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Report of the ASMO Workshop on Modelling of Contaminant Transport and Fate

4-7 November 1997, The Hague, The Netherlands

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ITLE:

Report of the ASMO Workshop on 'Modelling Transport and Fate of Contaminants'

BSTRACT:

he Environmental Assessment and Monitoring Committee (ASMO) of the Oslo and Paris Commission (OSPARCOM) ecided during its first meeting in March, 1994 that it was important to increase cooperation between contracting parties ith regards to modelling. Important issues included the scope and objectives of existing models and future coordination of odelling activities. In the organization of these modelling coordination activities, The Netherlands was selected as lead untry. To this end, it was decided to hold a series of three ASMO modelling workshops:

Use of models in environmental risk assessment of accidents in the shipping and offshore industries, 15-17 November, 1995
Modelling of eutrophication issues, 5-8 November, 1996
Modelling transport and fate of contaminants, 4-7 November, 1997

l workshops were held at RIKZ in the Hauge, The Netherlands.

is report gives the summary of the third ASMO modelling workshop on 'Modelling Transport and Fate of ntaminants'. Summaries of nine different contaminant transport models are presented together with results of the mparison exercises conducted for the workshop. A discussion of some comparisons and contrasts between models is esented and references for each model are given.

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	M.T. Villars		April 1998	approved by ASMO	M.R.L. Ouboter		T. Schilperoort	

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Summary

Introduction

The workshop on "Modelling of Transport and Fate of Contaminants" was the third in a series of workshops organised by the Environmental Assessment and Monitoring Committee (ASMO) of the Oslo and Paris Commission (OSPARCOM). The Netherlands, lead country for ASMO modelling cooperation, hosted the workshop, which was organised by Rijkswaterstaat - The National Institute for Coastal and Marine Management (RIKZ). The workshop was held on November 4-7, 1997 in The Hague, The Netherlands.

The modelling cooperation activities within ASMO include conducting an inventory of models relevant to the convention area, as well as holding 3 workshops relevant to the QSR-2000 process:

1995	Environmental risk assessment of accidents in the shipping and offshore industries;
1996	Eutrophication issues (nutrient concentrations, blooms, and foodwebs); and
1997	Pollutants (transport, routes and fate).

Six countries participated in the workshop: France, The Netherlands, Germany, The United Kingdom, Norway and Denmark.

Objectives

The objectives of the workshop were defined in the Terms of Reference as drawn up by ASMO at the second meeting of ASMO, April 1995. The general objective was to review the available models and current modelling activities used to assess contaminant transport and fate issues in the North Sea and other Convention waters.

Specific objectives were:

- to evaluate the agreement between model results and available in-situ data, (i.e. model validation), and
- to evaluate the responsiveness of models to anthropogenic input reduction.

Models Presented

A total of 9 models were presented by 7 institutes from five countries. Models were available for the following areas: Greater North Sea, Southern North Sea, English Channel and estuaries (Scheldt and Seine estuary). A listing of all the models presented during the workshop, including country and institute, is given in Table 1.

These models have widely different spatial and temporal scales, reflecting the different goals for which they were originally developed. The spatial variability ranges from the Greater North Sea (with a maximum grid size of 35 x 35 km) to estuarine scale with a spatial resolution (~ kilometers) to resolve steep concentration gradients, to no spatial variability (e.g. chemical equilibrium model).

The *temporal variability* of models also covers a range, from steady state (i.e. no temporal variability) to temporal resolution within a tidal cycle. The time resolution of the external forcings also affects the temporal variability of the models. The hydrodynamic models need external meteorological forcing (e.g. wind, tides) to drive the water circulation. The temporal scale of this forcing ranges from long-term average conditions, to actual meteorological (hourly, daily) data.

The models also have different focuses and strengths in terms of physical (hydrodynamics), chemical and biological/ecotoxicological processes. In terms of hydrodynamics, some models have detailed 3-dimensional computations of flow while others are 2-dimensional (depth averaged). Some have true meteorological forcings of short time scales, while some use monthly average conditions, or are even steady state (no time variation).

For the chemical and biological processes relevant to pollution transport and fate, models also incorporate very different degrees of complexity, reflecting the different goals for which they were originally developed. Processes range from simple (no) processes (i.e. simply transport of conservative contaminants), to detailed reactions including contaminant adsorption, desorption, sedimentation, resuspension, oxidation, reduction, volatilization, degradation, uptake in organisms and concentration in the food chain. A policy oriented model can calculate and rank the environmental risks of different contaminant compounds.

Despite the different focus of models, and some underlying differences, five of the North Sea models (numbers 1-5) were similar enough to allow direct comparison of model results and these were the focus of a model comparison exercise, described further below.

Table 1. Summary of models presented during the workshop

Country/Institute	Model Name	Model Area	Contaminants modelled
1. Germany/BSH	BSHcmod (circulation) BSHdmod.E (eulerian) BSHdmod.L (lagrangian)	North Sea and Baltic Sea	Cd
2. Norway/IMR	NORWECOM	Greater North Sea	Cd, PCB, atrazine, BaP, fluoranthene
3. UK/SOC	NOSTRADAMUS	Southern North Sea	Cd
4. NL/RIKZ and DELFT HYDRAULICS	SCREMOTOX	North Sea	Cd, PCB, atrazine, BaP, fluoranthene
5. NL/RIKZ and DELFT HYDRAULICS	ZeeBos	North Sea	Cd, PCB, atrazine, BaP, fluoranthene
6. Norway/SINTEF	PROVANN	North Sea	dispersed oil
7. France/IFREMER	PCB bioaccumulation model	Seine Estuary	bioaccumulation of PCB in sea bass food-web.
8. NL/RIKZ and DELFT HYDRAULICS	SAWES	Western Scheldt Estuary	Cd, PCB, atrazine, BaP, fluoranthene
9. France/EDF	TELEMAC/SUBIEF	Channel/Bay of Seine	radionuclides

Model Comparison Cases

Because the models were developed for different regions and different purposes, the workshop did not focus only on detailed test cases and output formats. Instead, a more 'loose' intercomparison was defined, focusing on validation results against field data and the responsiveness of models to changes in anthropogenic loadings. For five of the North Sea models which were similar enough, a specific model comparison exercise was conducted. The following analyses were presented.

1. Model Validation in domain of application

The first part of the workshop focused on the conceptual basis of the models in relation to the objectives for their development and on an evaluation of the agreement between model results and in-situ data. Cadmium (as a heavy metal) and PCB-153 (as an organic contaminant) were chosen as the main pollutants of focus, with atrazine, benzo(a)pyrene (BaP), and fluoranthene as additional compounds. Two of the models simulated dispersed oil or radionuclides instead.

In the model validation, a cost function equation was used as one method for giving quantitative measure of the agreement between model results with data. For the North Sea, field data from ICES for dissolved cadmium were made available for validation. Also, results from model validation using other field data were presented. For other regions, data from local monitoring programmes were used.

2. Model Comparison

Five of the North Sea models were the focus of a model comparison exercise. Where possible, comparison of model results with field measurements was also made. Data from the NERC North Sea Project (NSP) from 1988-89 was found to be the best available for this purpose. Seven locations throughout the North Sea were chosen and model inputs for river, offshore and atmospheric loads, boundary concentrations and model parameters were defined. The first model exercise focused on the year 1989 and consisted of:

- comparison of model results and data of salinity and Suspended Particulate Matter (SPM)
- comparison of model results and data of monthly cadmium concentrations
- comparison of model results (no data) of monthly PCB concentrations
- comparison of modelled mass balances of water, SPM, cadmium and PCB

The responsiveness of models to anthropogenic input reduction was the subject of the second part of the comparison exercise. Two reduction scenarios were considered in the exercise, namely:

- 50% reduction of cadmium loads (from rivers and atmospheric deposition)
- 50% reduction PCB-153 loads (from rivers and atmospheric deposition)

Summary of the comparison exercise for 1989

Comparison of model results with salinity and SPM on a yearly time scale (as mean value and range) shows general consistency between the models and good agreement with data at the selected locations. For salinity, the largest range in data and the most differences in models are for the coastal locations in the Dutch coastal zone and German Bight. For SPM, the largest range in the data is near the UK coast, most likely due to cliff erosion, and in the Dutch coastal zone and German Bight. None of the models have the same extent of variation as seen in the data.

The comparison on a monthly time scale for cadmium and PCB is intended to indicate how well the models perform at specific locations over a yearly cycle. Some general comments can be made:

- Five models could make calculations of cadmium concentrations. For dissolved cadmium, all of the modelled concentrations were quite similar (in the range of 0.01-0.03 ug/l) but were consistently *lower* than the measured field concentrations. Also, the modelled concentrations showed much less seasonal variation in concentrations than the data, where maximum concentrations in April-May were as high as 0.07 ug/l.
- For particulate PCB-153 there is no field data from NSP for comparison with model results. Data from other sources included ICES was also too limited for comparison. Three models could make calculations of the PCB concentrations. Model results were similar in the ranges of calculated concentrations and show that compared to cadmium, chemical processes result in much more seasonal dynamics in calculated concentrations .

From the results for cadmium, it can be concluded that there must be (an) additional source(s) of cadmium in the North Sea which all the models are missing. Sources can include cadmium flowing into the North Sea from outside the region as well as sources within the North Sea. Cold deep water flowing in from the North Atlantic can have higher concentrations than the surface water. One possibility presented during the workshop is that offshore drilling activities are contributing significantly to loads. Although this source is included in the calculations, there is still some uncertainty as to its magnitude. Preliminary analysis shows that the discharge of large volumes of production water in the Northern North Sea could be adding cadmium at a level comparable to the combined loads of all the rivers. Other potential sources of contaminants must also be considered, such as dumping of contaminated dredged sediments along the Belgian, Dutch and UK coasts (which was not currently included in the model exercises).

