analysis, it is crucial that independent sets of data from many different regimes be used to establish the model's credibility through rigorous statistical tests. Obviously, if the observational data are very limited, then all of it will be used in the calibration stage and a model validation will not be possible until further data sets become available.

It is also important to realize that good validation performance does not necessarily guarantee that any model will accurately predict future conditions. Some uncertainties will always remain in the model coefficients, the model variables, and the model structure itself (Simons and Lam, 1980). Therefore, models should be subjected to post-audits in which their predictions are tested with data obtained after an environmental control programme has been implemented. The purpose of this stage of validation is to check whether the model reproduces the expected changes. Unfortunately, post-audits rarely occur. Only recently has there been some activity in this phase of validation (Lam et al., 1987).

Clearly, modelling is heavily dependent on the availability of appropriate and reliable data. All too often, especially in ocean modelling, the lack of appropriate data impedes model development or prevents proper validation of models. Perhaps the best example is in the area of toxic chemical effects modelling, where the lack of appropriate data is a major constraint. Model users must therefore be cognizant of the issue of data quality. The best of models cannot make reasonable and accurate predictions if these predictions are based on imprecise or inaccurate input data. Although the adage 'garbage in - garbage out' has become common modelling jargon, it nonetheless provides an important cautionary note for potential model users. In many cases, the underlying cause of such a situation is that data used for model development were originally collected for a purpose other than modelling. If data collection programmes are more closely linked with modelling studies, then the constraints imposed by the lack of suitable data can be substantially reduced.

The most difficult problem, however, is proving that the model is robust, namely that it can predict extreme conditions. Since most validation data are collected under normal conditions, they are of little value in assessing confidence in the results of the model under extreme circumstances. A sensitivity analysis is then probably the most appropriate manner of determining the value of the model under such circumstances. If the correct parameterizations of the various processes have been included in the model and the confidence we have in our knowledge of these processes is high, then the model should be accurate under extreme conditions.

7. SUMMARY AND CONCLUSIONS

The purpose of this report is to recommend modelling techniques to be used to determine the transport, dispersion and fate of materials discharged into coastal environments. These techniques comprise one of the key elements of strategies required to effectively protect and manage the coastal marine environment. The Working Group was asked to address the following three terms of reference:

a) to evaluate the state-of-the-art of coastal (including continental shelf) modelling relevant to waste inputs by sea dumping or land-based discharges to such areas;

b) to determine which model parameters are site and source specific and which parameters are generic to different coastal situations and contaminants;

c) to recommend the types of model appropriate for specific coastal situations.

In meeting these objectives, we have tried to define what is meant by the coastal environment, examined how models have been built in the past, studied how the various processes have been parameterized and discussed how to go about constructing a model for a specific coastal situation and question.

Waste management questions are usually expressed in a form that requires the relationship between contaminant release rate and effects (e.g., risks to human health, effects on biological productivity, interference with marine amenities, etc.) to be adequately represented. However, such a relationship has two components: 1) the relationship between the release rate of a contaminant and its distribution in the environment; and 2) the relationship between exposure to the contaminant (the concentration field in the environment) and effects.

These two components can be illustrated rather simply by the following two equations that can be applied to determining the effect of a contaminant released to the environment:

$$\text{Exposure} = f(\text{source, behaviour, transport, fate, etc.}) \quad (7.1)$$

$$\text{Effect} = f(\text{toxicity, exposure}) \quad (7.2)$$

Modelling of the relationship between the contaminant release rate and its distribution in the receiving environment (Equation 7.1) constitutes the subject of this study. The relationship between effects and exposure (Equation 7.2), an essential part of environmental management, is outside the terms of reference of this study. Nevertheless, the nature of the exposure-effects model will clearly impose demands upon the environmental model to which it is coupled. For example, the physical and biological matrices in which contaminant concentrations need to be predicted by the environmental model are dictated by the origins of the pathways leading to the predominant effects.

There also exists the possibility of feedback from the exposure-effects model to the environmental model. For example it is impossible, without considering effects, to predict the concentration field if sufficiently high concentrations of a contaminant result in direct harm to biota thereby altering the biological structure of the system. Thus, a knowledge of the exposure effects relationship can influence the structure of the model.

For these reasons, the questions covering the relationships between contaminant release rates and distributions in the environment have had to be couched in general, rather than specific, terms.

There are far more monodisciplinary than multidisciplinary models in the research field but environmental management questions almost invariably involve aspects of a multidisciplinary nature. This is often the case simply because it is the consequences of a practice that are of primary concern, namely increased risks to human health, damage to marine ecosystems or interference with amenities. In the main, therefore, models conceived and constructed for the purposes of responding to environmental management questions are required to be multidisciplinary in order to provide suitable linkages to the effects or exposure model.

a) Evaluation of the state of the art of coastal modelling

Environmental management requires robust models. Transportability of models is also desirable. However, our knowledge of the complex processes potentially requiring to be represented in water quality models is extremely poor. There is therefore a continuing need for carefully-implemented, long-term, comprehensive research on the transport and fate of marine contaminants.

The Working Group undertook a literature survey to determine how extensive previous work in this area has been. The methods revealed in this survey have been incorporated into the discussions of parameterisation and model construction. It is clear that the state-of-the-art in waste disposal modelling is less advanced than that in a single discipline (e.g., hydrodynamics modelling). Some general conclusions can be made about the types of model that are available for addressing waste disposal problems:

i) Models of water circulation and related advection/diffusion processes within the water column are the most advanced. These are suitable for contaminants whose transport, dispersion and fate are primarily governed by the motion of the water, with the possible addition of a simple decay process;

ii) Sediment transport modelling tends to have been advanced on an engineering rather than a theoretical approach because of the need to deal with practical problems in the nearshore environment. There are few, if any, models which cover the movement of fine cohesive sediments across the entire continental shelf. Much work is presently being undertaken to try to parameterize the combined effects of waves and tidal forces on the erosion and deposition of sediments;

iii) The most frequently used biological transport models are based on conservation of mass. Complicated models of the complete marine ecosystem usually have many parameters whose values can be difficult to determine. It will probably be several years before these complicated models are useful in the solution of waste disposal problems;

iv) Most benthic transport models are one-dimensional in the vertical and very few consider horizontal variations in the seabed. If these variations are considered, the usual method is to couple these one-dimensional models through exchanges with the water column;

v) Much of the geochemistry introduced in waste disposal models is based on the K_d, or equilibrium partitioning, approach. In estuaries, the K_d may be allowed to vary with salinity, but in coastal seas it is usually assumed to be constant. Some contaminants change their oxidation state and become involved in organic cycling and various other complex reactions. Such processes are now included in the most sophisticated models but the reaction rates appropriate to specific environments are difficult to determine.

b) Site specific versus generic model parameters

The coastal shelf is a very heterogenous environment. This makes it very difficult to produce generic models but the processes involved can be considered generic. The parameterization procedures that are relevant to one situation may be equally applicable to other coastal regions. It will normally be the combination of processes and their relative importance that will distinguish one coastal model from that applied to a different region. However, the parameter values are often site-specific in coastal models, particularly those that integrate information in time and/or space and those meant to be used to represent effects on aggregated biological populations. In general, the values of several parameters in a model have to be selected on the basis of data obtained at the site. Hence, as a consequence of calibration, those parameter values are site specific.

c) Recommendations on types of model

There are two major reasons for embarking on mathematical modelling. The first is to gain insight (i.e., fundamental understanding) of the processes governing the movement of contaminants in the sea. The second is to produce answers to management questions with adequately-quantified confidence limits. The second objective should not be pursued until sufficient understanding has been achieved to ensure that confidence in the model solution is sufficient to meet the specifications defined by the managers.

One of the most important aspects of modelling is deciding exactly what the question is to be answered. Therefore, the management question has to be carefully analysed and the relevant model inputs and outputs determined. In some circumstances, a simple calculation can indicate whether or not there is a potential problem with a planned waste disposal activity, i.e., whether any limits on dose or effects are likely to be approached or exceeded. In other circumstances, only a rather complex model, taking account of all the important couplings between concentration fields and processes, is likely to provide the confidence limits required to answer the questions posed by environmental managers.

The management question should give an indication of the time and length scales of interest. These will govern the type of model to be selected. It should be clear from the above discussion that no single model is appropriate for all purposes and that a range of models is usually required. Also, suitable models can only be derived from a sound knowledge of the processes in the region of interest. This may require an observational programme prior to the modelling work to determine environmental conditions and subsequently to provide validation data for the model itself.

It must be emphasized that care is required in using models for management purposes. There is a significant danger of misusing models that are either too simple or too complex for the questions being asked. Despite claims to the contrary, the art of modelling has not yet reached the stage where expert systems (i.e., systems designed to be used by non-experts) can be blindly relied upon. All models have limitations. These cannot be fully understood without a minimum of expertise that needs to be transferred with the models.

For many years, researchers have attempted to model various aspects of marine systems. This has resulted in an improvement in the understanding of the processes and, as a consequence, in the reliability of models. An essential part of modelling is quality assurance, that is model verification, sensitivity analysis and model validation. Without the application of quality assurance procedures, confidence in model predictions is low and their use in answering management questions is dubious. Currently, not enough effort is being invested in quality assurance or, for example, the collection of field data required to support model validation. It is abundantly clear that this situation needs to be remedied; quality assurance must be considered as an integral part of the cost of creating a model, and not merely as an afterthought.

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Annex 1

COASTAL REGIMES

A1.1 Estuaries

The widest variety of sub-regimes of the coastal zone and associated physical conditions are found in estuarine areas. In general an estuary is defined as a semi-enclosed coastal body of water that has a free connection with the open sea and within which seawater is measurably diluted with freshwater derived from land drainage (Cameron and Pritchard, 1963). This definition applies to situations in which river discharge and precipitation exceeds water loss by evaporation. There exists another class of estuaries, termed 'negative estuaries', in which evaporation exceeds runoff plus precipitation. A large-scale example of such an estuary is the Mediterranean Sea. Less extensive examples, that occur predominantly in equatorial regions, are hypersaline lagoons.

Estuaries are usually classified on the basis of their physical oceanographic characteristics, particularly the magnitude of vertical mixing. This classification will be used here as a basis for explaining the diversity of processes operating in particular types of estuary, and the manner in which these processes influence model formulation and development.

The descriptive classification of estuaries depends on the relative intensities of tidal forcing and runoff influxes which affect vertical stratification within the estuary. Figure A1.1 shows an estuarine classification diagram (after Hansen and Rattray, 1966). Exemplar estuaries appear on this diagram as diagonal lines because the upper portions of these estuaries are less well mixed than the lower and because the river flow into the estuary varies. In the following sections the characteristics of the various classes of estuary, and the extent to which each type of estuary has different dominant processes operating within it, are described.

A1.1.1 Stratified estuaries

Freshwater entering an estuary tends to flow seawards across the surface of the estuary because of the density difference between the two mixing end-members. Entrainment caused by the turbulent flow of

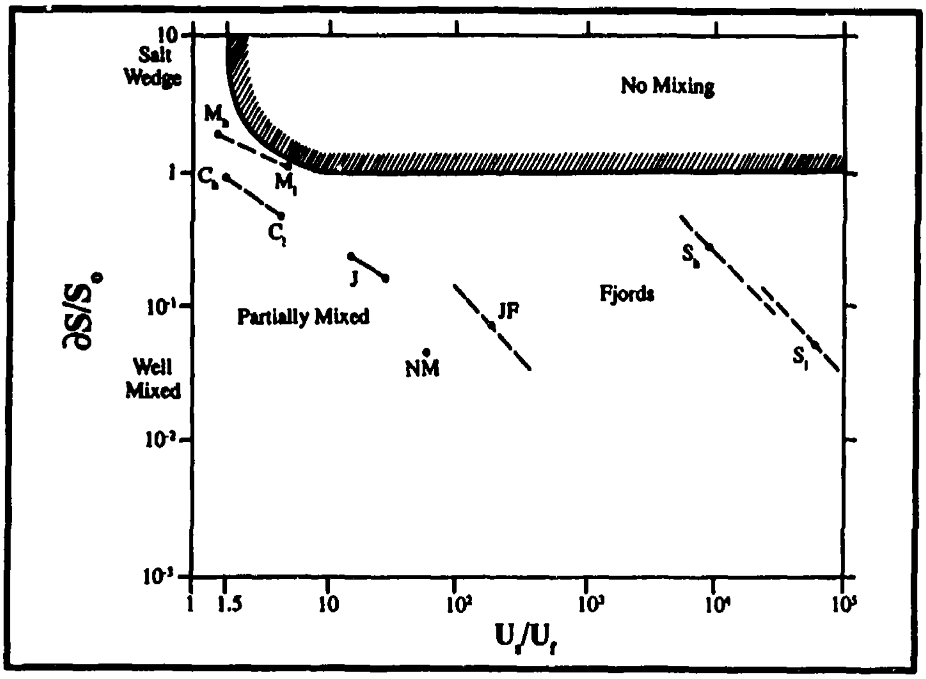

Figure A1.1. Estuarine classification diagram (after Hansen and Rattray, 1966) S is difference in salinity between surface and bottom, S_O is depth of mean salinity, U_s is the mean surface velocity, U_f is the mean flow due to river discharge. M = Mississippi River; C = Colombia River Estuary, J = James River Estuary; NM = Narrows of the Mersey Estuary; JF = Strait of Juan de Fuca; S = Silver Bay. Subscripts h and l refer to high and low river discharge.