The difference in seasonal variation between models and data is more difficult to explain. There are potentially chemical processes occurring which the models do not include, such as seasonal fluxes from the bottom sediment. Additionally, seasonally varying effects such as concentrations at the model boundaries, or discharges from sediment dumping (neither of which is in the models) could explain the pattern. A final possibility lies in a systematic error in the measurements.

The mass balance calculations give significant insight into some of the differences between models. The water mass balance shows that there underlying hydrodynamics of the models are different, as is also supported by the different focus on time scales, spatial scales, and meteorological forcings used in each model. Significant differences are also seen in the fluxes of SPM in the models, due to large conceptual differences in the way sediment matter is modelled. The interaction between the water column and bottom sediment and thus processes such as sedimentation and resuspension are quite different in the models. Also the composition of 'SPM' in the models is different, in some cases consisting of only inorganic material, while in others including organic and detrital material as calculated by an ecological module. One model had no SPM. Cliff erosion is also included in some models as a source of SPM.

The differences in water balance and sediment flux are reflected in the calculated mass balances for cadmium and PCB. The inflow in from the Straight of Dover, and outflow to the North were quite different, as were the fluxes due to sedimentation. For PCB, the loss due to volatilisation can be important, but not all of the models included this process. It should also be noted that despite defining river, offshore and atmospheric inputs for the comparison exercise, the models show differences in these values, most likely due to the different way in which they are able to incorporate input information.

Although there are differences in the mass balances given by the different models, the net transport over the boundaries for water, SPM, cadmium and PCB are in general agreement with the range of values found in literature.

Summary of responsiveness to load reductions

The results of the model responsiveness to anthropogenic load reductions from rivers and atmosphere are fairly consistent. For cadmium, a 50% reduction of loads generally has an effect of less than 15% in environmental concentrations at seven selected locations throughout the North Sea. The largest concentration decreases are seen in the coastal zones where rivers discharges are the largest contributing source of contaminants. The largest decreases are predicted in the Dutch coastal zone (maximum of 16%) where the influence of decreased Rhine River inputs is the highest. The smallest decreases (1-4%) are seen in the central North Sea, where river influence is small, and inflow over the boundaries is the largest contributing source of contaminants. In general, water flowing into the North Sea from the English Channel and Atlantic have a large contribution to the amount of cadmium in the North Sea.

It should be noted that some data from the Dutch coastal zone for the period 1980-1990 do show that there has been a significant decrease in environmental concentrations of cadmium corresponding to 50% reduction in the Rhine river inputs. However, an additional factor is the reduction in loads from dredged material dumping. The dredged materials were not included in the model simulations.

For PCB, the models predict a larger impact of river and atmospheric loads reduction, as high as 40-49% at some locations. This is primarily an indication of the relative importance of rivers as the contributing source of PCB to the North Sea, compared to inflow from the boundaries. As with cadmium, the largest reductions were generally in the coastal regions, where the influence of rivers is largest.

At this point in time, the responsiveness cannot be validated against field data.

Conclusions

The workshop has had a significant output with respect to:

1. An update of available models and data for marine contaminant issues in the Convention area
2. Validation and comparison of model results
3. Answers to JAMP questions on contaminant transport and fate issues in the Convention area, in particular the responses of the various models to anthropogenic input reduction scenarios

1. Update of available models and data

Models compared and evaluated at this workshop included models for:

- greater North Sea: BSHdmod.E, NORWECOM, SCREMOTOX, ZEEBOS and PROVANN
- southern North Sea: NOSTRADAMUS
- English Channel: Telemac/SUBIEF
- estuaries: SAWES and PCB bioaccumulation model

General descriptions, main characteristics, references and list of contact persons/institutes are available for all of these models. These models were all for the OSPAR region II (Greater North Sea). No models for other OSPAR regions were presented, and it is not certain if such models are available.

Important exchange and use of common datasets was made, namely:

- riverine input data on monthly basis
- atmospheric deposition data
- estuarine retention information
- ICES data
- North Sea Project data

2. Validation and comparison of model results

The exercises show that the cost function is a valuable method for performing model validation and model comparison, and can be widely used in the future. Overall results as to the goodness-of-fit can be summarized:

- water transport: mass balances show different fluxes into/out of North Sea.
- SPM: large scale fluxes still poorly understood, and are calculated very differently with the different models. However, the SPM flux is crucial for determining the fate of many contaminants, especially those which are largely adsorbed to particulate matter.
- cadmium: Despite differences in the models, calculated concentrations are similar and the general distribution pattern of dissolved cadmium over the North Sea is similar (as is the salt pattern). Also the relative responses to load reductions is similar. Models results are low and do not reflect the seasonal variability as shown in NSP field measurements.
- PCB and other organic pollutants: the data for model validation is not available.

Although there are differences in the mass balances given by the different models, the net transport over the boundaries for water, SPM, cadmium and PCB are in general agreement with the range of values found in literature.

3. Answers to JAMP questions

Despite the differences between models, and some of the limitations of the models which have been presented, the models show much agreement in calculated concentrations, and predictions of relative decreases in environmental concentrations due to load reductions. The models in their current state can offer significant insight into contaminant fates in the North Sea, including links between inputs and concentrations, and can thus be used to address the issues which are raised by the JAMP questions.

Recommendations

Further development and improvement of models can still be achieved. Specifically, further development for other Convention areas (outside of the North Sea Region II) is important.

One enhancement of the operational use of the models would be a more complete validation of the responsiveness of the models based on actual field data. Such a validation could improve the reliability of the models. Currently, field data on contaminants is very limited.

International coordination and cooperation should facilitate further validation of the models, including comparison exercises. OSPARCOM, ASMO or Regional Task Teams could provide the platform for such further developments. However, complete validation is limited by availability of field data. This data is especially lacking for organic pollutants. While a lot of data are accessible through ICES, they are primarily for coastal regions, and not in the 'open' North Sea. Additionally, the data are not available for monthly periods (or seasons) within a year. It is specifically these type of data which are needed for good model validation.

Sources of contaminants to the North Sea including the relative influence of boundaries should be better studied. The input from cold Atlantic deep water should be quantified.

Follow-up

The workshop participants aim to prepare the results for publication in a peer-reviewed scientific journal for broader publication.

Relation to QSR 2000

From the workshop, a good overview of the available models as well as a network of people working in the field of contaminant transport and fate modelling has been established. This network can be activated to respond to any questions raised, including specific questions within the framework of QSR 2000 and the regional QSRs. For this purpose, general questions pertaining to relevant issues will have to be posed by policy makers and their organisations, including ASMO and the RTTs. These questions will then need to be 'translated' into the specific questions which can be answered by models.

I Introduction and Objectives

1.1 Introduction

The workshop on "Modelling of Contaminant Transport and Fate Issues " was the third in a series of three workshops organized by the Environmental Assessment and Monitoring Committee (ASMO) of the Oslo and Paris Commission (OSPARCOM). The Netherlands, lead country for the ASMO modelling cooperation, hosted the workshop, which was organized by Rijkswaterstaat - The National Institute for Coastal and Marine Management (RIKZ). The workshop was held on November 4-7, 1997 in The Hague, The Netherlands.

OSPARCOM is the working commission set up under the Convention for the Protection of the Marine Environment of the North-East Atlantic (see Figure 1.1). This Convention has as its goals: the prevention and elimination of pollution, and protection against adverse effects of human activities. Fourteen European countries (Portugal, Spain, France, Belgium, The Netherlands, Germany, Denmark, Sweden, Norway, Iceland, Ireland, the United Kingdom, Switzerland and Luxembourg) as well as the European Union have signed the Convention.

OSPARCOM is divided into two main committees:

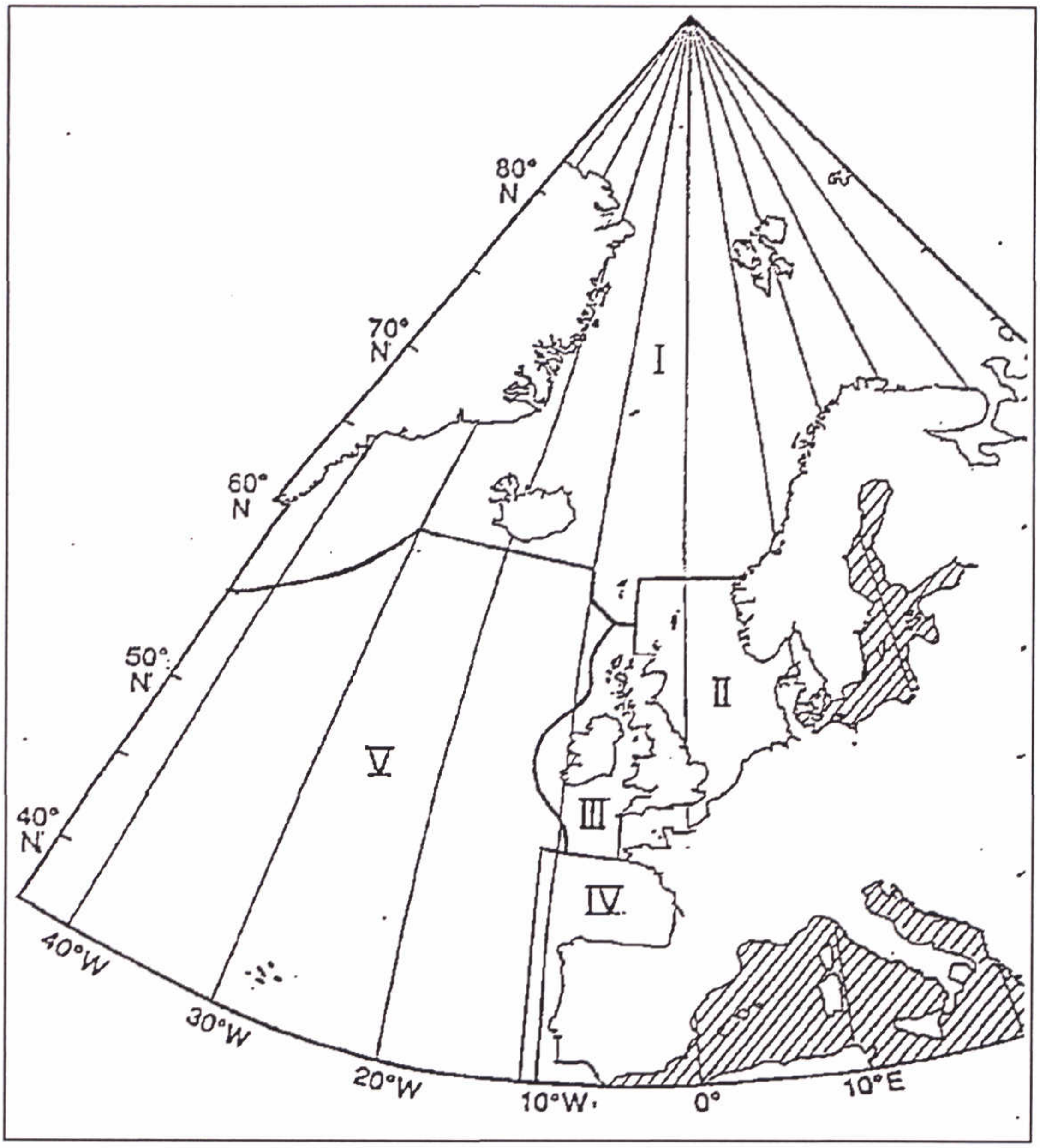
- ASMO (Assessment and Monitoring)
- PRAM (Programmes and Measures)