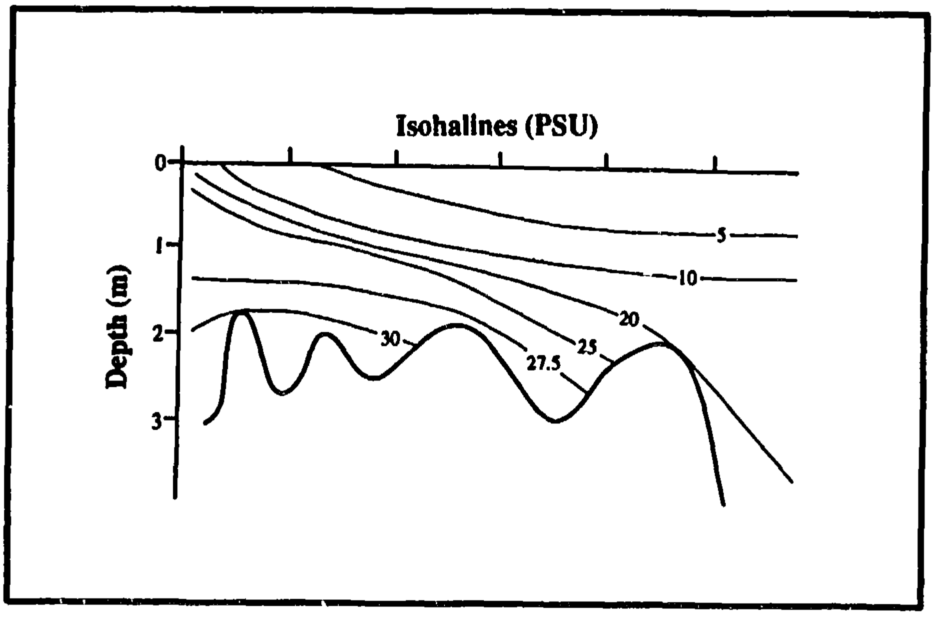

Figure A1.2. Longitudinal distribution of salinity in a salt-wedge estuary.

freshwater results in the saline subsurface water being mixed into the seaward flowing surface layer. To maintain the loss of saline water through entrainment into the surface layer a landward flow of seawater occurs into the salt-wedge estuary from offshore. This gives rise to a characteristically sloped halocline with salinity increasing seaward in the surface and with depth in the estuary (Figure A1.2). Estuaries with high river discharge in areas of restricted tidal movement can be expected to have salt-wedge estuarine characteristics where horizontal gradients are relatively small or negligible and vertical gradients are high.

A1.1.2 Partially-mixed and well-mixed estuaries

Tidal movements increase turbulence at the boundaries of an estuary as water enters and leaves the estuary during each tidal cycle. This increases the overall mixing in relation to that caused solely by entrainment. The net result is to reduce vertical and to enhance horizontal gradients in the isohalines. Systems in which this kind of behaviour is observed are referred to as a partially-mixed estuaries. Partially-mixed estuaries can have 'turbidity maxima' or regions of intense turbidity caused largely by asymmetry in the bottom tidal currents (Postma, 1967). This is a zone within which the suspended sediment concentrations exceed those downstream and upstream. It is located near the limit of salt intrusion and varies in position with alterations in river discharge. Particles in the turbidity maximum zone are supplied both by sediment discharge in runoff and by tidally-induced movement of sediments into and upstream in the estuary. Differential settling of particles within the turbidity maximum results in very effective size sorting and retention of a narrow size-range of particles within the zone of high turbidity. Fine particles are lost by advection in seaward-flowing currents and coarse particles are lost through landward sediment movement into the head of the estuary where shoaling occurs as coarse sediment is deposited continuously. The presence of the turbidity maximum can have an important effect upon particle-water exchange processes through the increased concentration of particles. In addition, the periodic resuspension and settling of sedimentary particles increase the rates of exchange of chemicals between the sediments and water. This occurs because of increased contact between sediment particles and water and by the stripping of poorly consolidated surficial sediment particles thereby exposing sub-surface sediments.

When the turbulent energy of the tidal current breaks down the stratification caused by the density differences between saline and fresh waters, the estuary becomes vertically homogeneous. It is still possible for there to be lateral inhomogeneities in these estuaries since lateral mixing may be non-uniform.

In tidally-influenced estuaries, such as the partially- and well-mixed estuaries, sediment movement can be quite intense. There is usually a depositional zone just above the limit of salt intrusion and a landward movement of coarse particulate material through bed-load transport. Thus, it is not uncommon to find that, in the absence of dredging, the volume of such an estuary will decrease with time as sediments accumulate and cause shoaling.

A1.1.3 Fjords

Fjords are a special estuarine type of deep, usually narrow, coastal inlets. Most have sills at their entrances that restrict the exchange of deep water between the fjord itself and the exterior coastal zone. Tidal oscillations tend to affect only the surface layer and entrainment is the main process responsible for mixing. Thus, fjords are in most respects similar to salt-wedge estuaries in that the surface salinity increases with distance seawards and the deep water constitutes the salt wedge. The deep waters usually show little lateral inhomogeneity in composition. When the sill is shallow, the deep water will be replaced infrequently when the density of water at the sill depth exceeds the density of bottom water within the fjord. Between these infrequent replacements of deep water, entrainment and turbulence result in a decreasing density of deep water with time and it is the rate of this decrease in density that mostly determines the frequency of deep water replacement. 'Classical fjords' are those in which replacement of deep water is sufficiently infrequent that the deep water becomes anoxic. However, there are a large number of fjords that do not fit this mould in that the rate of residual vertical mixing, or the variations of water density at the sill depth, are sufficiently large and frequent to permit relatively frequent deepwater replacement. In such cases, and in fjords where the downward transport of organic matter into the deeper layer is relatively small, the deep water remains oxygenated at all times even though it will undergo excursions in concentration reflecting the mixing and advection patterns. It is, however, very common for the sedimentary column within a fjord to be almost entirely anoxic with perhaps a thin oxygenated layer at the surface if the overlying water remains oxygenated throughout the year.

A1.1.4 Hybrid estuaries

Some estuaries can be subdivided into sequential zones in which different characteristics exist. An example is the St. Lawrence Estuary, where the landwardmost section of the estuary (the upper estuary) is partially-mixed and the downstream section (the lower estuary) is stratified and is most analogous to a salt-wedge estuary. The lower estuary in this case is almost fjord-like with almost horizontal isohalines that are transversely sloped due to horizontal inhomogeneities.

A1.1.5 Transverse characteristics of estuaries

In the classification scheme referred to above there is an implicit assumption that the circulation is two dimensional and that there are no differences in the velocity or density fields across the estuary normal to the main flow. This is a simplification that can mask the extent of transverse inhomogeneity. The transverse circulation is created by a balance between topographic effects, the Coriolis force and the lateral density field. If the estuarine cross section is not uniform along its axis, flow velocities can increase with distance landward and the main flow will be preferentially deflected to the deep channel. If the estuary is horizontally curved, flows will be directed to the edges due to inertial forces and this can effect the lateral cross section. Coriolis effects will result in a tendency for the seaward moving flow to keep to the right bank of the estuary in the northern hemisphere and to the left bank in the southern hemisphere. In well-mixed estuaries the mixing is so intense that gradients in residual circulation are essentially confined to the horizontal plane. In such cases the seaward-flowing mixed water and the landward-flowing salt water are often separated by banks into ebb and flood channels. Vertical variations in salinity are small and transverse effects then become all important. The effects of transverse variations on dispersion in estuaries has been dealt with by Fischer (1972; 1976) and Smith (1978).

A1.2 Inshore embayments

Embayments may be found on the inshore margins of continental shelves. Relatively narrow and/or shallow passages may inhibit water exchange between the embayment and the open shelf. Otherwise, circulation is usually driven by freshwater inflow or longshore drift.

Long Island Sound, located on the east coast of the U.S., represents a semi-enclosed embayment on an inner continental shelf (Riley, 1952). The sound is elongated east-west with a length of about 160 km; the maximum width is about 30 km. While maximum depth is about 100 m, the mean depth is only 20 m. There is an interchange with open shelf water through a series of passes on the eastern end; in the west, there is only limited exchange with New York Harbor.

The Sound receives fresh water from several rivers along the northern shore. Low salinity water (<30 parts per thousand) is found along the north coast which tends to move westward while it mixes offshore. Tidal currents are moderate enough to permit a weak seasonal thermocline with slight vertical gradients of salinity, dissolved oxygen and nutrients. In shallow regions where there is little river discharge, tidal mixing tends to break up any stratification.

The major feature of the non-tidal circulation is a 2-layer system in which the upper layer, freshened by river discharges, moves eastward out of the sound; the lower layer contains more saline water from the continental shelf which flows westward into the sound along the bottom. In addition to riverine input of nutrients, the inflow of shelf water along the bottom also provides nutrients to the sound.

Small-scale circulation features are controlled by bottom and shoreline topography interacting with todal and wind-driven currents. The net result appears to be a set of three eddies. These eddies circulate water counterclockwise in the east and west end of the Sound; the eddy in the center circulates clockwise.

A1.3 Open continental shelf

Open continental shelves are most influenced by pelagic circulation. However, major fresh water inputs and turbulence induced by wind energy affect the flows more than in the deep ocean because of the relative shallowness of the shelf.

A1.3.1 Example of a wide shelf

The continental shelf along the southeastern U.S. is shallow (<75 m) and is geomorphologically isolated from the adjacent shelf north of Cape Hatteras, North Carolina and the narrow shelf south of Cape Canaveral, Florida (Atkinson et al., 1985). The coast forms a gently curving bight with a zone of riverine discharges located along the central one-third of the bight, hereafter called the South Atlantic Bight, (SAB). The width of the shelf varies from a few kilometres off Cape Hatteras and Cape Canaveral to nearly 200 km off Georgia in the center of the SAB. The large latitudinal range results in large variations of climate ranging from subtropical to temperate.

The SAB is divided into three regions based on topography and forces driving the circulation. The inner shelf (water depth <20 m) is dominated by tidal currents, river discharges, local winds and interaction with estuaries. A coastal frontal zone, characterized by a band of low salinity water at the surface, is a semi-permanent feature along the central one-third of SAB's inner shelf. Tidal currents dominate inner shelf circulation accounting for approximately 80-90% of the total kinetic energy.

The middle shelf (water depth between 20 - 40 m) is dominated by local wind forcing. The mean flow is northward and is influenced episodically by the coastal environment of the inner shelf and the offshore environment of the Gulf Stream. The middle shelf is vertically mixed in autumn and winter and can be stratified from time-to-time in spring and summer as a result of decreased wind mixing, cross-shelf advection of low density water from the inner shelf and subsurface intrusions of upwelled Gulf Stream water.

The outer shelf (water depth between 40-75 m) is dominated by Gulf Stream fluctuations and wind stress. The Gulf Stream influences circulation by eddy-like fluctuations which distort the western edge of the Gulf Stream and propagate northward along the outer shelf and slope at speeds of 40-50 km d^{-1}.

Gulf Stream fluctuations induce upwelling along the outer shelf which brings in water that is characterized by high nitrate concentration. The nutrients can be introduced along the surface in winter when the shelf water is relatively cold and dense or can flow in along the bottom in summer when the shelf water is relatively warm and light. This continental shelf represents an example where accurate portrayal of the offshore boundary condition, incorporating the Gulf Stream fluctuations, is a critical prerequisite to accurately modelling the shelf environment.

A1.3.2 Example of a narrow shelf

The continental shelf along the Pacific coast of the southern Japanese Islands (about 1200km along the shore line) ranges in width from less than 1km up to 25km. The maximum shelf depth is about 200m at the continental slope edge. Surface sediments overlying the continental shelf are mostly composed of sand. Beyond the continental slope edge, there is a steep slope which reaches a trough, the Nankai trough, in which depths of more than 4500m are found. There are two ridges, the Kyushu-Palau in the south of the Japanese Islands and the Izu-Ogasaware to the north, which cut across the continental shelf and extend toward the southeast. Both ridges have many sea-mounts as well as several islands in the latter ridge.

There are about 10 major rivers with yearly freshwater runoffs ranging from 20 to 200 $m^3 s^{-1}$ (10-year average) that empty onto the Japanese continental shelf. The maximum runoff from these rivers occurs mostly in the rainy (from the middle of June to the middle of July) and typhoon (August and September) seasons. Speeds of the river runoff flow are generally rapid due to short river distances and steep slopes. Along the shelf edge, warm western boundary current, the Kuroshio, flows towards the northeast at a speed of up to 2.5m s^{-1}(Stommel and Yoshida, 1972). The transport of the Kuroshio attains values as large as 30-60 10^6 m^3 s^{-1} in the area off the continental shelf.

Because of the meandering of the Kuroshio along the narrow continental shelf, the Japanese shelf is often partly or entirely (both in area and depth) exposed to direct influences of the main or branch streams of the Kuroshio. Such influences are frequently felt at the shelf edge, and often extend even into nearshore areas. Many eddies occur along the boundary between the Kuroshio and coastal water, which cause vertical turbulence and the uplift of nutrients from the subsurface waters. Similar effects due to vertical turbulence are also occasionally observed around sea-mounts, islands and peninsulas. Offshore movements of the Kuroshio are accompanied by extensive turbulence of the water masses in the area between the Kuroshio and the shelf. Nutrient supply by this turbulence stimulates biological production.

A cold water eddy often appears in conjunction with large offshore meanders of the Kuroshio. The eddy is a few tens of kilometres to over 100km in width and is located within the shelf area between the Kuroshio and the coast. The eddy remains at a given location for long periods of time, up to a few months to several years or more. Such a large cold water eddy influences the water on the continental shelf from the surface to the bottom.