One of the objectives within ASMO is modelling cooperation. A general goal has been to make a comparison of results of applications of existing models. This would ultimately lead to a continuous and updated overview of models applicable for the 5 regions of the Convention area, and a network of modelling groups to be activated for model comparison exercises.

In the organization of these modelling coordination activities, a 'focal point' contact person has been chosen per country. This person is someone who should have a good overview of national modelling activities. The ASMO Modelling activities include conducting an inventory of models relevant to the convention area, as well as holding 3 workshops relevant to the QSR-2000 Process:

1995 Environmental risk assessment of accidents in the shipping and offshore industries;
1996 Eutrophication issues (nutrient concentrations, blooms, and foodwebs); and
1997 Pollutants (transport, routes and fate).

Six countries participated in this third workshop: France, The Netherlands, Germany, The United Kingdom, Norway and Denmark. A full list of workshop participants is given in Appendix B.



The five OSPAR regions:

- Region I: Arctic waters
- Region II: Greater North Sea
- Region III: Celtic Seas
- Region IV: Bay of Biscay and Iberian coast
- Region V: Wider Atlantic

Figure 1.1 The 5 OSPAR Convention regions

1.2 Objectives

The context and goals of the workshop have been drawn up by ASMO in the Terms of Reference (TOR), as given in Appendix A.

The need for modelling activities in the OSPAR Convention area has been identified for contaminant transport and fate issues in Section II ('Issues to be taken into account in development and implementation of the Joint Assessment and Monitoring Programme') and Annex 5 ('Issues for inclusion in the regional assessment for region II: Greater North Sea) of the OSPARCOM ASMO 1995 Summary Record. The JAMP issues raised with reference to modelling are:

- What are the fluxes and environmental pathways in the marine environment?
- Where do persistent pollutants ultimately end up?
- Which quantities of pollutants enter the Region (i.e. region II) from outside?
- What is the time lag between input reductions and reductions in field concentrations?

The context of the workshop has been to review the available models and current modelling activities with a view towards the preparation of the QSR 2000 (North Sea Quality Status Report 2000), and gaining perspective on the reliability, accessibility and applicability of available models.

The workshop has objectives for significant output with respect to:

- an update of available models for contaminant transport and fate issues in the Convention area
- Answers to JAMP questions on contaminant transport and fate issues in the Convention area, in particular the responses of the various models to anthropogenic input reduction scenarios
- Common strategy for cooperation on further model development and application, also with the aim of contributing to the Quality Status Report (QSR) 2000.

1.3 Approach

The main features of all the contaminant transport and fate models were inventoried with the help of a model questionnaire prior to the model workshop. Additionally, all the models were presented during the workshop. A brief description and a summary table of important characteristics are presented for each model in Chapter 2.

It was decided that a form of model intercomparison activities would be the best means to gain more information about the capabilities of each of the models and to quantitatively compare the available models. Since models cover different geographic regions and contain different model parameters, a strict model comparison could not be made. Instead, the workshop has focused on:

- an evaluation of model validation in the domain of application using a cost function (i.e. comparison of model results with available in-situ measurements)
- an evaluation of model responsiveness to specified reductions in anthropogenic loads.

Model validation exercises involved comparing model results of salinity, suspended particulate matter and cadmium concentrations with available field data from the North Sea Project. Model results for PCB-153 were also compared, but insufficient field was available for validation. The cadmium validation was made using a defined 'cost function'. The cost function is an equation that can be used to calculate the goodness of fit between model and data in an objective manner. This exercise primarily gives an indication of how well a model represents what is observed in the natural system. When different models use the same cost function for validation with the same data set, it is possible to compare the goodness of fit of the different models by comparing cost function results (i.e. which model best represents the natural system). The model validation results are presented in Chapter 3.

Model responsiveness exercises involved simulating a reduction scenarios for riverine loads. A base case for anthropogenic loads of cadmium and PCB-153 was defined (year 1989), as well as a load reduction scenarios (50% reduction). The responses of the different models to the contaminant reductions were then compared. Such an exercise gives an indication of the changes that can be expected in the natural system due to a realistic policy decision, and illustrates the role that predictive models can play in marine management. Additionally, the responsiveness illustrates many of the characteristics of the models. The model responsiveness results are presented in Chapter 4.

Based on the results of the model exercises and the discussions held during the workshop itself, some conclusions and recommendations are brought forward in Chapter 5.

2 Models Presented

2.1 Computational Models

There is a wide variety of models that can be used for modelling of contaminant transport and fate issues. These range from a steady state chemical equilibrium model for calculating bioconcentration in a food chain, to fully 3D hydrodynamic-chemical models for the greater North Sea, to a model for simulating complex estuarine chemical gradients, to an ecotoxicological risk assessment model. The models make different assumptions about the importance of certain processes, and require different types of inputs at various levels of spatial and temporal detail.

Table 2.1. Summary of models presented during the workshop

Country/Institute	Model Name	Model Area	Contaminants modelled
1. Germany/BSH	BSHcmod (circulation) BSHdmod.E (eulerian) BSHdmod.L (lagrang.)	North Sea and Baltic Sea	Cd
2. Norway/IMR	NORWECOM	Greater North Sea	Cd, PCB, atrazine, BaP, fluoranthene
3. UK/SOC	NOSTRADAMUS	Southern North Sea	Cd
4. NL/RIKZ and DELFT HYDRAULICS	SCREMOTOX	North Sea	Cd, PCB, atrazine, BaP, fluoranthene
5. NL/RIKZ and DELFT HYDRAULICS	ZeeBOS-tox	North Sea	Cd, PCB, atrazine, BaP, fluoranthene
6. Norway/SINTEF	PROVANN / DREAM	North Sea	dispersed oil
7 France/IFREMER	PCB bioaccumulation model	Seine Estuary	bioaccumul. of PCB in sea bass food-web.
8 NL/RIKZ and DELFT HYDRAULICS	SAWES	Western Scheldt Estuary	Cd, PCB, atrazine, BaP, fluoranthene
9. France/EDF	TELEMAC/SUBIEF	Channel/Bay of Seine	radionuclides

The *focus of the models* can be characterized by their level of attention to:

1. physical transport (hydrodynamics) including coupling with meteorology
2. chemical processes
3. biological effects/ecotoxicology

While all three of these aspects are important for making a complete assessment of chemical transport and fate, there are no models which cover everything. Thus, one method of categorizing the models is to specify the degree of focus on each of these points, as has been done qualitatively in Table 2.2 by giving each model a ranking of high, medium, low or no for each topic.

In terms of physical transport processes (hydrodynamics), some models have detailed 3-dimensional computations of flow coupled to actual meteorological forcings (e.g. wind), while others are 2-dimensional (depth-averaged), or even 1-dimensional (along the length of an estuary) with variable levels of meteorological forcings.

The chemical and biological processes range from simple (no) processes (i.e. simply transport of conservative contaminants), to detailed reactions including contaminant adsorption, desorption, sedimentation, resuspension, oxidation, reduction, volatilization, degradation, uptake in organisms and concentration in the food chain.

In addition to the different focus of the models, they have also been designed for different *spatial scales* ranging from the North Sea (with a maximum grid size 35 x 35 km), to estuary scale with a spatial resolution (~ kilometers) to resolve steep concentration gradients, to no spatial variability (e.g. PCB bioconcentration model).

The *temporal variability* of models also covers a range, from steady state (i.e. no temporal variability) to temporal resolution within a tidal cycle. The time resolution of the external forcings also affects the temporal variability of the models. Specifically, the models which include physical transport (hydrodynamics) need some sort of external forcing (e.g. wind, tides) to drive the water circulation. The temporal scale of this forcing ranges from long-term average conditions, to actual meteorological (hourly, daily) data.

Table 2.2 Characterisation of models based on physics, chemistry and biology/ecotox

Country/Institute	Model Name	Focus		
		physics/ hydrodynamics	environmental chemistry	biology/ ecotoxicology
1. Germany/BSH	BSHcmod (circulation) BSHdmod.E (eulerian) BSHdmod.L (lagrang.)	high	low	none
2. Norway/IMR	NORWECOM	high	medium	none
3. UK/SOC	NOSTRADAMUS	medium	medium	none
4. NL/RIKZ and DELFT HYDRAULICS	SCREMOTOX	low	medium	high
5. NL/RIKZ and DELFT HYDRAULICS	ZeeBOS-tox	medium	medium	none
6. Norway/SINTEF	PROVANN / DREAM	medium	medium	high
7 France/IFREMER	PCB bioaccumulation model	none	medium	high
8 NL/RIKZ and DELFT HYDRAULICS	SAWES	low	high	none
9. France/EDF	TELEMAC/SUBIEF	high	medium	none

North Sea Models

1 *BSHcmod, BSHdmod.L, BSHdmod.E (BSH, Germany)*

BSH has two dispersion models which can be used for calculation of contaminant transport: BSHdmod.L and BSHdmod.E. Both of these models require results of the hydrodynamic (circulation) model BSHcmod as input. This 3-dimensional model calculates dynamic parameters of current, water level, temperature and salinity in the North and Baltic Sea in three nested grids (1 nautical mile (nmile) inshore of the German Bight and western Baltic; 6 nmiles further offshore; and 12 nmile outside of this area). In the vertical, up to 10 layers area used. The model is forced by tides, external surges, wind stress, surface pressure, waves, heat fluxes between atmosphere and water as well as fresh water input from large rivers. Temperature, salinity and ice coverage are calculated prognostically. The model runs operationally once a day and is driven by meteorological forecasts (48 hours ahead).

The spreading of substances can be calculated with the (Lagrangian) drift/dispersion particle tracking model “BSHdmod.L” or the (Eulerian) advection diffusion model “BSHdmod.E” using the stored current, water level and wind field data calculated in the hydrodynamic model. In the Lagrangian model, the particles are transported as a result of advection by currents and turbulent diffusion, which is simulated by a Monte Carlo method. Simulations are possible for conservative substances, drifting objects and oil. Chemical processes are included for the simulation of oil dispersion and for first-order decay. In the Eulerian model, the finite difference method is used to solve the advection diffusion equation. There are two options for diffusion coefficients, using constant values, or variable data from the circulation model. Currently, only simulations for passive conservative substances is possible. There is no modelling of suspended (organic) matter or process of adsorption/desorption of contaminants to suspended matter.

2 *NORWECOM (IMR, Norway)*

NORWECOM is a coupled physical-chemical-biological model (NORWegian ECOlogical Model) of the greater North Sea. The coupled model system is based on a physical model (Princeton Ocean Model) which calculates the 3-dimensional velocity field, temperature, salinity, turbulence and water level. The model is forced by actual atmospheric pressure and windstress (6 hour hindcasts from the Norwegian Meteorological Institute - DNMI), tide at open boundaries, freshwater runoff, and in/outflow at open boundaries. It is thus able to represent vertical exchanges realistically.

In the chemical-biological part of the model, nutrient and algae dynamics are simulated. The processes of primary production, respiration, phytoplankton mortality, mineralization, sedimentation and resuspension are included, to simulate two types of algae (diatoms and flagellates), 3 inorganic nutrients (nitrogen, phosphorous and silicate), 3 forms of particulate organic matter and oxygen. The chemical (pollutant module) builds on the results of the physical and biological module (full 3-D hydrodynamics are used to transport the contaminants). Atrazine is modelled as a dissolved passive tracer, although it is recognized that it will have some adsorption to particulate matter, and can thus settle to bottom sediments. Cadmium is found both in the dissolved phase and adsorbed to particulate matter, and the distribution is determined by the use of an equilibrium sorption equation (K_d). An equilibrium model based on the octanol-water or K_{poc} partition coefficient is used to calculate the distribution of PCB-153 and PAH between the dissolved phase and the particulate phase.

3 *NOSTRADAMUS (SOC, UK)*

NOSTRADAMUS incorporates separate, though linked transport sub-modules for water, suspended sediment, plankton and metals. **(i) Water transport:** The transport and mixing (advection and diffusion) of conservative tracers are based on the 2-D vertically integrated models developed for NW European shelf seas. The mixing model employs a 35 x 35 km grid. Residual water circulation in the hydrodynamic model was determined by the dominant M_2 tidal component and by wind forcing, principally from the west and south, based on spatially-averaged monthly mean wind fields for the observation phase of the North Sea Project (NSP). Monthly mean residual velocities (tide plus winds) for each grid cell from the hydrodynamic model are used in the mixing model to determine advection. Tidal current amplitudes for each grid cell are used to determine diffusion. **(ii) Suspended sediment transport:** Suspended sediment within the water column is composed of both inorganic (ISPM) and organic SPM (OSPM) particles, the latter itself comprising living and detrital (dead) components. The organic fraction is generated within the biological transport module described below. Concentrations of ISPM are altered by conservative mixing, and by inputs from rivers and cliff erosion, exchange across the open sea boundaries, and tide and wind induced resuspension and settling of particles. **(iii) Biological transport:** This component of the model is concerned with the production, remineralization and transport of organic matter. The overall aim is to generate concentrations of both living and detrital OSPM, which when added to ISPM yields a value for total (T) SPM; it is these latter values which are used to influence metal phase partitioning. As with ISPM, concentrations of OSPM are changed following mixing by exchange of material at model boundaries, including resuspension and settling, and microplankton growth and decay. **(iv) Metal transport:** Concentrations of dissolved and particulate metals are changed by conservative mixing, exchange across the model boundaries and solid-solution phase transfer. The latter exchange is driven by the use of distribution coefficients derived from NSP observations.

4 *SCREMOTOX (Rijkswaterstaat and Delft Hydraulics, The Netherlands)*

SCREMOTOX is a screening model for toxic substances in the North Sea. It has been developed as a collaborative effort between several Dutch institutes including Delft Hydraulics, Rijkswaterstaat, TNO, and the Ministry of Public, Spatial Planning and Environment. The goal of the model is to serve as a screening tool for the evaluation of ecotoxicological risks of the emissions of toxic substances into the North Sea. As such, the model has been designed to be easy to use (menu driven, with a graphical user-interface), have a short run-time (~10 seconds on a Pentium PC), and to provide a ranking of evaluated substances based on their environmental risk.

Three input options are available for definition of emissions: (1) based on EC production or use (based on E-Uses method), (2) based on loads to river and atmosphere, and (3) based on direct loads to the North Sea from rivers, disposal sites, off-shore activities, shipping, and atmospheric deposition. All emissions are input as yearly averaged values only. Atmospheric deposition can be calculated based on source-receptor relations (EU-TREND model) to specific North Sea zones, it can be specified directly to the North Sea (a fixed gradient over North Sea is assumed), or it can be given as emissions per country to atmosphere. Inflow over the boundaries is also included based on user-defined boundary concentrations.

The model hydrodynamics are steady-state, based on residual flows with an average wind (7.5 m/s SW) forcing, and are calculated on a curvilinear grid (EU-PROMISE model). Chemical processes include adsorption/desorption to silt (inorganic) and POC, volatization, degradation and sedimentation/resuspension. Output includes not only concentration fields, but PEC/NEC fields, relative contributions from sources, and ranking of substances for different zones according to PEC/NEC ratio or NEC exceedence probability factor.

5 *ZeeBOS-TOX (Rijkswaterstaat and Delft Hydraulics, The Netherlands)*

ZeeBOS-TOX is part of a Decision Support System (DSS) for the assessment of heavy metal and organic micropollutants in the North Sea. The toxic substances model can be used with two different model grids: the Continental Shelf, or the Dutch coastal region. The Continental Shelf version of the model has been presented in the ASMO workshop. The objective of the DSS is to correctly simulate the existing pollution conditions and assess different pollution reduction measures and strategies. Gaining insight into the relative importance and contribution of pollution from different sources is a goal, as is risk analysis and comparison of (calculated) water quality concentrations with standards.

The water circulation is calculated from a 2-dimensional (depth-averaged) hydrodynamic model. Using measured monthly wind values from the 'de Kooy' monitoring station as forcing, residual currents are calculated by interpolation from 9 pre-calculated hydrodynamic conditions. Physical/chemical processes include, advection, diffusion, sorption to POC, DOC and inorganic matter, sedimentation, resuspension, volatization, and first-order degradation. POC fields are taken from the ZeeBOS-eutrophication model which calculates detritus carbon and phytoplankton concentrations. DOC fields are determined separately by means of a conservative calculation with the ZeeBOS-TOX model. Inorganic suspended matter is one of the state variables calculated by the model. Pollutants can adsorb to inorganic suspended matter (heavy metals) or POC and DOC (organic micropollutants) as calculated using equilibrium sorption equations (Kd, Kpoc).

6 *PROVANN (SINTEF, Norway)*

The model PROVANN is developed for analysis of environmental fates and biological effects of low level pollutant discharges resulting from release of production water from North Sea oil platforms. It actually comprises 3 modules which calculate: transport and fate of pollutants, migration/movement and exposure model (fisheries), and individual effects and population dynamics model. The hydrodynamic information needed to drive the transport and fate module is obtained from the Norwegian Meteorological Institute (DNMI). The spreading of substances (dispersed oil) is calculated with a Lagrangian particle tracking model, where particles are transported as a result of advection by currents and turbulent diffusion. The resulting concentration fields are used as input to the migration/movement and exposure module, which calculates the distribution of individual organisms. This results in exposure histories for various organisms. Individual effects are calculated by the population dynamics module.