Winds (particularly northwest prevailing winds in winter), tides and freshwater input are also driving forces on the Japanese continental shelf. The latter two may not be as effective when compared to the wind and fluctuations of the Kuroshio. The surface seasonal thermocline disappears in the winter and a portion of the upper water column is then mixed vertically.

Similar narrow shelves are found along the east side of the Japanese Island ridge, in the western Pacific Ocean, along the west coast of North and South America, and in the coastal areas of Africa. However, these regions are not characterized by a strong ocean boundary current such as the Kuroshio.

A1.4 Marginal Seas

There are a number of marginal seas that may be treated as entities for modelling in relation to waste management questions. We provide here just two examples of such seas. The first in the Baltic, a shallow shelf sea with restricted exchange with the North Sea. The second is the North Sea which has greater hydrographic exchange with offshore waters.

A1.4.1 Example of a marginal sea with a sill: the Baltic Sea

The Baltic Sea (Figure A1.3) is a semi-enclosed shelf sea having restricted exchange with the North Sea through the Belt Sea, the Kattegat and the Skagerrak (the Danish Straits). It is commonly divided into

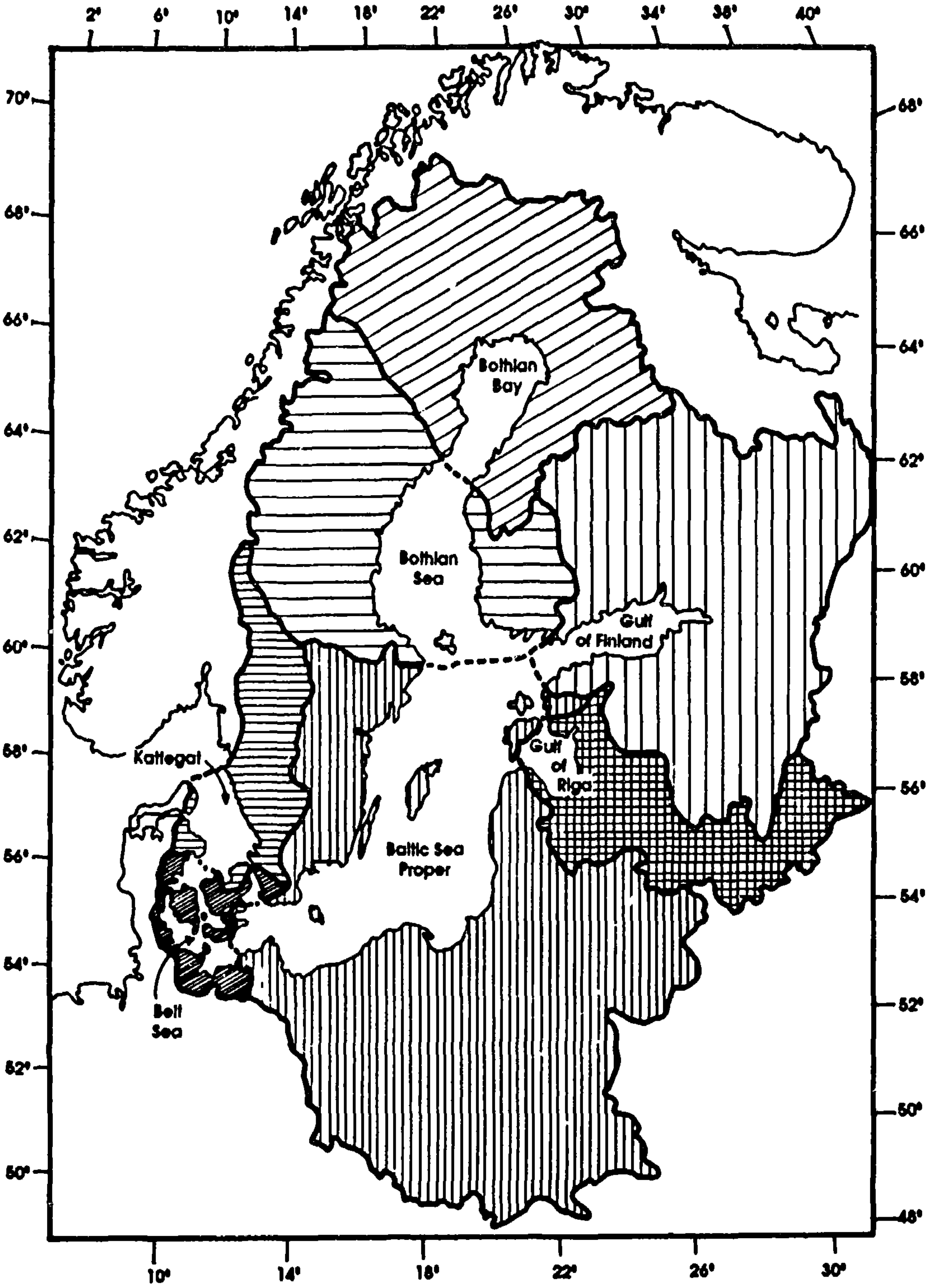

Figure A1.3. The drainage basin and subregions of the Baltic Sea and its transition area. The drainage areas for the subregions are distinguished by hatching.

geographical sub-areas, namely Bothnian Bay, the Bothnian Sea, the Gulf of Finland, the Gulf of Riga, the Baltic proper and the Belt Sea with many of these basins being separated by sills. Bothnian Bay, which contains several areas of depth exceeding 100 m with the deepest part 147 m, is separated from the Bothnian Sea by a sill of about 30 m depth. The Harnosand Deep in the northern part of the Bothnian Sea is 230 m deep, while much of the eastern central Bothnian Sea exceeds 100 m depth. The Landsort Deep north of Gotland is the deepest place in the Baltic proper with a depth of 459 m while the Gotland deep to the east of Gotland is 245 m deep. Despite the existence of several relatively deep basins, the mean depth of the Baltic proper is only 65 m, that of the Bothnian sea 68 meters and Bothnian Bay 43 m. The deep water salinity is $3\text{-}7^{o}/oo$ in the Gulf of Bothnian, $5\text{-}9^{o}/oo$ in the Gulf of Finland and $10\text{-}13^{o}/oo$ in the Baltic Sea Proper. The connection between the North Sea and the Baltic Sea through the Danish Straits has a maximum passage depth of 18 m and the presence of this sill accounts for the very limited exchange between the two adjacent seas. Indeed, it has been noted that the Baltic Sea is more like a fjord than an estuary (Kullenberg, 1981).

The fresh water supply to the Baltic Sea generates a brackish surface layer of outflowing water, while inflowing subsurface water forms layers of more saline deep and bottom waters. Although the internal circulation is weak, low salinity surface water is concentrated along the western side (the Swedish coast) and high-salinity deep flows predominate on the eastern side of the basin. The deep water replacement is restricted by the topography of the basin. The inflow of deep water is continuous over the Darss Sill and provides a continuous source of salt and oxygen to the deep water. Sometimes strong pulses of inflowing deep water are generated by special meteorological conditions.

A permanent oxygen deficiency exists below the permanent thermocline as a result of the pronounced stratification of the Baltic (Figure A1.4). The permanent halocline presents an effective barrier to convection but shear stress, especially where the halocline intercepts the bottom, gives rise to some vertical mixing. The transport of oxygen downwards through vertical circulation appears to be comparable with that supplied by horizontal advection from the Danish Straits (Gargas et al, 1977). Anoxic conditions were first detected in 1931 in the Gotland Deep, but lowering dissolved oxygen concentrations had been recorded in the Landsort Deep in the 1890s. The Gotland Deep exhibits pronounced

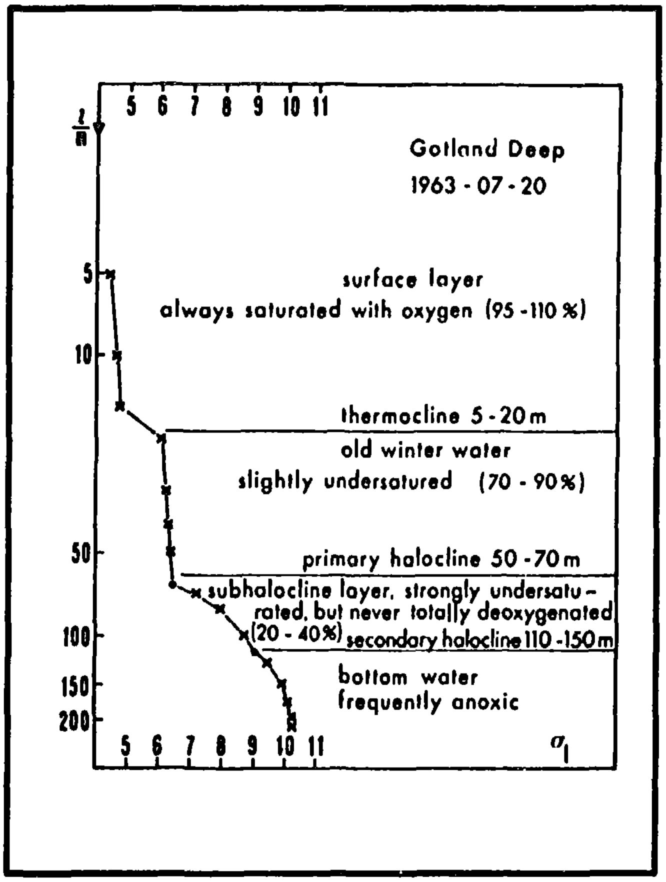

Figure A1.4. Stratification of water in the Baltic Proper. Ordinate is depth in metres and the abscissa is relative density minus unity.

short-term variations in redox potential, but there is a long-term trend towards continuously reducing oxygenation of this basin since 1900. The Gulf of Bothnia differs from other parts of the Baltic Sea in these respects. The amount of saline water entering the Gulf of Bothnia is a larger proportion of the volume of that basin than is the case with the Baltic proper. Furthermore, the salinity of water entering the Gulf of Bothnia, which is essentially surface water from the Baltic proper, is only slightly greater than Bothnian Sea water and no sharp halocline is produced. The less-pronounced density gradient and thermal convection in winter, which occurs throughout the water column, has resulted in the maintenance of dissolved oxygen levels at 60-80% saturation. Nevertheless, there is evidence of a long-term trend of reduced oxygen levels since 1900.

A1.4.2 Example of a marginal semi-constrained sea: the North Sea

The North Sea is a rather shallow shelf sea with an average depth of less than 100 m. It has an open boundary to the North Atlantic Ocean, to the English Channel, and to the Baltic Sea separated by land boundaries (Figure A1.5). The North Sea can be divided roughly into two parts, a southern and a northern part, the separation line being 56°N. The southern part has an average depth of only 37 m. The average depth in the

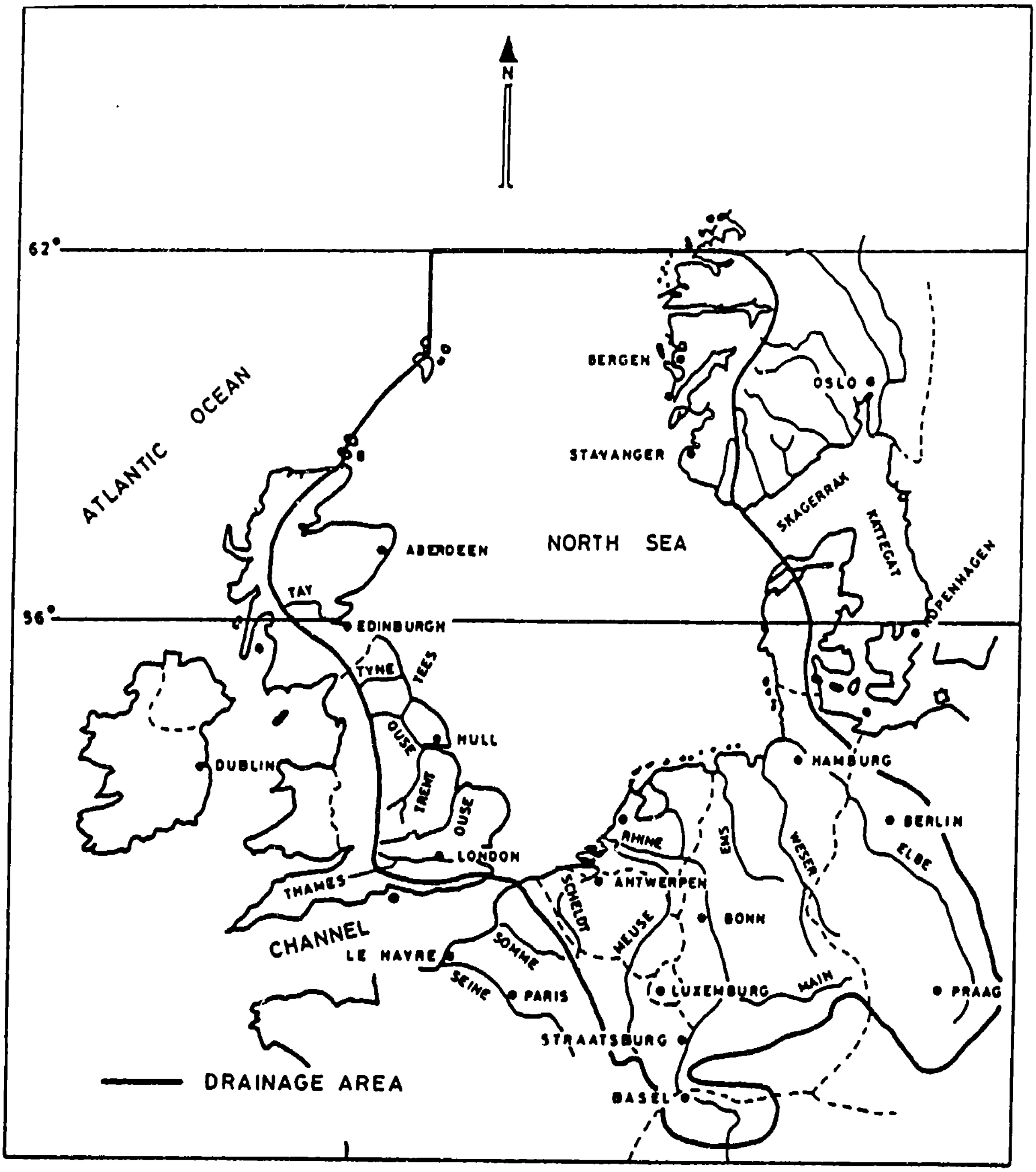

Figure A1.5. The North Sea Area.

northern part increases towards the north to well over 100 m, but depths greater than 200 m are only found off the Norwegian coast.