Other Models

7 *PCB bioaccumulation model (IFREMER, France)*

This is a generic modelling framework for the bioaccumulation of PCB in a sea bass food-web, which includes biological, environmental and chemical parameters. The model has been developed/applied in the Seine Estuary. The sea bass (*Dicentrarchus labrax*) is chosen as the top predator of a very simple food web. Bioaccumulation is modelled via uptake from water or uptake via diet. Factors that increase bioaccumulation via uptake from water are: direct absorption, diffusion, adsorption, and respiration. Diet uptake includes food (lower level of the food web) and sediment. Factors that decrease bioaccumulation are excretion, biotransformation, growth, and reproduction.

In the model, the food web is structured in six biological compartments, together with contaminant concentration in the water column and in suspended particulate materials (detritus). The sea bass is the top predator in a three-level food chain. The mid-level consists of small crustaceans and gobies, which have been shown to be the main constituents of a sea bass diet. The lower level consists of zooplankton. The zooplankton take up contaminants from the water column, direct ingestion of chemicals on suspended particles and from phytoplankton. Contaminants enter the biological cycle adsorption onto solid inert particles or living materiel (passive partitioning). For detritus, the distribution of organic contaminants is modelled as a function of the octanol/water partition coefficient and the organic carbon fraction. For phytoplankton, the distribution is modelled as a function of the octanol/water partition coefficient and the lipid content of phytoplankton. For each of the organisms in the food web, an equilibrium equation is solved which includes direct uptake of PCB by the animal from water, uptake from food, and loss via excretion and decrease in concentration due to growth. The model needs parameters for specific chemicals (e.g. Kow), and those associated with organism ecology (growth, respiratory, nutrition rates, etc.).

8 *SAWES (Delft Hydraulics, The Netherlands)*

SAWES is an estuarine water quality model, which is built into a complete Decision Support System (DSS) for the Scheldt estuary. The DSS includes an information system (database of emissions, measured concentrations and user functions), model system (hydrodynamic and sediment transport model, waste load model and SAWES), plus an analysis system (for definition and assessment of different management strategies, analysis of effects in water and sediment quality, and evaluation of water quality). The SAWES water quality model has been established to assess the relation between emissions and water quality for the whole estuary, through the seasonal cycles. It is a deterministic and dynamic model with an emphasis on chemistry.

The water and sediment quality is based on a transport model for dissolved and suspended constituents. For dissolved compounds the advection diffusion equation is used. The model schematization is 1-dimensional. The hydrodynamic coefficients are tidally averaged and the water level is fixed at its average value. The tidally and cross-sectionally averaged velocity is derived from a mass balance equation for fresh water inputs into the estuary. The dispersion coefficient, bringing into the model the tidal mixing, is derived from a mass balance for chlorides. The model includes a number of water quality processes that contribute to the oxygen balance and the nitrogen cycle, including the exchange of oxygen and carbon dioxide with the atmosphere, decay of BOD, ammonification, nitrification and denitrification. Algae are also included in the model, as they affect the oxygen balance, the nutrient cycles and the adsorption of trace metals (via pH effect).

Metal related processes include the formation of metal sulphides under reduced conditions, the oxidation of metal sulphides with increasing oxygen concentration (seaward direction), and equilibrium partitioning between dissolved and adsorbed metal fractions (on organic and inorganic particles). The particulate metal forms (sulphides or adsorbed) can be sedimented or resuspended. The model has been calibrated based on measured chemistry of the Scheldt estuary. The distribution coefficient (Kd) is a function of the pH and alkalinity, which are calculated by the model. The modelling of organic pollutants includes partitioning to particulate organic matter, volatilization, aerobic and anaerobic degradation.

9 *TELEMAC/SUBIEF (EDF/France)*

The Telemac and SUBIEF models are used to simulate the fate of radionuclides discharged from La Hague and 4 nuclear power plants in the Bay of Seine region (Flamanville, Paluel, Penly and Gravelines). TELEMAC is a 2-dimensional hydrodynamic model for calculating the circulation of the region. It is used to calculate residual circulations for 30 tidal and wind conditions in the Channel and south of the North Sea. Real winds and tides are used as forcings, and interpolation of the residual circulations are made on a tide by tide basis. The residual currents computed by TELEMAC for the given tide and wind conditions are interpolated and are used by SUBIEF to reproduce the long-term dilution of radionuclide tracer. Suspended matter and sediment are implemented In SUBIEF (by erosion and deposition fluxes) and contaminants may interact with them (equilibrium sorption/desorption). the radionuclide fluxes from historical discharge data are incorporated. The advection, diffusion and decay of the radionuclides are thus calculated.

In Table 2.3, the important characteristics of the models in terms of strengths and weaknesses (as seen by the model developer/user) are summarized. Literature references for each model indicating the institute and scientists involved are given in Chapter 6.

Table 2.3.1 Summary of strengths and weaknesses of contaminant models (BSHdmod.L)

Model Name BSHdmod.L

	PROS	CONS
Spatial Resolution	3-dimensional (up to 10 layers), 4 nested grids, fine resolution (1 nm) in German Bight and Western Baltic Sea	coarse resolution (20 km) outside German Bight and Western Baltic
Temporal Resolution	15 minutes tidal cycle is resolved	time consuming
Forcing	currents and water levels calculated by the operational circulation model	no hindcast data (uses forecast data)
	wind data of German Weather Service (stored together with current data)	problems with input in larger areas (many particles necessary)
	point sources for input of substances	
Processes	calculations possible for: a) passive conservative substances b) drifting objects c) different types of oil	no calculations for particulate material possible
	d)backward calculations possible	
	advection (currents from circulation model) and turbulent motion (Monte Carlo method) (for a-d)	parameterization of turbulence close to the coast problematic
	wind drift, stranding (for a, b, d)	
	oil processes (for c): spreading, evaporation, emulsification, horiz. and vert. dispersion, sinking	
	sharp gradients are maintained	
Validation	several drift experiments with different drifters	
	good results in real pollution cases: - APRON PLUS packages in 1994 - oil pollution in June 1996 - River Odra flood in summer 1997	
Usability (Availability, transportability, publications, etc.)	Mainly developed for short-term forecasts (up to 1 months)	problems with calculation of concentrations (many particles necessary)
	model runtime for 24h: approx 4 min (short runtime allows many scenarios)	model runtime and output increases with increasing particle number
	water of different sources can be marked and traced	calculations for periods > 1year troublesome
	transport times can be calculated	
	model is used for different areas(North Sea, Baltic Sea, Wadden Sea, SMHI)	
	PC-version also available	

Table 2.3.1 Summary of strengths and weaknesses of contaminant models (BSHdmod.E)

Model Name BSHdmod.E

	PROS	CONS
Spatial Resolution	3-dimensional, 3 nested grids, fine resolution (1 nm) in German Bight and Western Baltic Sea	coarse resolution (20 km) outside German Bight and Western Baltic
Temporal Resolution	15 minutes tidal cycle is resolved	
Forcing	currents, water levels and eddy coefficients calculated by the operational circulation model	no hindcast data (uses forecast data)
	initial concentration field and mass input or concentrations at sources	
Processes	advection and turbulent motion (uses stored data of currents, water levels and eddy coefficients)	Only simulations for passive conservative substances possible (at the moment)
	new transport algorithm with small numerical diffusion (Kleine, 1993)	
Validation	good results during river Odra flood in summer 1997	
Usability (Availability, transportability, publications, etc.)	Mainly developed for calculations with large scale input	water of different sources cannot be distinguished
	developed for simulations periods > 1 week	calculations for periods > 1 year troublesome (loading of stored current and turbulence data)
	model runtime for 24h: approx 8 minutes (short runtime allows many scenarios)	quite new, no publications

Table 2.3.2 Summary of strengths and weaknesses of contaminant models (NORWECOM)

Model Name NORWECOM

	PROS	CONS
Spatial Resolution	Large-scale version covers whole shelf with grid size of 20km x 20 km	Continental coastal plume cannot be resolved with 20km x 20km resolution
	Fine-scale modules can be set up anywhere and be coupled to large scale model	Fine-resolution (4km) modules (now) cover only the Skagerrak, Kattegat and parts of the eastern North Sea
	Fully 3D model able to simulate important physical and biological vertical gradients and fluxes	Computer expensive simulations
Temporal Resolution	Resolves the daily cycle (15 min.); important for short term events (hours)	
Forcing	Has 'realistic' meteorological forcing and hydrodynamics, including variable inflow of Atlantic water	
	Surface waves from wave forecasting model	
Processes	Sedimentation and resuspension included	Sedimentation / resuspension results not yet validated
	Effect of surface waves, tidal currents and wind forced currents included in the sedimentation resuspension formulation.	
	POC is calculated by the primary production module.	DOC specified in a very simplistic way
	Contaminant particulate/dissolved partitioning, K_{poc} for organic and K_d for metals.	K_d partitioning concept crude
	Flexible model structure, easy to include processes missing	No degradation and volatilisation for organic contaminants
Validation	Generic process formulations and parameterizations taken from scientific literature; no tuning to local data has been performed.	Computer expensive simulations limit detailed sensitivity analysis
Usability (Availability, transportability, publications, etc.)	Fortran 77 and 90 code	Requires large computer resources
	Several refereed papers have been / are being published on validation and model behaviour for physics/biology	No publications on the contaminant module.

Table 2.3.3 Summary of strengths and weaknesses of contaminant models (NOSTRADAMUS)

Model Name NOSTRADAMUS

	PROS	CONS
Spatial Resolution	2D - simple	2D-vertically averaged
	Model grid matches resolution of North Sea Project (NSP) data used to test model output	Model grid coarse: 35 km * 35 km
	Covers southern North Sea	Cannot resolve steep gradients in coastal zone
Temporal Resolution	Calculates daily changes	Appropriate timescales 1-3 weeks
Forcing	Tidal and wind forcing determine advection	Tidal and meteorological residuals control advection. Meteo residuals varied monthly by sinusoidal scaling factor.
	Tidal amplitudes control dispersion	
	Wind forcing relevant to NSP period	
Chemical processes	Initial conditions from NSP data	
	Open sea boundary values from NSP data	
	River inputs from relevant to NSP period. Effects of estuarine transformations of river inputs parameterized in some cases	
	Atmos. inputs use NSP data	Dry deposition has only spatial variation (no temporal) Wet deposition has only temporal variation (no spatial)
	Metal solid/solution partitioning from NSP data	Kd partitioning concept crude
	Wind/wave and tidal resuspension of seafloor sediments included	
Simulations	Salinity, inorganic and organic SPM, dissolved and particulate metals (Cd, Cr, Cu, Ni, Pb, Zn)	
Validation	Extensive testing against NSP data (1988-89), Extensive sensitivity testing undertaken	
Usability (Availability, transportability, publications, etc.)	Fortran 77 Code, PC based	Available (with DETR agreement?)
	Fast run times (steady state in <2hrs CPU time	
	Model description and results published in scientific literature and sponsors report	

Table 2.3.4 Summary of strengths and weaknesses of contaminant models (SCREMOTOX)

Model Name SCREMOTOX

	PROS	CONS
Spatial Resolution	fine resolution, curvilinear grid (PROMISE) 2D (vertically averaged)	
Temporal Resolution		no temporal resolution; model calculates long-term average steady state
Forcing	3 different methods for specifying emissions shipping lanes, offshore, disposal sites, atmospheric deposition can be included	fixed emission locations Northern UK rivers not included
Chemical Processes	sedimentation, volatilization, adsorption, desorption, first order decay	yearly averaged POC field
Validation	validated for 5 years of data on 10 monitoring locations along the Dutch coast	
Usability (Availability, transportability, publications, etc.)	includes Aquapol database	
	generic set of process descriptions and parameters	
	model runtime ~ 5 seconds (Pentium Pro)	
	can estimate missing values (compound properties and emissions)	
	ranks compounds according to ecotoxicological risk in the North Sea	
	little knowledge required of user	

Table 2.3.5 Summary of strengths and weaknesses of contaminant models (ZEEBOS-Tox)

Model Name ZeeBOS-Tox

	PROS	CONS
Spatial Resolution	Greater part of the North Sea, fine resolution grid including the Channel	2DH (i.e. vertically averaged) does not resolve coastal gradients
Temporal Resolution	Model capable of predicting monthly, seasonal and yearly trends	
	Steady state and dynamic	
Forcing	POC from eutrophication model DOC from separate calculation (modelled as conservative substance)	Wind conditions of one coastal location.
Processes	Slow desorption kinetics can be included	Simple bottom kinetics
	Sorption, sedimentation, volatilization, first-order degradation	Parameters constant in time and space
Validation	1990/ 1993,1994	
Usability (Availability, transportability, publications, etc.)	Process formulations available from process library	
	Part of a DSS for the North Sea	
	Model gives output of fluxes for all processes (optionally aggregated in time and space)	
	Model runtime for 1 year = 0.3 hr CPU (Pentium PC)	
		Until now no publications in scientific literature

Table 2.3.6 Summary of strengths and weaknesses of contaminant models (PROVANN)

Model Name PROVANN/DREAM

	PROS	CONS
Spatial Resolution	3D - varying according to problem considered.	May be poor resolution locally when large areas are involved
Temporal Resolution	Time steps from days down to minutes. Simulation time max. 1-2 years.	Spatial reliability poorer when time step is increased.
Forcing	Winds and ambient 3D and time varying current fields. Simulating in real time.	Winds and currents must be corresponding in time/space
	Currents and wind fields may also be generated from computer programme.	Density effects are expressed through mixing coefficients.
Physical processes	3D current advection, turbulent mixing, effects from winds on mixing, effects from stratification on mixing, near field fixing, 3d and time varying concentration fields from multiple sources	Concentration fields are calculated based on Lagrangian particle tracking. Number of particles used may be limiting the resolution.
Chemical processes	Effects from evaporation of matter from the sea surface, dissolution from droplets, adsorption to biota, deposition on the bottom and different biodegradation processes	Simulates the 3D multi-source concentration fields for one compound at a time (tracer, dispersed oil, some specified dissolved chemicals)
Biological processes	Budgets for adsorption, intake, bioaccumulation and depuration in zooplankton/fish. Calculation of environmental loads (doses) on communities of biota	Inputs are dependent on a description of, or information on the presence of biota in time and space.
Validation	Concentration fields have been compared against produced water releases measured both locally and on a regional scale with good result.	No verification on the biological and chemical part as yet.
Usability (Availability, transportability, publications, etc.)	Model runs on a PC. Chemical data base, graphics and GIS in colours follow the calculations. Model has been used offshore Norway and abroad. The model has been under continuous development for many years, and still is, in particular the biological/chemical part.	Calculations over a time span of more than a year may be time consuming. Also, the 3D and time varying current database may require a lot of storage capacity in the computer (or on the net).

Table 2.3.7 Summary of strengths and weaknesses of contaminant models (SAWES)

Model Name SAWES

	PROS	CONS
Spatial Resolution	(1-D) Model resolves the steep spatial gradients along the length of the Scheldt Estuary. The model contains all chemistry needed to describe profiles of concentrations along the estuary.	no resolution laterally across the estuary; no morphological units regarded. Resolution does not allow analysis of near field effects of dredging
Temporal Resolution	monthly-seasonal-yearly changes	high-frequency changes not resolved
Forcing	all forcing functions derived from database	(simple) hydrodynamics: fresh water balance, tidal mixing by dispersion
Chemical processes	Water quality processes for oxygen balance, nitrogen cycle and algae dynamics; alkalinity and pH are calculated	
	Kd for metal sorption a function of macrochemistry (pH, salinity and alkalinity) determined by the basic laws of thermodynamics.	Understanding of the chemical model and interpretation in detail needs the involvement of an experienced specialist in the field of chemical modelling.
	Model gives a good understanding of the basic phenomena determining the complex behaviour of Phosphorous.	The phosphorous model is typically a research model, rather than a standard user model
	The model offers a frame for further study of the sources and fate of pesticides in the Scheldt estuary	Pesticide processes are not tested by comparison with measurements because of a lack of data.
	The model contains all essential processes describing the fate of 'other' organics (i.e. PCB's, PAH's)	Some phenomena in the concentration profile of heavy PCB's are not (yet) understood
Validation	Being calibrated on the year 1987 and 1991, the model describes the water quality of 1980-1991; an extensive parameter analysis has been carried out to investigate the range in process fluxes describing the measured water quality	
Usability (Availability, transportability, publications, etc.)	Water quality model part of a Decision Support System (DSS) with waste load model, data base of emissions, concentrations, and user functions, and analysis tools	
	use of a process library sustains a relatively quick extension of water quality processes	
	Model gives output of fluxes for all processes, thus offering a good explanation of the model results	

Table 2.2.8 Summary of strengths and weaknesses of contaminant models (TELEMAC/SUBIEF)

Model Name TELEMAC/SUBIEF

	PROS	CONS
Spatial Resolution	finite element grid with refined elements near the Coast	the area studied is only the Channel and the South North sea
Temporal Resolution	long term simulations (up to several years)	the model does not resolve the tidal cycle
Forcing	Radionuclides fluxes known from real historical discharge data catalogue of residual currents computed for 30 tide and wind conditions	Daily averaged wind assumed to be spatially uniform (wind characteristics measured at Le Hague)
Processes	nuclear decay of radionuclides the interaction between contaminants and suspended matter/sediment can be taken into account if relevant.	
Validation	the model results have been compared to field campaigns realised in Sept. 1990, and Sept. and Nov. 1994.	
Usability (Availability, transportability, publications, etc.)	the computed residual currents can be used to model the long term dilution of other types of contaminants. model runtime for 7 years = 3 hours on a workstation	until now no publications in scientific literature (only internal reports)

2.2 Additional Presentations

In addition to the presentations on specific models an additional presentation was given on the AQUAPOL data base.

AQUAPOL data base

The AQUAPOL data base was presented by Mr. Arie de Vries of RIKZ, the Netherlands. The data base contains several thousands of physical, chemical and major reactivity properties of contaminants, which determine their fate and effects in freshwater, estuarine and marine environments. The database has been developed in cooperation between several Dutch academic, technical and governmental research institutes. The development was commissioned by the Dutch Ministry of Transport, Public Works and Water Management in 1993.

In addition to general physical/chemical properties such as melting point, boiling point, heat of fusion and heat of vaporization, the database also includes evaluated experimental values of parameters which are especially important in the field of environmental chemistry: vapour pressure, aqueous solubility, Henry's Law constant, octanol-water partition coefficient, bioconcentration factor, gas-aerosol partition, sediment-water and DOC-water partition coefficients. The rate parameters for photochemical quantum yields, hydrolysis and oxidation, and biodegradation in water are also included. Compounds can be selected by CAS-registry number, class, synonym and SMILES notation. Selection of substance properties under certain environmental conditions (e.g. temperature or pH range) is also possible.

The quality of the data is evaluated by a newly developed score method which quantifies the reliability of the analytical chemical technique and the experimental methodology used to obtain the data, and the statistical uncertainty of each value. Quantitative-Structure-Property and Activity Relationships (QSPRs and QSARs) are also incorporated, for calculation of physical-chemical properties, environmental partitioning and reaction tendencies based on chemical structure.

AQUAPOL runs under Microsoft Windows operating system and includes a graphical user-interface and an on-line help facility. The database is available from the National Institute for Coastal and Marine Management (RIKZ) in the Hague, via Mr. A. deVries: (a.dvries@rikz.rws.minvenw.nl).