The water movement in the North Sea is dominated by a semi-diurnal tide. Typical tidal currents range from 2-3 m s^{-1} near the Straits of Dover to less than 0.5 m s^{-1} in the north. The complexity of the tidal system is reflected by the existence of three amphidromic points for the semi-diurnal tidal component. The influx of saline ocean water through the Straits of Dover is estimated to be 1.4(±0.3) 10^5 m^3 s^{-1} (Otto, 1983). The influx of fresh water from Dutch and Belgian rivers is about two orders of magnitude smaller, i.e. only 3 10^3 m^3 s^{-1}. Although small in quantity, this fresh water is important to the water quality along the Dutch and Danish coasts as it moves to the north in a narrow belt. Large quantities of nutrients are released into the North Sea by nutrient-rich rivers such as the Rhine, the Meuse, and the Scheldt. These nutrients are transported to the north by the residual flow, but algal blooms occur in most parts of the North sea.

A1.5 The Arctic Shelves

The dominant characteristic of the Arctic and Antarctic Oceans is their very cold environment. Both regions experience considerable cooling and sea ice plays a major role in determining many of their features. The differences between the two oceans are, however, perhaps more striking than the similarities. The Arctic Ocean (north of Fram and Bering Straits) is an enclosed ocean whereas the Antarctic Ocean has open boundaries. The topographically constrained exchange of water between the Arctic Ocean and the rest of the world's major oceans is in marked contrast to the Antarctic where exchange is not strongly restricted, and the waters formed there enter the deeper layers of the major oceans. The Arctic Ocean is largely covered by ice much of the year whereas the Antarctic Ocean undergoes considerable seasonal variation in ice cover. Finally, the Arctic Ocean is bordered by vast continental shelves with a large input of fresh water from rivers; whereas, there is little fresh water input into the seas surrounding Antarctica.

Sea ice plays a major role in determining many of the features of the Arctic Ocean. In central regions, where ice is present year round, and in shelf regions during the winter season, the ice cover greatly inhibits wind mixing. The Arctic ocean is generally a low energy regime, with many fewer and smaller near-surface eddies than are found elsewhere. Prevailing winds drive the ice and are believed to cause the anti-cyclonic gyre associated with the Beaufort Sea (Colony and Thorndike, 1984). Seasonal ice formation over the continental shelves produces the water that forms the halocline over much of the Arctic Ocean (Aagaard et al., 1981; Melling and Lewis, 1982; Midttun, 1985) and to a large degree determines the chemical characteristics of not only the shelf water, but also the water in the halocline (Jones and Anderson, 1986).

The Arctic Ocean continental shelves are large, comprising about one-third of the total area of the Arctic Ocean. They experience quite different conditions from those found in the central regions of the Arctic Ocean. Much of the shelf area is ice-free during part of the year. There is a large fresh water source from rivers as well as from sea-ice melt water. Shelf areas are relatively active biologically. All of these affect the chemical properties of the shelf water and subsequently other water masses as the shelf water advects into central regions.

Sea-ice formation over the continental shelves may be the driving process by which the continental shelves most influence the chemical characteristics of water masses both on the shelves and in the central Arctic Ocean. The cold, relatively saline halocline in central regions of the Arctic Ocean almost certainly results from shelf processes. As sea-ice is formed especially during the onset of the winter season, brine is excluded from the nearly pure ice phase, forming brine pockets that eventually drain out of the ice into the underlying water. The brine produced in this way mixes with the water on the continental shelves to form cold, saline water which then advects into central regions carrying with it chemicals from shelf waters, particularly those near the sediment-water interface where the dense water will tend to pool before leaving the shelves (Jones and Anderson, 1986). The production of brine also mixes the water column over the shelves during ice formation. In the summer season, sea-ice meltwater is a source of fresh water for all of the Arctic Ocean, and is probably the main source for some regions especially in and to the north of the Barents Sea (Anderson et al., 1988a; Tan et al., 1983). Sea-ice thus plays a major role in determining distributions of chemicals both over the shelves and in central regions of the Arctic Ocean. There are also possible chemical effects that the changing of phase between ice and water can have. In general, there will be separation of dissolved constituents as well as isotopic separations when such phase changes occur. In Arctic conditions, isotopic changes are small (Tan and Strain, 1980); however, several laboratory experiments dating back to the early part of this century show that there is a preferential precipitation of some salts from sea water as it is frozen and ice is formed. In spite of these convincing laboratory studies, evidence for preferential precipitation being an important process in nature is lacking. While enrichment of some salts was measured in natural samples in the Arctic Ocean, to date there is no evidence that this preferential precipitation is significant in determining distributions of chemicals in the Arctic Ocean (Anderson and Jones, 1985a; 1985b), though it could be important in the Sea of Okhotsk (Lyakhin, 1970).

The chemical characteristics of shelf water that have been revealed by studies in central regions are determined mostly by four processes: sea-ice formation and melt, river run-off, biological production, and interactions between the sediments and overlying water. River run-off introduces several materials into the ocean including some trace metals, artificial and naturally occurring radionuclides, and calcium carbonate, the latter being of special interest in global carbon budgets. Biological processes over the continental shelves influence distributions of carbon and nutrients in central regions of the Arctic Ocean, and from these together with measurements of transient tracers, one can make assessments of the annual rate of new production. Two studies, one based on total carbonate distributions (Anderson et al., 1988b) and one on oxygen distributions (Wallace et al., 1988) have resulted in estimates of a shelf-averaged new production. These estimates are consistent with and perhaps more representative of new production estimates for Arctic regions than those based on more conventional, local productivity measurements (Subba Rao and Platt, 1984).

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Annex 2

DETAILS ON PARAMETERIZATION OF PROCESSES

A2.1 Introduction

Additional details of the parameterization of processes and interaction between processes for coastal zone modelling are given in this annex. The organization follows that of Chapter 4. First, the parameterization of the different transport models is discussed. Next, the interactions between these transport models, including details on the use of equilibrum partition factors for decaying contaminants, are discussed. The annex ends with a parameterization of the source terms for specific chemical compounds.

A2.2 Hydrodynamic transport models: momentum transfer

Energy dissipation at the sea bed can be parameterized in two ways. First, a quadratic law of bed friction is used in which bed stress is related to the current one metre above the sea bed through a drag coefficient derived from observations (Davies and Furnes, 1980). With such a parameterization, it is not possible to resolve the near-bed logarithmic layer. In the second approach, the logarithmic bottom boundary layer is resolved, and energy dissipation at the sea bed is related to bed shear and eddy viscosity (Davies, in press).

In the majority of three-dimensional tidal models, the diffusion of bed-generated turbulence is parameterized through a coefficient of vertical eddy viscosity. In shallow water, where the turbulent Ekman boundary layer extends to the sea surface, eddy viscosity A_z is parameterized by (Bowden et al. 1959),

$$A_z = 0.0025hu$$

where h is water depth and u is the magnitude of the instantaneous tidal velocity. In deeper water, where the thickness of the Ekman layer is limited by rotation, Davies and Furnes (1980) suggested the use of the relationship

$$A_z = K u^2 / f$$

with $K = 2.0 \times 10^{-5}$ (a dimensionless coefficient), and f is the Coriolis parameter. A recent parameterization (Davies and Jones, 1988), which may be appropriate for both shallow and deep water, is

$$A = 0.0025\ u\ d \qquad \text{(A2.1)}$$

where d is the thickness of the bottom boundary layer, given by,

$$d = 0.3\ u_* / f \qquad \text{if } d < h$$

$$\text{or} \quad d = h \qquad \text{if } d > h$$

where u_* is the bed frictional velocity.

Validation of these tidal models, and hence the appropriateness of these various parameterizations, requires a comprehensive deployment of current meters in both the horizontal and vertical. However, as the majority of tidal current variation occurs in the near-bed region, increased emphasis on near-bed tidal measurements is required. The closer to the bed measurements are made, the greater the influence of bottom topography, and the finer the model grids will need to be.

In the case of wind-induced circulation, the downward diffusion of the wind's momentum due to small scale processes must also be parameterized. Early calculations parameterized the downward diffusion of wind momentum via eddy viscosity related to the wind-induced and tidally-induced current (Davies, 1976). Models of this form, successfully reproduce the temporal and spatial variations of currents occurring during JONSDAP '76, and were subsequently used in contaminant transport studies, in particular in determining flushing times for various regions of the North Sea based upon seasonal wind fields (Davies, 1982).

The role of the surface wind/wave field in transferring wind momentum to depth was omitted from Thorpe (1984) and Kitaigorodskii et al.,(1983), although subsequent idealized calculations (Davies, 1986) suggest it will be important in determining near-surface currents in deep water. Also, the level of turbulence at depth due to wind and tidally-induced currents will be significant in diffusing the wind's momentum to depth (Davies, 1986). The intensity of surface wind and the rate at which its momentum is diffused to depth, together with tidal- and wind-induced currents, will be particularly important in determining the bed stress during a major wind event. In addition to these effects, bed turbulence associated with the surface wind/wave field can significantly enhance bed stress (Grant and Madsen, 1979; Christofferson and Jonsson, 1985). This enhanced bed stress will cause substantial sediment movement in many situations.

Under stratified conditions, the rate of diffusion of wind momentum to depth is significantly influenced by the intensity of stratification. The physical processes whereby the wind's momentum can erode the thermocline and subsequently cause it to deepen are very complex and are usually parameterized in terms of entrainment velocity and Richardson number.

In the case of tidal motion, internal tides can be generated at the interfaces between layers of different density. In models of internal tides, the retarding force which one layer exerts upon the other is usually parameterized by an interfacial friction coefficient.

A2.3 Sediment transport models

The various processes of sediment transport are formulated in mathematical terms and the parameterizations involved are discussed starting with the formulation of bed load and suspended load.

A2.3.1 Bed-load transport

Bed load comprises sediment transport of grains that roll, slip and saltate over the bed. Bed load occurs in a confined narrow zone above the bed, and its thickness is limited by the saltation height of particles. Research in river engineering has established a direct relationship between the bed load, q_b, and the bed shear stress, τ_b:

$$q_b = \alpha \, \tau_b \, (\tau_b - \tau_{cr}), \qquad \text{(A2.2)}$$

where α is a coefficient to be determined during the calibration phase of the model. The motion of grains starts when the value of τ_b exceeds the critical bed shear stress, τ_{cr}, which for unidirectional flow is given by the Shields diagram (Shields, 1936). In most practical bed transport formulae only a few parameters are important and these can often be put into two dimensionless parameters (van Rijn, 1984a; Ackers and White, 1973). Parameter values for Equation (A2.2) have been experimentally derived by Van Rijn (1984a), Engelund and Hansen (1967) and Ackers and White (1973).

From the bed-load transport a so-called reference concentration, c_a, for the bed is found by dividing the bed load by an effective bed-particle velocity and an effective bed-zone thickness. Several formulae exist in the literature, but all are related by some equivalent roughness height for the effective bed-zone thickness and an effective bed-particle velocity proportional to the bed-shear velocity (Bijker, 1965; Van Rijn, 1984a). Bed load transport is influenced by short wave action. For ways of dealing with this see Bijker (1965). The formulae which determine the bed load transport assume that particle size can be characterized by a mean particle diameter. If the grain-size distribution is more complex, bed load transport equations can be set up for grain size intervals which are subsequently treated as separate quantities.

A2.3.2 Suspended sediment transport

The concentration of suspended sediment, cohesive and non-cohesive alike, is usually described with an advection-diffusion equation analogous to those discussed in Section 4.2. To solve this transport equation the initial sediment concentration and the conditions at all boundaries of the domain must be prescribed. The boundaries are the inflow and outflow boundaries in the vertical, the free surface of the water column and the bed boundary.

At inflow boundaries the suspended concentration or the influx of material must be prescribed across the whole inflow plane. The concentration, c, can, for instance, be taken from a larger area model or from measurements. At outflow boundaries the flux or the concentration can be prescribed. If neither one is known, a so-called free stream outflow boundary condition can be prescribed, i.e.,

$$\partial^\alpha c / \partial n^\alpha = 0 \qquad \text{(A2.3)}$$

where α = 1 or 2 and n is the outward - directed normal to the boundary. The physical interpretation of this boundary condition for α = 2 is that diffusion in a direction normal to the boundary is neglected. At the free surface, the normal flux through the surface is set equal to the atmospheric influx of material (which is frequently set to zero).