3 Model Validation

Model validation exercises involved comparing model results with different sets of measurement data and in one case using a defined 'cost function' to measure the goodness of fit between model and data. This exercise primarily gives an indication of the 'goodness of fit' of the different models, i.e. of the model representation of what is observed in the natural system, and also allows a comparison between models.

For the North Sea Models, results were originally compared with ICES data and later with the North Sea Project (NSP) data set collected in 1988-89 (NERC, 1992). The focus was on heavy metal and organic micropollutant contaminants, with cadmium and PCB-153 chosen as examples. For the estuarine and Channel models, no comparative validation exercise could be performed. Instead, the validation studies performed for each separate model using the regional data were presented.

3.1 Model validation exercises

For the North Sea models, the validation exercises focused on the year 1989. For this year, the inputs (river runoff, atmospheric deposition, etc.) were known and more importantly, there was a set of North Sea monitoring data from the North Sea Project. This data set has the most complete spatial and temporal coverage of the North Sea and allowed several different comparisons of the model results with measured values. As such, the model validation focused on three approaches:

1. Seasonal (monthly) variations in concentrations of cadmium and PCB at selected NSP locations;
2. Yearly average concentrations of salinity, suspended particulate matter (SPM), and cadmium at selected NSP locations;
3. Yearly mass balances for the North Sea (water, SPM, cadmium and PCB).

Table 3.1 Overview of the comparative validation exercises performed by North Sea Models

	BSH-dmod	NORWE-COM	NOSTRA-DAMUS	SCREMO-TOX	ZEEBOS-TOX
Monthly Means and Yrly Ave. Conc.					
Cadmium	X	X	X	X*	X
PCB	-	X	-	X*	X
Yearly Average Concentrations/ Cadmium Cost Function					
Salinity	X	X	X	X	-
Total SPM	-	X	X	X	-
Cadmium	X	X	X	X	X
Mass Balances for S. North Sea					
Water	X	X	X	X	-
Cadmium	X	X	X	X	X
SPM	-	X	X	X	-
PCB	-	X	-	X	X

X = validation exercise performed with the model
- = no validation exercise performed
* = yearly average concentration only

The North Sea Project Data

The North Sea Project (NERC, 1992) had as its ultimate aim, the development of a suite of prognostic water quality models to aid management of the North Sea. Required information in order to meet this aim was a complete seasonal cycle of data which could be used to formulate, drive and test the models, as well as identify and quantify sources and sinks determining the cycling and fate of individual constituents. This aim led to the NSP data sampling project which was conducted from August 1988 to October 1989, covering the southern North Sea region (south of 55.5°N). Many physical and chemical parameters were measured, including salinity, Suspended Particulate Matter (SPM), and cadmium which are relevant for this modelling exercise. Seven locations from the NSP monitoring data were selected for comparison with the model results (Table 3.2). The locations are shown in Figure 3.1.

Table 3.2 Selected North Sea Project monitoring locations

NSP data set				
	location name	**location description**	**latitude**	**longitude**
1.	AM	UK coast	52.09	1.84
2.	AG	Dutch coast	52.62	4.33
3.	BB	South Central NS	53.50	3.00
4.	BU	German Bight S.	54.42	6.71
5.	CP	Central NS	55.50	2.59
6.	CG	German Bight N.	55.50	7.33
7.	DZ	UK coast/SW North Sea	54.33	1.50

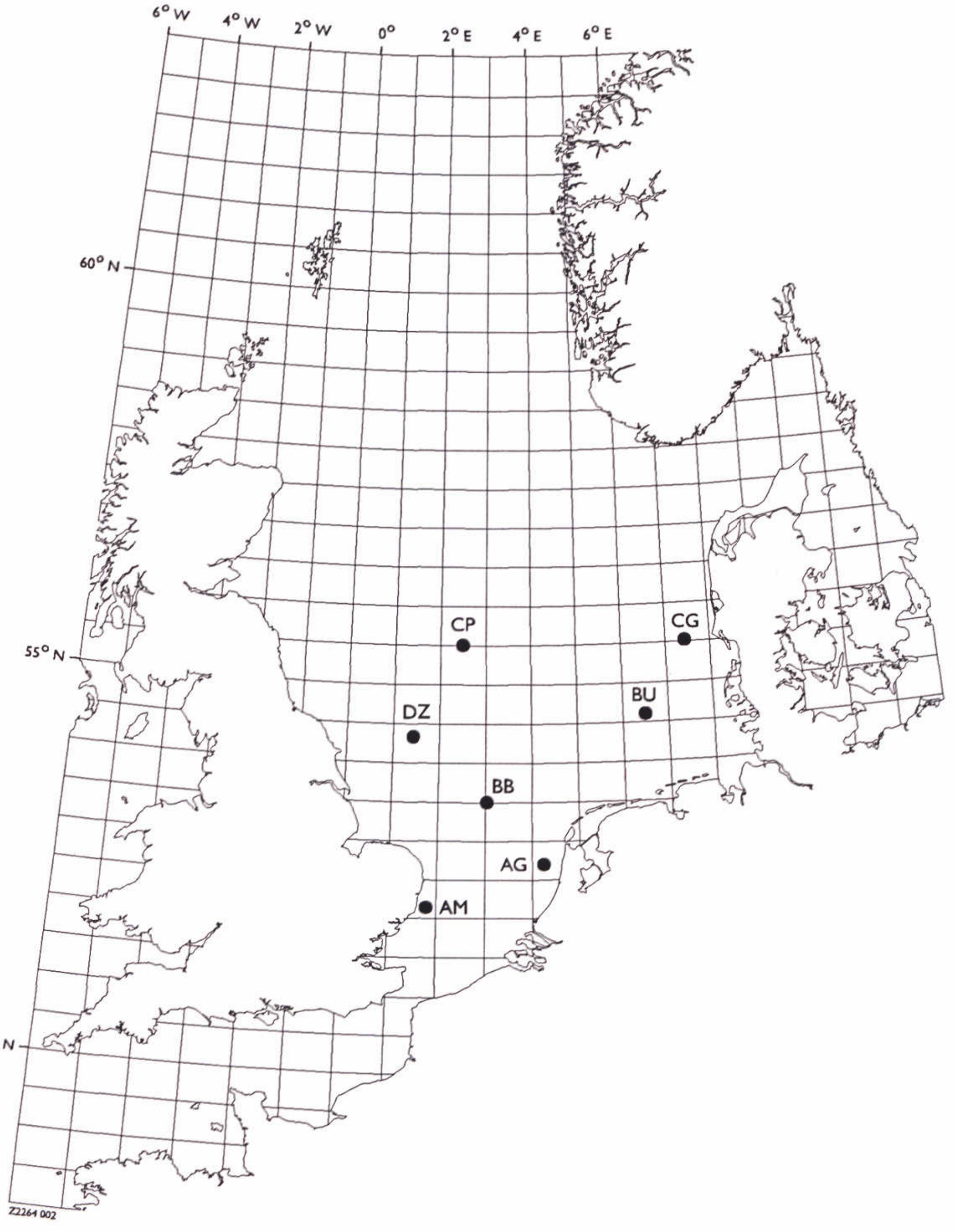


Figure 3.1 Locations of the seven North Sea Project (NSP) monitoring locations used for comparison with model results

Definition of the base case model simulation

In order to make the model simulations comparable, the different North Sea models were all provided with consistent input data and model parameters regarding the modelled contaminants:

1. River flows (m^3/s)
2. River concentrations (ug/l)
3. estuarine retention (%)
4. atmospheric deposition ($g/km^2/yr$)
5. offshore loads (tons/yr)
6. boundary concentrations (ng/l)
7. water quality process parameters

Data for all the North Sea river inputs (both flow and concentrations) were provided for 1989. Concentrations of both river particulate matter and contaminants were given. Also, to account for sedimentation of particulate matter and contaminants in river estuaries, 'retention factors' were provided for each river.

Table 3.3 Retention of sediment and contaminants in North Sea estuaries

River	**Sampling station**	**Estuarine retention (%)**		
		Cd	**PCB-153**	**fluvial SPM**
New Waterway (Rhine/Meuse)	Maassluis	20	32	45
Dutch WaddenSea	Lake IJssel (fresh water)	12	71	85
Scheldt	Schaar van Ouden Doel	55	84	80
Ems	Herbrum	35	84	85
Weser	Intschede	26	68	80
Elbe	Grauerort	59	81	85
Thames	Teddington Weir	31	67	60
Humber	7 stations in 7 tributary rivers	10	50	20
Wash	fresh water area	32	88	85
Tyne	Wylam	6	15	15
Tees	Worsall	9	16	15
Forth	fresh water area	54	78	85
Other rivers (Ness, Medway, Tweed, Tay, Glomma, Gota)	fresh water area	30	50	60

Source: Zwolsman, 1994.

Additional loads to the North Sea from offshore drilling activities and atmospheric deposition were also provided. Contaminant concentrations at the boundaries of the modelled area were provided. Finally, water quality process parameters were given. These values are presented in the tables below.

Table 3.4 Offshore loads to the North Sea

Coordinates	**Production water (m^3/yr)**	**Cd concentration (mg/l)**	**Load (tons/yr)**
60.5 N; 1^E	$150 * 10^6$	0.1	15
57N; 3.5^E	$50 * 10^6$	0.1	5

Source: Rye, 1997; Rye et al., 1998; E&P Forum, 1993. (tons=10^3 kg)

Table 3.5 atmospheric deposition to the North Sea

	Cadmium	PCB total	PCB-153
North Sea (508126 km^2) ton/yr	20 $^{1)}$	1.2	0.06
g/ km^2/yr	**39.4**	2.36	**0.12**

Source: Baart et al., 1995; Grieken et al.,1996.

$^{1)}$ Baart et al., 12.4 ton/yr; van Grieken et al., 27 ton/yr

The **bold** figures have been used in the models.