The bed boundary condition must reflect the difference between cohesive and non-cohesive sediment. For non-cohesive sediment the boundary condition is not applied on the bed itself but at a small distance, a, the effective thickness of the bed load transport zone equal to half the dune height (van Rijn, 1984b). What is actually prescribed depends on several site and problem-specific aspects. If there is a local equilibrium between the suspended sediment concentration and the bed (or if the horizontal grid size is larger than the adjustment length for equilibrium) either the reference concentration or a zero flux can be prescribed, i.e.,

$$c(x,y,z=a,t) = c_a, \tag{A2.4}$$

or

$$w_s\ c + \epsilon_z\ \partial c/\partial z = 0, \tag{A2.5}$$

where c_a is the mean concentration of sediment over the near bed zone, also called the reference concentration, w_s is the particle settling velocity and ϵ_z is the vertical sediment diffusion coefficient. Usually, either one of these conditions is used in practical applications. If more information is available, a boundary condition proposed by Cheng (1984) can be applied :

$$w_s\ c + \epsilon_z\ \partial c\ /\ \partial z = \alpha\ w_s\ (c-c_a) \tag{A2.6}$$

where the parameter α is to be determined by calibration.

For cohesive suspended sediment, the bed-boundary condition reflects the cohesiveness of the bottom sediment :

$$w_s\ c + \epsilon_z\ \partial c\ /\ \partial z = q_d - q_e, \tag{A2.7}$$

where q_d and q_e are the deposition and erosion rates to be described below.

The sediment diffusion coefficients, ϵ_x, ϵ_y and ϵ_z, are usually related to the diffusion coefficients for dissolved matter, but in practical applications only ϵ_z is relevant. Van Rijn (1984b) applied a parabolic distribution for ϵ_z :

$$\epsilon_z = \beta \, \phi \, z / h \, (1 - z / h) \, \kappa \, u_* h, \qquad (A2.8)$$

where κ is von Karman's constant, β is a factor to describe the difference between momentum and particle diffusion, and ϕ expresses the damping of turbulence by the sediment. More refined models apply a turbulence closure sub-model to find the eddy viscosity coefficient for the transfer of momentum and dissolved matter and relate these to the diffusion coefficient for sediment (Sheng, 1986; Koutitas, 1986).

The formulae presented above pertain to a three-dimensional problem. In many situations, however, a formulation of lower dimensionality can solve the problem as well. In most cases a two-dimensional model in the horizontal plane is used, but in some specific cases a two-dimensional laterally-averaged model is required (siltation of ship channels, for instance). The common procedure to go from the full 3-D equations to the lower dimensional model is to integrate the 3-D equations over the coordinate direction to be suppressed, apply boundary conditions at the integration boundaries, approximate averaged products by products of averaged quantities plus some residual term, and express these residual terms in the averaged quantities (usually through some kind of dispersion coefficient). The two-dimensional horizontal formulation in conservative form reads :

$$\frac{\partial(hc)}{\partial t} + \frac{\partial(uhc)}{\partial x} + \frac{\partial(vhc)}{\partial y} = \frac{\partial}{\partial x}\left(\epsilon_x h \frac{\partial c}{\partial x}\right) + \frac{\partial}{\partial y}\left(\epsilon_y h \frac{\partial c}{\partial y}\right) + P \qquad (A2.9)$$

where c, u, v , and P are the depth-averaged concentration, depth-averaged flow components, and the depth-averaged source and sink terms, respectively. ϵ_x and ϵ_y are the eddy diffusion dispersion coefficients for suspended sediment in x- and y-directions, reflecting the influence of approximating depth-averaged products by products of averaged quantities. The depth-averaged source and sink term, P, now reflects explicitly the exchange processes with the bottom, i.e.,

$$P = q_d - q_e , \qquad (A2.10)$$

where q_d and q_e are the bed erosion and deposition functions. When using Equation A2.9, new parameterizations need to be applied that pertain to the flow field and to dispersion coefficients for dissolved matter. These coefficients, ϵ_x and ϵ_y, can be constant, calibrated in the process of modelling, or a function of the friction velocity, e.g.,

$$\epsilon_x = \alpha \bar{u} h \text{ and } \epsilon_y = \beta \bar{v} h \qquad \text{(A2.11)}$$

where α and β are site specific and to be determined during calibration. More elaborate turbulence closure models use additional equations to determine these transport coefficients (Sheng, 1986; Koutitas, 1986).

A2.3.3 Grain size distributions

If the grain-size distribution of the bed load or of the suspended load is not well represented by one mean particle diameter, separate equations should be used for each grain-size interval. Essentially the same formulae are used but the parameterization of the various processes now pertain to grain- size intervals (Cheng, 1984). Exchange of particles between grain-size intervals is usually neglected.

A2.3.4 Gravitational settling

The settling velocity, w_s, of suspended sediments generally depends on the specific weight and shape of the particles. Only at very small concentrations is the settling velocity independent of the concentration (Stokes-range). There are expressions for settling velocity depending on the mean particle diameter (Koutitas, 1986) At higher concentrations, w_s is a function of the concentration itself (Mehta, 1984; Teisson and Latteux, 1986; Burt, 1984) :

$$w_s = k\, c^n, \qquad \text{(A2.12)}$$

where k depends on the sediment composition and is of the order of 0.001, and n is between 1 and 2. Teisson and Latteux (1986) report a value of 4/3 for the Loire Estuary, and Mehta (1984) reports a value of 1.29 for

Maracaibo mud. For still higher concentrations settling is hindered and the settling velocity is written as :

$$w_s = w_{so} (1 - kc)^m , \qquad \text{(A2.13)}$$

where m is approximatively 5 and k must be determined in the calibration process. Thorn (1981) reports for the Severn Estuary :

$$w_s = 0.513 \quad c^{1.29} \quad \text{mm s}^{-1} , \qquad \text{for } c < 5 \text{ gl}^{-1}$$

and

$$w_s = 2.2 \ (1 - 0.008 \quad c)^{4.65} \quad \text{mm s}^{-1} , \quad \text{for } c > 5 \text{ gl}^{-1}$$

Settling velocities are site specific, i.e., there does not exist a 'typical fall velocity'. Burt (1984) reports values for estuaries ranging from 0.1 - 10 mm s^{-1}; see also Mehta (1984).

A2.3.5 Critical bed shear stress

The critical bed shear stress for the initiation of motion of non-cohesive sediment can be taken from Shields' diagram (Shields, 1936). If surface waves are important, this diagram can still be used if the orbital wave velocity is known. For cohesive sediment, the critical bed shear stresses related to erosion and deposition are sediment- and size-specific and need to be determined from measurements.

(a) Erosion

There are two modes of erosion: surface and bulk erosion. Surface erosion is the rupture of individual particles from the bed by the shearing forces of the turbulent flow. Bulk erosion occurs when rupture occurs beneath the bed surface (liquification, for instance) and relatively large volumes of sediment are eroded. Surface erosion is the dominant process under weak to moderate bed stress. Bulk erosion is dominant under severe conditions. Surface erosion can be related to critical shear stresses, whereas bulk erosion must be treated as an instantaneous process and is difficult to model (Hayter, 1983; 1984). The rate of surface erosion is usually set proportional to the excess shear stress above the shear strength, i.e. :

$$q_e = M \ (\tau_b \ / \ \tau_{cre} - 1), \text{ for } \tau_b > \tau_{cre} \qquad \text{(A2.14)}$$

where τ_b is the bed shear stress and τ_{cre} is the critical bed shear stress related to erosion. Both M and τ_b are sediment and site specific. Teisson and Latteux (1986) report for the Loire Estuary :

$$M = 0.55\ (0.001\ c_b)^3 \quad , \quad (c_b \text{ in g } l^{-1})$$

and a critical bed-shear velocity ranging from 0.7 cm s^{-1} to 3.1 cm s^{-1} for recently deposited and consolidated sediment, respectively. Basic to all modelling of erosion is that the coefficient of proportionality, M, and the critical shear stress are specific to sediment type, grain-size specific and these two parameters must be calibrated in the process of modelling. See Mehta (1984) and Thorn and Parsons (1980) for recent reviews.

(b) Deposition

If suspended sediments were composed of non-interacting particles and were to settle in still water, the deposition rate would simply be the product of the settling velocity and the concentration. However, when particles interact and the flow is turbulent, not all particles will either reach or remain on the bed. The rate of deposition, q_d, is usually set proportional to the excess bed shear stress related to deposition :

$$q_d = -\, w_s\, c\, [1-(\tau_b\, /\tau_{crd})], \text{ if } \tau_b < \tau_{crd} \qquad \text{(A2.15)}$$

where τ_{crd} is the critical bed stress for deposition. If the suspended sediment concentration increases, deposition is hindered. Other formulations exist in literature and are summarized by Mehta (1984). The critical bed shear stress related to deposition is site (turbulence level) and sediment specific.

Flocculation influences the particle size distribution and the settling velocity. This process is included in the parameterization if the settling velocity, w_s, is calibrated with in situ measurements. Cheng (1986) applied a model proposed for smoke and dust to arrive at an explicit expression for the influence of flocculation on the settling velocity.

(c) Short wave influences

Short waves can strongly influence both bed load and suspended sediment transport. The most straightforward way to include this is to take the orbital wave velocity into account in the near-bed velocity. Most probably, this procedure should also be applied equally to both the critical bed shear stresses for erosion and deposition. Sheng (1986) applied a separate sub-model to formulate the wave-current boundary layer.

(d) Consolidation

Newly-deposited cohesive sediments consolidate over time, resulting in an increase in the specific density and the critical shear stress for erosion. More refined models for cohesive sediment transport apply so-called layered-bed models to describe this process of consolidation in some detail (Hayter, 1984, 1986; Teisson and Latteux, 1986). In a layered-bed model, the bed is divided into several layers each with distinct properties. Newly deposited sediment is added to the top layer; after some time, hours or days, this sediment is consolidated to the density of the second layer, the second layer to that of the third, and so on. Each layer has its own specific density and critical shear stress for erosion. Obviously, much in situ information must be available to arrive at parameters that can be used in this formulation.

(e) Bioturbation

Sea bed stability can be influenced by biogenic activity. The top layer of sediment can be reworked thereby changing the bottom roughness. Grant et al (1982) determined critical shear stresses for erosion for natural marine sediments (fine sand) and for abiotic sediments of virtually the same characteristics. For the natural sediment, the critical shear stress for erosion is reported to be up to twice the value predicted from Shields curve. Though biogenic activity is important, precise (in situ) measurements are necessary to quantify the influence in a given situation (Grant et al, 1982).

(f) Sand waves, dunes, and wave-ripples

Literature exists on modelling the onset of bed form instabilities resulting in the formation of wave-ripples, dunes, and sand waves. Models exist that describe sand transport on these bed forms, but these models have not progressed to the point that they would be useful for practical waste management applications (Richards, 1980).

(g) Episodic events

Episodic events, such as severe storms and extreme waves, can be formulated in mathematical terms, but their influence on (suspended) sediment transport is very site specific. A possible way is to treat their influence as an instantaneous process and to redistribute the sediment between bed and suspended load and continue the computation. If the event lasts for an appreciable period of time, this redistribution must be repeated (Ariathurai, 1974; Hayter, 1933).

A2.4 Biological transport models

(a) Introduction

The purpose of this section is to survey a number of mathematical formulations (parameterizations) which are used in modelling (i.e., quantifying) biological processes. Discussions of the biological oceanographic processes that are the basis of these parameterizations can be found in Parsons et al. (1984), Cushing and Walsh (1976) and Longhurst (1981). With the exception of the basic conservation principle, there are no fundamental laws of physiology or ecology, and the parameterizations described hereafter are to be viewed as empirical. The implication of this remark is that even if a given parameterization is deemed applicable in different environments (i.e., pseudo-generic), the actual values of the parameters will frequently be site-specific and require appropriate determination.

A number of commonly-used parameterizations for the processes of biological uptake of nutrients, carbon fixation by primary production, grazing by herbivors, bioturbation in sediments, etc., are illustrated in the following sections.

(b) Nutrients

Typically, the uptake of nutrients by phytoplankton is modelled using a formulation that relates the specific rate of nutrient removal to the ambient concentration of the nutrient. The form most generally used is the Michaelis-Menten uptake relationship

$$V = \frac{V_m N}{K_s + N} \qquad \text{(A2.16)}$$

where V_m is the maximum specific uptake (time^{-1}) of the nutrient, N, and K_s is the half saturation constant which represents the nutrient concentration at which $V = V_m/2$. Values for V_m and K_s are determined from experiments and vary considerably for different phytoplankton species. The above formulation does not take into account the changes in nutrient uptake that can occur in response to changes in internal cell nutrient pools and general cell physiology. Much recent experimentation has indicated that phytoplankton show a preference for certain forms of the same nutrient, e.g., nitrogen as nitrate or ammonium. There are no clear guidelines to suggest how this process should be modelled. However, ammonium inhibition of nitrate uptake is usually modelled with a function that decreases nitrate uptake by phytoplankton with increasing ammonium concentration. Nutrient uptake can also be a non-linear function of ambient temperature.

(c) Primary production

Photosynthesis is the process by which phytoplankton fix carbon. Parameterization of this process is required in models that are concerned with quantifying phytoplankton growth. Photosynthesis is described by a rate that is usually expressed as the ability of the phytoplankton to produce a quantity of fixed carbon per quantity of chlorophyl a in a given time (mgC mgchla^{-1} time^{-1}). This rate is then modified by the availability of water temperature, light and nutrients.

Photosynthesis versus light intensity relationships for marine phytoplankton, determined from experiment, show three characteristics: a linear increase in photosynthetic rate at low light intensity; a maximum rate at some intermediate value of light intensity; and inhibition of photosynthesis at higher light intensity. One approach to modelling this process is of the form

$$P = P_m \frac{I}{I_k} \exp(1 - I / I_k) \qquad \text{(A2.17)}$$

where P is assimilation, P_m is the maximum assimilation, I is the light intensity, and I_k is the light intensity corresponding to P_m. This relationship exhibits the desired characteristics of the photosynthesis versus light response. However, it is only one of many forms that can be used. Jassby and Platt (1976) and Platt et al. (1977) evaluate and discuss the many diverse relationships that are used to parameterize phytosynthesis versus light responses by marine phytoplankton.

For modelling studies, the photosynthesis-light response in respect to other biological constituents must be in terms of a specific rate ($time^{-1}$). This requires ratios (e.g., C:N, C:Chl a) to convert to the appropriate units. The photosynthetic rate can be modified by the available nutrients and temperature.

The parameterization of phytoplankton growth can be achieved in different ways. It can be assumed that growth is determined by the factor (light, nutrients, temperature) that is present in a limiting quantity at a particular time or location. This is an restatement of Liebig's Law of the Minimum. It can also be assumed that growth can be represented by a multiplicative function that includes the effects of all factors. With this approach, growth is regulated by several quantities.

The quantity of interest in ecological studies is the net production at a given trophic level. If gross primary production is obtained from experimental studies, then it is necessary to include a respiration term in the phytoplankton growth formulation to account for cell metabolism cost. This process is usually assumed to be proportional to the phytoplankton biomass and is modelled with a linear term in which a portion of the biomass is lost at each time. However, respiration is a complex function of cell physiology, as well as other processes.

(d) Grazing

Grazing on phytoplankton by higher trophic levels represents a major process by which a contaminant can be transferred up the food chain. This process could be parameterized by a linear function that is proportional to the biomass of the phytoplankton and the grazer. However, experimental studies have shown that ingestion by herbivores tends to approach a maximal rate as the available food concentration increases. The usual approach used to parameterize grazing is an Ivlev formulation

$$\text{grazing} = R_m \, [1 - \exp(-\delta \, P)] \tag{2.18}$$

where R_m is the maximum ingestion rate and δ is a parameter affecting the initial increase of grazing with increasing food concentration, P. Modifications to this grazing response function allow for a feeding threshold, selective feeding behaviour and food quality. Introduction of a feeding threshold is done by modifying the exponential so that there is some food concentration, P_o, below which grazing ceases. This modification is sometimes necessary in models to prevent grazing of the phytoplankton to extinction. The feeding threshold implies a refuge for the phytoplankton at low food concentration.

Much recent experimental work has shown that herbivores actively select certain sizes or types of particles for food. This is introduced in a model by the use of selectivity coefficients (Vanderploeg and Scavia, 1979) that modify the existing biomass, P, to account for the grazers' preference for certain size ranges of particles. The phytoplankton concentration is then transformed to an effective food concentration. This may then be further modified to indicate the quality of the effective food concentration.

(e) Secondary production

The starting point in modelling the amount of secondary production associated with a particular system is to parameterize the portion of ingested food that is assimilated by the organism. Typically, two approaches are used for this. The first simply assumes that a constant fraction of the ingested food is assimilated in a given time. This takes the form in the model of a parameter that modifies the ingestion formulation discussed in the previous section. The second approach assumes that the assimilation efficiency of the animal depends on the ambient concentration of food. One example is an assimilation efficiency, Aff, of the form

$$\text{Aff} = 0.3 \, (3 - 0.67 \, \text{Ing}) \tag{A2.19}$$

where Ing is the ingested food. The above form gives an assimilation efficiency that is a maximum at low food concentration and decreases asymptotically to approximately 70% at high food concentrations.

The portion of the ingested food that is not assimilated is taken to represent faecal pellet production. In terms of modelling the transfer of a contaminant through a marine system, this process could be quite important. If the contaminant is not in a form that is assimilated by the organism, faecal pellets represent a mechanism for rapid transport of the substance to the sea bottom. Ingestion of faecal pellets by the detritus feeders also represents a process by which a contaminant can be transported within the food chain.

Excretion by secondary producers represents an important recycling process for marine systems. For some systems, excretion can be the primary source of nitrogen. In models, this process can be parameterized as a linear loss, with some specified rate, from the secondary producers. However, this is not a very realistic approach because experimental studies have shown that excretion rate is related to food concentration, animal size, developmental stage, etc. A better approach is to use experimentally-derived relationships that relate excretion rate to animal size or food concentration. For example, excretion, exc, can be parameterized as

$$\text{exc} = a\,(\text{effective food conc}) + b. \qquad \text{(A2.20)}$$

This gives an excretion rate that depends on effective food concentration. When food is not available, excretion continues at some rate, b, which represents the basal metabolism costs to the organism. Excretion may also have a dependence on temperature.

Modelling the transfer of a contaminant through secondary producers may require parameterization of the developmental stages of a specific organism. If this is the case, then formulations like those above need to be developed for each developmental stage or category (several stages) to be included in the model. This type of model necessitates the addition of formulations that describe the transfer of one developmental category to the next. For example, egg production by adults and development from one juvenile stage to the next need to be modelled.

If a steady state exists, the system of ordinary diferential equations reduces to a set of algebraic equations. Box models are useful for investigating bulk transfers and are fairly easy to implement. These models do not usually require sophisticated numerical techniques or substantial computer resources to obtain solutions.

If the spatial dimension is of concern either because the physical environment controls biological processes, or because the biological processes include migration, a model comprising a set of partial differential equations is required. The most complete model of this type would include three spatial dimensions and time. However, this complexity is not usually necessary. Often, a truncated model (two spatial dimensions and time) is adequate to address the questions of interest. Output from this type of model gives distributions of the contaminant (or whatever state variable) and thus provides additional realism that is not possible with box models. These models, however, can require sophisticated numerical techniques for solution and substantial computer resources.

A2.5 Benthic transport models

(a) Bio-diffusion

The most common description of uptake and mixing of tracers or contaminants in the sea bed is the use of the diffusion analogy. It is hypothesized that burrowing organisms cause mixing in the sediments in such a way as to create a net flow of contaminant down the gradient in concentration (c.f. molecular and eddy-diffusion). The bioturbational flux is thus related to the concentration gradient by a constant of proportionality, the biodiffusion, biomixing or bioturbation coefficient, D_b,

$$\text{Flux} = - D_b \, \partial C / \partial z \qquad \text{(A2.21)}$$

where $\partial C/\partial z$ is the contaminant gradient. The coefficient is not known *a priori* but must be determined from observations by examining the distribution of a tracer down a sediment core with no *in situ* production. Ideally, under steady conditions, the concentration profile is an exponential curve decreasing away from the sediment-water interface, reflecting the balance between mixing and decay.

$$\frac{d}{dz}\left(D_b \frac{dC}{dz}\right) = \lambda C \qquad \text{(A2.22)}$$

where λ is the decay constant. Hence

$$C = C_o \exp\left(-z \left(\frac{\lambda}{\bar{D}_b}\right)^{1/2}\right)$$

where C_o is a constant. For coastal water measurements, values for D_b of 42 ± 16 $cm^2 a^{-1}$ are found (Kershaw et al., 1988).

A simple constant of proportionality has proved to be inadequate for describing some tracer profiles in sediment cores. Depth dependent biodiffusion coefficients, based on ideas of changing density of organisms with depth, have been tried, but these do not necessarily show any improvement over the constant value. The problem arises when biological activity causes sediment to be moved over relatively large distances (conveyor-belt feeders).

(b) Burial

Most benthic transport models use a coordinate system which is fixed relative to the sediment-water interface. However, if there is a net sediment deposition on, or erosion from, the sea bed, these axes will move in space admittedly by a very small distance (1-2 cm a^{-1}). The effect is represented on the moving axes by a burial (downward) or erosion (upward) velocity which is added to the sediment velocity generated by the biological activity.

At steady state

$$d(D_b\ dC/dz)/dz = \lambda\ C + w\ dC/dz \qquad (A2.23)$$

where w is the sediment burial velocity. Hence,

$$C = C_o \exp\ (\ (w- (w^2 + 4\ D_b\ \lambda)^{0.5})\ z\ /\ (2\ .\ D_b))$$

(Berner, 1980).

(c) Conveyor-belt feeders

The treatment of head-down (i.e., feeding at depth and moving sediment to the surface) and head-up (i.e., surface feeders defaecating in their burrows) feeders is very similar from a mathematical view point. The important pieces of information needed are the depths at which the organisms feed and defaecate and the rate of their activity. These give the rate of sediment movement and the distance over which it is moved. This enables a 'feeding function' to be constructed that describes the depth distribution of particle ingestion and egestion. From this can be deduced a sediment movement speed, arising from sediment being removed from one depth and deposited at another. For example, at steady state, an upward conveyor-belt mechanism can be represented by:

$$d(w\ c)/dz + (K_E + \lambda)\ c = 0 \qquad (A2.24)$$

and

$$dw/dz = -\ K_E \qquad (A2.25)$$

where K_E is the fraction of material moved from depth z and w is the induced sediment velocity (Boudreau, 1986; Robbins, 1986).

Conveyor-belt feeders, or other organisms in the sea bed, may also cause some local disturbance of the sediment inducing a diffusional type of mixing on top of the conveyor-belt movement. Thus, for a proper description of the contaminant distribution in the sea bed both the conveyor-belt feeding function and some small diffusivity may be required. The diffusivity has the effect of smearing the peaks in concentration which can occur at the base of the feeding region (egestion layer for surface feeders) when this has been moved by the induced sediment velocity. Again, the method of determination of the biodiffusion coefficient (now only part of the description of the system) has to be by fitting to the observations although this may be complicated by the lack of precise knowledge of the feeding function.

(d) Sediment description

So far the discussion of the parameterization has implicitly assumed that the sediment is treated as a single phase continuum. The sea bed consists of particles of different size with interstitial water. As with suspended particulates in the water column, there is exchange of contaminant between particles and water. It may be necessary to model the two phases separately. This can be done by introducing the concept of porosity which is related to the fraction of solids per unit volume. Biodiffusion, burial and conveyor-belt mechanisms can easily be reformulated to deal with the amount of sediment moved, using the fraction of the volume occupied by the sediment derived from the porosity. If there is compaction of the sediment with depth, porosity will be depth-dependent.

The interstitial water can be treated in a similar manner to the sediment particles, using porosity, but the amount of water moved by the biota and the mixing of the water within the sediment could be different from that of the particles. Consequently, a similar formulation can be constructed for the water, but there remains the problem of determining a different set of rate coefficients in the equations from those for the sediment particles. In practice, the coefficients are usually taken to be the same for lack of better information.

Within the sea bed, particle grain size and organic content change. This will affect the attractiveness of particles for ingestion by organisms. The small particles are often ingested in preference to the larger ones, causing a grading of the sediment grain size during mixing. Particle selectivity can be modelled by a 'feeding selectivity factor', so that the actual feeding rate is proportional to that for the whole sediment. The selectivity factor can be related to the ratio of the concentration of the contaminant on the ingested material to that on the sediment in the feeding site. Thus, if the ratio is unity then the animal shows no preference, but if it is less than one, particles with a lower contaminant concentration are being selected, and vice versa for values greater than one. As small particles usually adsorb more contaminants than larger ones, a selectivity factor greater than one would indicate a preferential feeding on smaller particles.

The discussion of parameterization for the near field holds for the far field. However, with many contaminant profiles in the sea bed it is often difficult to distinguish between the results of a conveyor-belt description of biological mixing and biodiffusive mixing. For example, a steady-state upward conveyor-belt mixing leads to homogenization of contaminant profiles for increasing removal frequencies (faster conveyor) relative to the non-biological sediment burial. Consequently, biodiffusion remains a useful tool in certain circumstances when details of the distribution of the contaminant in the sea bed are not required but only the rate of removal of contaminant to the sea bed, the inventory in the sea bed and the rate of release back into the overlying water.

(e) Geochemistry

All the above discussion has assumed that the sediments are oxic, whereas, in many circumstances, at a depth of a few centimetres oxygen is wholly depleted. A number of chemical reactions then take place which influence the mobility of substances within the seabed. For example, manganese precipitates in oxic conditions and redissolves under anoxic conditions. In such cases, the pore water above the redox boundary contains low dissolved manganese and pore-water below the boundary is high in dissolved manganese. Precipitation above the redox boundary and diffusion from below results in a dissolved manganese concentration peak just above the boundary. It may therefore be necessary to represent the sea bed by a number of layers depending on the chemical conditions which occur. As conditions in the overlying water column change, the depths of the redox boundary may also alter, potentially resulting in either trapping or release of contaminant incorporated in the seabed. It may be necessary to resolve the detailed chemistry but, in some circumstances, a two-level seabed model with the interface between them at the redox boundary position may suffice.

(f) Pore water pumping

The exchange of contaminant with the seabed may be enhanced by the presence of burrows. Changes in hydrostatic pressure across a burrow system may pump water physically through the burrows, but also biota within the burrow can increase the flushing of water. In experimental studies of deposit feeders, Aller and Yingst (1985) found that there was an increased diffusion in the pore water in the upper sediment layers in the presence of macrofauna. Using a 2-dimensional model which could represent the abundance, size and depth of burrowing, they found that it was possible to describe the apparent time variation in this increased diffusion and also the larger values of diffusion measured at longer times in their experiments. A simple non-local parameterisation suggested by Emerson et al (1984) effectively mimics the behaviour of their more complicated model for typical non-steady state and steady-state cases.

A2.6 Coupling between transport models

A2.6.1 Biota-water interactions

Although strictly outside the field of geochemistry, biological interactions with substances in solution or on particles in coastal zone systems include aspects that are actually chemical in nature. The major interactions that must be represented in coastal zone models for the present application are:

1) biological uptake and incorporation of substances into biological materials;

2) the subsequent release of incorporated substances to solution during decay of marine organisms after death.

Although, it might be assumed that the uptake of substances from solution by living organisms would differ from the processes of adsorption onto dead biogenic material and inorganic particles, this assumption has been recently questioned (Fisher, 1986). It appears that uptake of metals by both living and dead phytoplankton is similar and that these associations are in accordance with Freundlich adsorption isotherms (Fisher et al, 1983, 1984; Fisher 1985). Nevertheless, if relative equilibrium between the particulate and dissolved phases of constituents can be assumed, as has been argued above, it becomes immaterial for modelling purposes whether the uptake is from solution or from particles or whether the process is active or passive. It can be assumed that disturbances of the dissolved-particulate equilibrium due to biological uptake are rare. This seems to be an eminently sensible assumption for long time-scales even if it may be untrue for short, e.g., diurnal or multi-day, time scales. Even when disequilibria occur, they involve disturbances smaller than an order of magnitude (e.g. dissolved nitrate). Such assumptions would permit the use of so-called biological concentration factors for typical coastal zone organisms to be introduced into the modelling process to take account of interactions of substances between the dissolved and non-biological particulate forms of substances and the biological phases. In this sense the 'biological concentration factor' becomes analogous to a partition coefficient but applies to the relationship between the concentration of the substance in organisms (or a particular type of organism) and the dissolved concentration of the substance in the surrounding water.

The regeneration or dissolution of substances from decaying biological material is largely a passive chemical process. The amounts of organic and inorganic biogenic material that are regenerated will depend heavily on factors such as the depth of the water column and sedimentation rate. However, it can often be assumed (except under circumstances of small water depth and/or high sedimentation rate) that most of the nitrogen and phosphorus associated with the organic material is regenerated in a manner that returns these chemicals to the euphotic zone, for re-assimilation, at a rate depending upon the vertical circulation. Other constituents will be regenerated at rates intermediate between the nutrients and that of the organic carbon itself. The inorganic biogenic material will generally be much less completely regenerated but clues as to the extent of such dissolution can be obtained from an examination of the local sediment composition and the extent to which intact burial of skeletal or exo-skeletal material is occurring.

A2.6.2 Sediment-water interactions

(a) Partition coefficients for decaying contaminants

Partition coefficients are related to the steady state of an exchange process. For a process that includes decay, a steady state might never be reached as concentrations decrease and approach zero at large times. For many cases, a partition coefficient, defined as the ratio of the concentrations, can be used (O'Conner, 1988). The following example is provided.

A decaying contaminant, a nuclide, is dissolved in the water phase and adsorbed to particles and the nuclide is exchanged between the water and the particles through sorption and desorption processes. The equations describing this process are given by:

$$\frac{\partial N_p}{\partial t} = k_1 N_w - k_2 N_p - \lambda N_p \qquad \text{(A2.26)}$$

$$\frac{\partial N_w}{\partial t} = - k_1 N_w + k_2 N_p - \lambda N_w \qquad \text{(A2.27)}$$

concentrations becomes

$$\frac{C_p}{C_w} = \frac{K_1 V_w}{K_1 m_p} \quad (= R_d\text{, see below}) \qquad \text{(A2.28)}$$

(b) Parameterization using K_d

The distribution ratio, R_d, is the ratio of the amount of the substance per unit mass of solid to the amount of the substance per unit volume of solution and therefore has units of Length^3 Mass^{-1}. It is purely an empirical representation of the partitioning between solid and solution phases and does not imply equilibrium. In laboratory experiments, R_d is used in a manner that neither implies reversibility nor equilibrium but we can still use the concept in assumed-reversible situations. In cases where equilibrium conditions prevail, or equilibrium is intrinsically assumed, as is common in the deep marine environment, the term distribution coefficient or partition coefficient (K_d) is commonly used.

It should be noted that although a sorption experiment or field measurement of particulate-water partitioning may represent truly equilibrium conditions, and thus the partitioning may be correctly represented as an equilibrium partition (or distribution) coefficient K_d, this coefficient is not a universal constant and only applies to the partitioning under fixed conditions, such as of temperature, concentration, pH and Eh. The distribution coefficient has the same form and units as R_d but implicitly applies to situations in which steady-state equilibrium applies. Various models have been used to relate the amounts of a substance adsorbed to particles to the concentration of the substance in solution under certain, usually isothermal, conditions. The most commonly used model is the Freundlich isotherm model which can be expressed as

$$A = B\ C^N \tag{A2.29}$$

where A is the amount of solute adsorbed per unit weight of solid; C is the equilibrium solute solution concentration; and B and N are constants.

We can apply this approach to the characterization of adsorption reactions to a situation in a column of coastal zone water of depth h to determine the vertical removal flux of a substance as follows:

First-order removal of a substance (in trace concentration) by settling particles (F) in a well-mixed water column is a function of the vertical flux of settling particles (S) in the following manner:

$$h\ dC_t/dt = -\ \alpha_t\ C_t\ h = -\ S\ X = F \tag{A2.30}$$

where α_t is the first order removal rate constant of the substance from the water column, C_t is the total concentration of the substance in the water column and X is the concentration of the substance in settling suspended particles.

Then

$$\alpha_t = S\,X/C_t\,h = S\,K_d/[h(1 + K_d\,C_s)]$$

Where

$$C_t = C + X\,C_s$$

if $K_d\,C_s \ll 1$, then

$$\alpha \approx S\,K\,/h_t$$

$$\text{or } \log \tau_t = -\log \alpha_t = -\log K_d - \log(S/h)$$

Where C is the dissolved concentration of the substance, C_s is the particulate matter concentration, K_d is the distribution ratio of the substance between particles and water and τ is the residence time. If a water column is not well-mixed on the time-scale of removal, α_t would need to include a rate constant for the finite rate of mixing.

This model for removal of substances from solution by association with particles and subsequent sedimentation can be tested by application to coastal zones, and indeed to the entire ocean, by determining the rate constant α_t or its inverse, the residence time of the substance τ_t. If equilibrium conditions apply and K_d is truly an equilibrium constant, there should be a linear relationship between τ_t and the particle removal rate (S/h) in a range of differing systems with the relationship having a slope of unity (-1) on a log-log scale. This, for example, is the case for particle reactive zinc in a variety of lakes (Santschi, 1984). This may not be the case if the apparent K_d (i.e. truly an R_d in which no assumptions of equilibrium conditions are made) varies significantly. A similar plot for thorium in marine environments does not show a plot with unit slope but one having a smaller slope (Santschi, 1984). This can be rationalized on the basis of changing R_d for thorium from smaller values in nearshore systems to larger values in deep-water environments because attainment of an adsorption-desorption equilibrium is a slow process. This does not prevent the use of an assumed equilibrium partition coefficient for representing particle-solute exchanges in sub-systems of the marine environment as long as the constant is appropriate to that environment and does not vary widely within the sub-system.

For the many elements for which equilibrium can be assumed throughout the marine environment, the partition coefficient can be estimated on the basis of τ_t. Recent work (P.A. Yeats, private communication) has shown that, when care is taken in selecting accurate data for the construction of oceanic mass-balances, it is possible to obtain a great deal of uniformity and consistency between K_d [derived from the existing natural partitioning of the elements between deep-ocean water and pelagic clay sediments in a similar manner to that used by Li (1981) and Whitfield and Turner (1979, 1981)] and residence time, τ_t, estimates for elements in the ocean. This provides the possibility of being able, not only to rationalize effective partition coefficients for the entire ocean for well-studied elements (and, if the particle-solute interaction is in steady-state throughout the ocean, determine universal marine K_d values for these elements) but also to determine the effective K_d values for poorly understood elements. This has a great deal of utility in modelling of particle-solute interaction processes in the coastal zone. Clearly, however, as stated above, some elements have slow kinetics for these interactions and such an approach would have to be used with care in these cases.

Information on the extent of disequilibrium in coastal systems can be gained from laboratory equilibration experiments of the type carried out by Nyffeler et al. (1984) in which the distribution coefficients for various elements was followed over a period of about 100 days under both adsorptive and desorptive conditions. These authors were able to demonstrate that the distribution coefficient for Na, Zn, Se, Sr, Ag, Cd, Sn, Sb, Cs, Ba, Hg, Th and Pa was constant after a few days of equilibration whereas Be, Mn, Co and Fe exhibited changing distributions over the entire 100 day adsorption period. Nevertheless, the changing distribution coefficients of these latter elements could be modelled on the basis of an additional first-order lattice reaction for the sorbed element on particles.

(c) Applications to coastal zone models

There are two major advantages of coastal zone systems that provide significant benefits in respect to representing particle-solute interactions in such systems. The first is that water residence times (flushing times) are in the range of days (estuaries) to a few months (marginal seas, excepting those with stagnant deep-water layers such as the Baltic). This then represents the time-scale over which particle-solute interactions need to be represented. This range of time-scales is close to that which can be represented in laboratory equilibration experiments to determine exchange reaction rates. This means that it is often possible to carry out laboratory simulations of particle-solution interactions on time-scales similar to those of interest in respect to typical coastal zone systems. Thus, even if K_d is not really an equilibrium constant, it can be applied to determine adsorption-desorption exchanges in these systems on the basis of partition coefficients derived directly from laboratory experiments. The second advantage is that coastal zones generally contain the highest particle concentrations of all marine environments, possibly excluding benthic boundary nepheloid layers. Since the adsorption reaction rate is proportional to the suspended particulate concentration, there is a larger probability that equilibrium is actually attained in such systems. This provides greater confidence that, for substances for which only generic K_ds can be obtained, it is likely that these will be adequately approached in coastal systems because of the larger particle concentrations. This of course must be tempered with the correspondingly shorter time for reactions to attain equilibrium because of the limited residence time of water in the system.

It should be emphasized that all that has been said with regard to particle-water exchanges and to characterization of particulate transports applies only to the exchangeable phase of substances on particles. The lattice constituents of rock mineral matrices, such as aluminosilicate weathering products, are not generally involved in exchanges within the marine environment at all. Thus, the measurement of particle-associated contaminants should be applied to the non-matrix components of those contaminants. Alternatively, allowance must be made for the detrital (lattice mineral) phase composition of particles. Furthermore, it also means that the only particles of interest in respect to particle-water exchanges are the silts and clays since larger particles have very small exchange capacities or specific surface area for adsorption in relation to mass.

It is concluded that, in general, an assumption of equilibrium conditions for the interactions between particles and solutes can be made for most coastal zone areas and constituents. This permits the characterization of exchange equilibria between particles and solution with an (assumed) equilibrium partition coefficient K_d. Care would need to be taken in situations in which an assumption of equilibrium conditions is not valid. Clues as to the acceptability or not of an equilibrium assumption can be gained from existing information on the nature of constituent distributions in the coastal zone, especially within estuaries which will exhibit the highest likelihood of non-equilibrium distributions. Even in cases where it is known that the equilibration takes considerable time, as for example with beryllium, manganese, cobalt, iodine, iron and arsenic, it may still be possible to make equilibrium assumptions while ensuring that the partition coefficient is appropriate to the specific environment to which it is to be applied.

A2.7 Diagenesis: water-sediment interactions

The theoretical aspects of the properties and transport of substances within an accumulating sedimentary environment are presented in Berner (1980). The general area of relevance to this study is that of early diagenesis which deals with the changes in sediments, as a result of physical, chemical and biological processes, following their deposition from water, but before deep burial.

When considering the time (t) and depth (x) changes of a property, p, in the sediments, it is necessary first to define a reference coordinate system. There are two potential origins for the depth coordinate - either a given layer in the sediments or the sediment-water interface. The first remains fixed in space and time; whereas, the second changes with sedimentation rate over time. Transformation from one origin to the other is given by:

$$\frac{dp}{dt} = \left(\frac{\partial p}{\partial t}\right)_x + w\left(\frac{\partial p}{\partial x}\right)_t \qquad \text{(A2.31)}$$

where w is the rate of burial of the layer below the sediment-water interface. Subscripts denote no change in the associated dimension. Under steady-state conditions, with no compaction, this is equivalent to the sedimentation rate.

In the absence of diagenesis, the changes in p with depth are due to temporal changes at the time of deposition. Thus,

$$dp/dt = 0 \quad \text{(no diagenesis)} \tag{A2.32}$$

and

$$(\partial p/\partial t)_x = - w\ (\partial p/\partial x)_t \tag{A2.33}$$

Under these conditions and w invariant with time, it is possible using equation A2.33 to determine the original rate of change of p at the time of sedimentation. At the other extreme, let us assume that all changes in p with depth are due to diagenesis. In other words, w is constant and there have been no other fluctuations of the delivery of p to the surficial sediments with time. This produces a condition of constant upper boundary condition and steady-state diagenesis where p at a given depth remains constant. That is:

$$(\partial p/\partial t)_x = 0 \tag{A2.34}$$

and

$$dp/dt = w\ (\partial p/\partial x)_t \tag{A2.35}$$

There is a third possibility. This occurs when there is a steady-state distribution of the property with depth, but no diagenesis. Under these conditions,

$$(\partial p/\partial t)_x = 0 \tag{A2.36}$$

and $dp/dt = 0$ (A2.37)

thus

$$(\partial p/\partial x)_t = 0 \tag{A2.38}$$

This results from either the presence of non-reactive p in the sediment or rapid attainment of equilibrium at the time of deposition both resulting in no change of p with depth.

The general equation for diagenesis is derived from mass-conservation on a volume of sediment:

$$\partial C_i/\partial t = - (\partial F_i/\partial_x) + \sum R_i \tag{A2.39}$$

where C_i = concentration of solid or liquid component i in mass per unit volume of total sediment;

F_i = flux of component i in terms of mass per unit area of total sediment per unit time;

R_i = rate of each diagenetic, chemical, or radiodecay reaction affecting i in terms of mass per unit volume of total sediment per unit time.

Fluxes are of two types, diffusive and advective. Thus,

$$F_i = - D(\partial C_i/\partial x) + VC_i$$

Where D is the diffusion coefficient; and V is the vertical velocity relative to the sediment-water interface.

Berner's (1980) treatise goes on to parameterize the influences of compaction and changing porosity on pore-water advection, the bulk diffusion of pore-waters and solids within the sediments and the diffusion of substances at the surface of solids, the correction of Fick's Laws of diffusion for electrical effects and tortuosity, analogues to diffusion arising from the movement of substances by infaunal biological activity and advective and diffusional transport across the sediment-water interface, approaches to representing the movement of chemical constituents resulting from redox gradients in the sediments.

A2.8 Parameterization of the source term

A2.8.1 Nature of source

Various aspects of the approach to coastal zone modelling for the purposes of establishing relationships between release rates and doses depend upon the nature of the source function involved. In this context the term 'dose' is used in a generic manner to imply the biological effects of a particular practice or contaminant release to a coastal environment. Some characteristics of the source and its method of disposal will imply constraints upon the approach and actual modelling procedure used to establish the dose-release rate relationship. These characteristics can be divided into those that involve the form and composition of the material entering the coastal marine environment and those that relate to the disposal procedure (i.e. the method, rate and place of disposal). These two aspects can then be characterized in a manner that constitutes a source function.

In addition, environmental concerns often pertain to specific chemical compounds. Different chemicals behave differently. Even for the same category of chemicals, e.g., chorophenols, the derivatives (e.g. tri-, tetra- and pentachlorophonols) have different characteristics such as sorption and photolysis. They need to be treated individually according to their chemical properties. A further complication is that, depending on the presence or absence of other chemicals, chemical reaction may or may not occur. Data availability is a major factor in formulating the interactions among these forms.

The method of ocean disposal is an important consideration in the construction of models. Whether it is a large bulk dumping over a short span of time, or whether it is a coastal discharge through a submerged diffuser, the problem of parameterizing the input conditions exists.

A2.8.2 Bulk sources

If the contaminant is introduced in a free form, modelling of its behaviour can be carried out on the basis of representations of the various processes (physical, chemical and biological) that control its behaviour. However, in most situations, the contaminant will be a constituent of some other host material when it enters the marine environment and it is necessary to include in the modelling representations of the way in which the contaminant(s) of interest is retained in the host material and the extent to which it is transformed and released to become associated with other phases in the receiving environment. It should be noted that there will be cases in which the substance of interest is not a specific contaminant but a type of material or mixture (e.g. sewage sludge). It is conceivable that it might be desirable to model the behaviour and transport of such materials in bulk form rather than dealing with individual constituents (contaminants) in those mixtures.

As a first step in defining the nature of the source term it will generally be necessary to identify the contaminant(s) of interest in the sense of determining which constituents of a waste are likely to be important in alternately limiting the scale of the activity. Usually, this is a fairly straightforward procedure which can be based upon either a knowledge of the composition of the material to be disposed of or from previous experience with the disposal of similar types of waste material. Even in the case of poorly-defined classes of waste material, like acid mine-wastes and sewage sludge, it is possible to identify specific constituents that are likely to impose the largest threat to human and animal populations in the receiving environment and its surroundings without great difficulty.

The next steps are to define the bulk nature of the host material in which the specific contaminant of interest is located when it enters the coastal marine environment and to characterize the manner in which the constituent (contaminant) of interest is retained or released from the host material.

The bulk forms that a material, intended for disposal into the coastal zone, may take are liquid and solid or a mixture of these. The solid forms can range from massive bulk forms to fine particulates, each of which will clearly have differing behaviour in the receiving environment and from which the contaminant may be mobilized and exchanged with other forms. Liquid forms may be aqueous or other miscible liquid or non-miscible forms. At one extreme of this spectrum of material types, water, the dispersion of the liquid, but not necessarily its constituents, can be dealt with wholly by consideration of the physical oceanography of the receiving system. Similarly, at the other end of the spectrum, bulky and insoluble solids can also be considered to be mobilized wholly by physical oceanographic forces. Other host materials of either liquid or solid forms are also moved wholly by physical forces but, for these materials, other processes become important controlling factors in their behaviour and these may depend upon certain characteristics of the host material such as its physical and chemical composition.

These factors include first the manner in which the specific contaminant of interest is retained in the host material both physically and chemically, the chemical conditions in the source (e.g. pH and Eh), the manner in which the contaminant is transformed or decays, and the nature of the non-physical interactions within the receiving environment. These can be characterized as reactivity terms characterizing chemical and radioactive decay, dissolution/precipitation, other aqueous-particulate exchange, and biological uptake, transformation and release. In this way, both the nature of the association between the contaminant of interest and its host waste form and the release of the contaminant from the waste form and its subsequent interaction with other materials in the receiving environment can be characterized for modelling purposes.

A2.8.3 Disposal procedure

The disposal practice itself will also influence the source term function required for modelling of the transport and effects of contaminants. Material may either be discharged into freshwater streams or through marine discharge pipelines, or dumped in packaged or unpackaged forms. In any rigorous examination of transport in coastal receiving waters, atmospheric transport and deposition would also need to be considered as an input to the system. However, this form of disposal has been excluded from this discussion since it is unlikely that any deliberate use of coastal waters for waste disposal via the atmosphere would occur. The only notable exception to this is incineration of wastes at sea where the source provides inorganic matter (HCl) and recombinant organic compounds that enter the marine environment through atmospheric despostion. (This method of disposal is expected to be banned in the 1990s as a consequence of decisions in both regional (Oslo) and Global (London) Marine Environmental Protection Conventions.) Thus, in practice, the only forms of disposal entertained within this analysis are direct discharge and dumping, the latter meaning the dropping overboard of wastes in packaged or unpackaged form from a vessel .

The second aspect of either route of disposal concerns the dimensions of the source. This can either be a point source of small dimensions compared with those of the receiving system, a line source where one dimension of the source is significant in relation to the dimensions of the size of receiving environment, or a diffuse or widespread source where the introduction of materials to the system occurs over dimensions comparable with the receiving environment. Examples of the latter case would be widespread dumping throughout the receiving environment or diffuse runoff that enters the system from a number of diverse line or point sources (GESAMP, 1987). The dimensions of the source would need to be considered in the modelling carried out in order to faithfully reflect transport of material from the source(s). Finally, the timing of the releases of material to the receiving system also needs to be characterized. Releases can be essentially continuous, fluctuating or discontinuous. Continuous releases are the simplest type to represent in models although fluctuating releases do not provide much greater complexity in modeling. Discontinuous releases, of either the single event or separated event form, where the release time is short compared with the intervals between releases, are the most difficult to accommodate in models. Frequent, discontinuous releases can sometimes be characterized as fluctuating releases if the time of release is long compared with the interval between releases and the flushing time of the receiving system.

A2.8.4 Specific chemical compounds

There are numerous types of chemicals entering the coastal zone. Several attempts have been made to classify these chemicals. From a modelling point of view, however, it is convenient to consider the different chemicals according to their properties and their environmental impacts. Thus, most models are designed to simulate the transport, pathways, fate and impact of the following classes of chemicals: radionuclides, metals, organic toxicants, nutrients and pathogens.

It must be emphasized again that most discharge effluents contain chemicals belonging to more than one of these classes. While models have been constructed using the whole effluent or bulk source approach (Young et al., 1985), many models are still chemical-specific. The chemical-specific models are developed by assuming reactivity terms specific to the chemical chosen. Thus, there are always restrictions in extending these models to other chemicals. For example, tritium models (e.g. Lam and Durham, 1984) generally assume that tritium is released in liquid form in a liquid host (water) so that the only important reactivity term is radioactive decay. The extension of such a model to other radionuclides may not be straightforward. For example, Technetium (^{99}Tc) has a long half-life (2.1×10^5 years) and exists in different oxidation states including the pertechnetate anion TcO_4 form. Simulation of this radionuclide calls for at least the hydrodynamic model and biological uptake/reactivity terms.

Similarly, models designed for the Fe(II) compounds in liquid form must be modified if it is applied to the Fe(III) compounds in solid form. In addition to the inorganic forms, metals also form organic complexes in seawater (e.g. alkyl lead and organo-cadmium complexes). A large class of toxic chemicals is organic in nature, e.g. chlorinated phenols, DDT, triazines, chlorophenoxyacetic acids, polycyclic aromatic hydrocarbons, clorinated benzenes and Malathion. Many of these are pesticides or their residues which enter the coastal zone from land-based effluents or through sea dumping. The organic toxics and the various forms of specific chemicals require special model formulation (Stepien et al., 1987) as many of the reactivity processes are not fully understood.

In contrast, model development for the nutrients has been quite extensive, particularly for eutrophication problems (e.g., phytoplankton blooms oxygen depletion and odours). Typical nutrient compounds influencing primary production include orthophosphate, nitrate and ammonium. These eutrophication models are fairly well developed and often include many chemical and biological variables, i.e. they are not restricted to one specific chemical. On the other hand, models developed for bacteria, viruses and other pathogenic or nuisance organisms are not as advanced, although many coliform models have been used for sewage outfalls.

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MEETING DATES

(1) IAEA Headquarters, Vienna, 27-31 January 1986

(2) Sidney, Canada, 4-10 September 1986

(3) Delft, The Netherlands, 11-15 May 1987

(4) IAEA, Headquarters, Vienna, 8-12 February 1988

(5) IAEA, Headquarters, Vienna, 7-11 November 1988

(6) IAEA, Headquarters, Vienna, 13-17 March 1989

(7) IAEA, Headquarters, Vienna, 6-10 November 1989

GESAMP REPORTS AND STUDIES

The following reports and studies have been published so far. They are available from any of the organizations sponsoring GESAMP.

1. Report of the seventh session, London, 24-30 APril 1975. (1975) Rep.Stud.GESAMP, (1):pag.var. Available also in French, Spanish and Russian

2. Review of harmful substances. (1976) Rep.Stud.GESAMP, (2):80p.

3. Scientific criteria for the selection of sites for dumping of wastes into the sea. (1975) Rep.Stud.GESAMP, (3):21p. Available also in French, Spanish and Russian

4. Report of the eight session, Rome, 21-27 April 1976. (1976) Rep.Stud.GESAMP, (4):pag.var. Available also in French and Russian

5. Principles for developing coastal waster quality criteria. (1976) Rep.Stud.GESAMP, (5):23. Published also as UNEP Regional Seas Reports and Studies No. 42

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7. Scientific aspects of pollution arising from the exploration and exploitation of the sea-bed. (1977) Rep.Stud.GESAMP, (7):37p.

8. Report of the ninth session, New York, 7-11 March 1977. (1977) Rep.Stud.GESAMP, (8):33p. Available also in French, Spanish and Russian

9. Report of the tenth session, Paris, 29 May - 2 June 1978. (1978) Rep.Stud.GESAMP, (9):pag.var. Available also in French, Spanish and Russian

10. Report of the eleventh session, Dubrovnik, 25-29 February 1980. (1980) Rep.Stud.GESAMP, (10):pag.var. Available also in French and Spanish

11. Marine pollution implications of coastal area development. (1980) Rep.Stud.GESMAP, (12):22p.

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13. Interchange of pollutants between the atmosphere and the oceans. (1980) Rep.Stud.GESAMP, (13):55p.

14. Report of the twelfth session, Geneva, 22-29 October 1981. (1981) Rep.Stud.GESAMP, (14):pag.var. Available also in French and Russian

15. The review of the health of the oceans. (1982) Rep.Stud.GESAMP, (15):108p. Published also as UNEP Regional Seas Reports and Studies No. 16

16. Scientific criteria for the selection of waste disposal sites at sea. (1982) Rep.Stud.GESAMP, (16):60p.

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18. Report of the thirteenth session, Geneva, 28 February - 4 March 1983. (1983) Rep.Stud.GESAMP, (18):50p. Available also in French and Spanish

19. An oceanographic model for the dispersion of wastes disposed of in the deep sea. (1983) Rep.Stud.GESAMP, (19):182p.

20. Marine pollution implications of ocean energy development. (1984) Rep.Stud.GESAMP, (20):44p.

21. Report of the fourteenth session, Vienna, 26-30 March 1984 Rep.Stud.GESAMP, (21):42p. Available also in French, Spanish and Russian

22. Review of potentially harmful substances. Cadmium, lead and tin. (1985) Rep.Stud.GESAMP, (22):114p. Published also as UNEP Regional Seas Reports and Studies No. 56

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24. Thermal discharges in the marine environment. (1984) Rep.Stud.GESAMP, (24):44p. Published also as UNEP Regional Seas Reports and Studies No. 45

25. Report of the fifteenth session, New York, 25-29 March 1985. (1985) Rep.Stud.GESAMP, (25):49p. Available also in French, Spanish and Russian

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31. Report of the seventeenth session, Rome, 30 March - 3 April 1987. (1987) Rep.Stud.GESAMP, (31):36p. Available also in French, Spanish and Russian

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