Table 3.6 Boundary concentrations for Strait of Dover and Northern Atlantic

	Cadmium total (ng/l)	PCB-153 total (ng/l)
Strait of Dover	25	0.003
Northern boundary	15	0.002

Source: Statham et al., 1993; Ras et al., 1996

Table 3.7 Model parameters for partitioning of contaminants to suspended matter and volatilization

Parameter (unit)	Cd	PCB-153
K_d (l/g)	30	
K_{poc} (log l/kgOC)		6.8
He (Pa.m^{-3}.mol^{-1})		10
k_{deg} (d^{-1})		1.0*10^{-6}

Source: Aquapol database (RIKZ, 1996)

With a consistent set of model input data and model parameters, the model comparison exercise allows differences in results to be attributed to inherent differences in the flow, model approaches, concepts and internal processes affecting pollutant transport and fate.

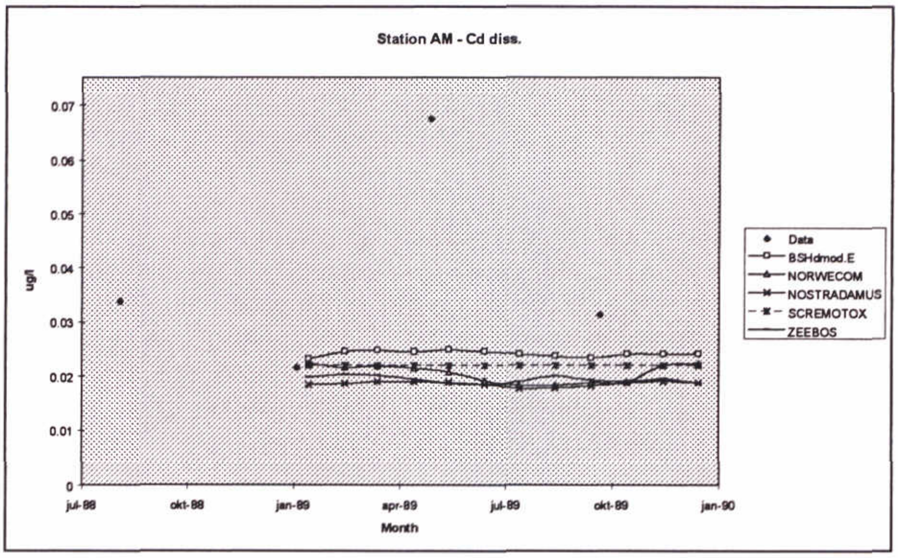
Furthermore it gives a range of results which are then indicative of the ability of models in general to reproduce the conditions measured in nature, and to be used to answer management and policy questions. This last point is addressed further in the next chapter, on model responsiveness.

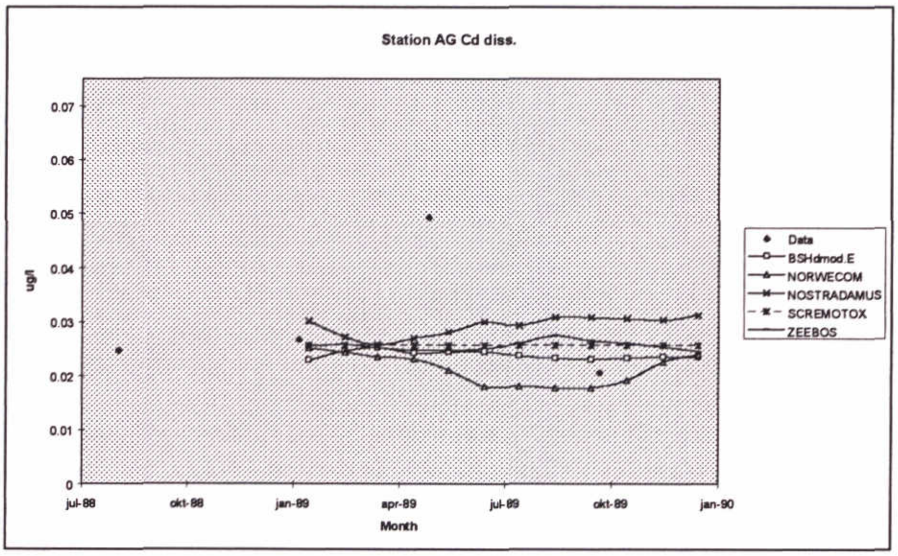
3.2 Seasonal variations

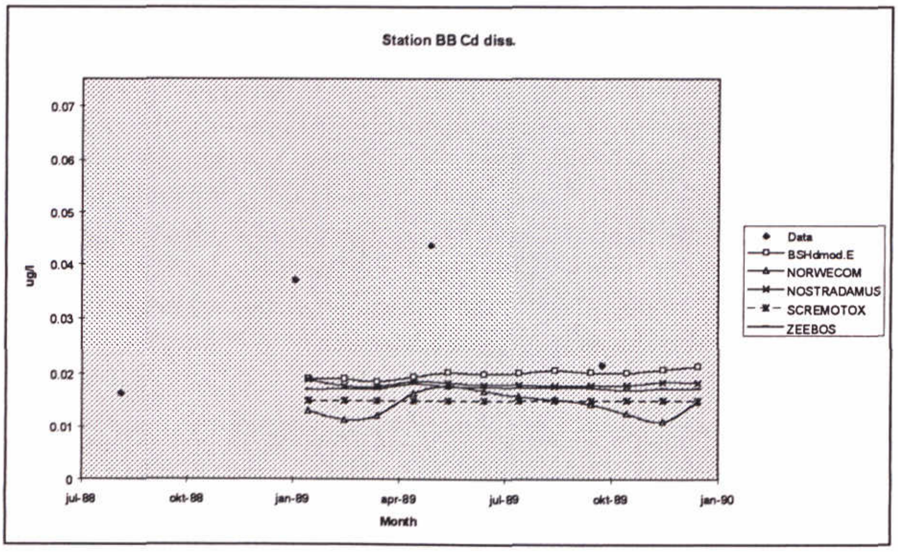
For each of the seven selected locations, the models have predicted the monthly average concentrations and standard deviations of cadmium (as dissolved cadmium in ug/l) and PCB-153 (as concentrations adsorbed to particulate organic carbon in mg/kg Organic Carbon).

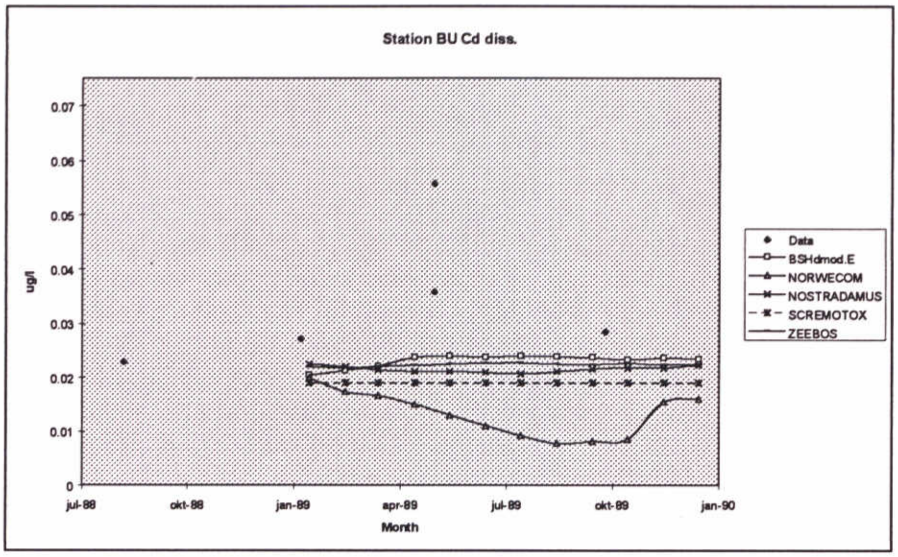
Model Results Cadmium

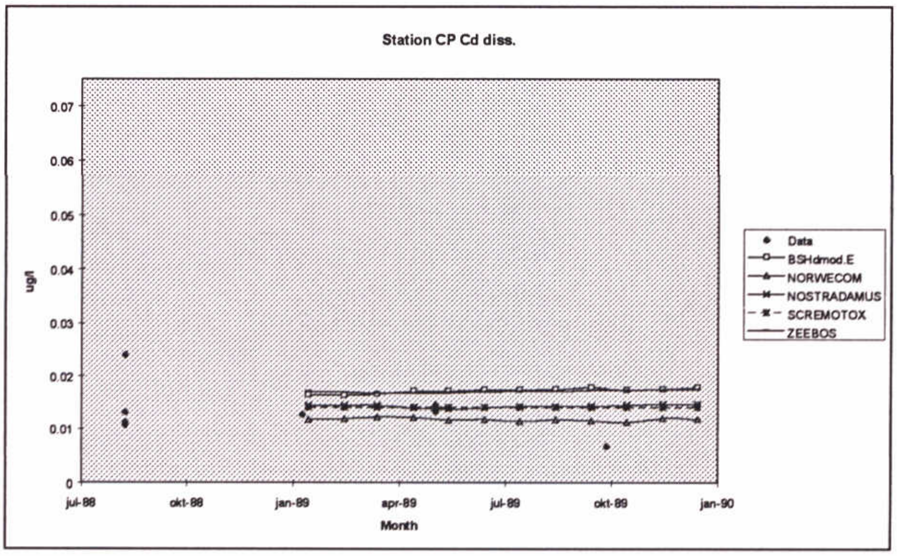
The model results for cadmium together with the NSP measurement data are plotted for each location in Figure 3.2. The calculated results from SCREMOTOX are the same for every month, as this steady-state model gives only a single (yearly average) result. For the other models, the monthly average values are plotted.

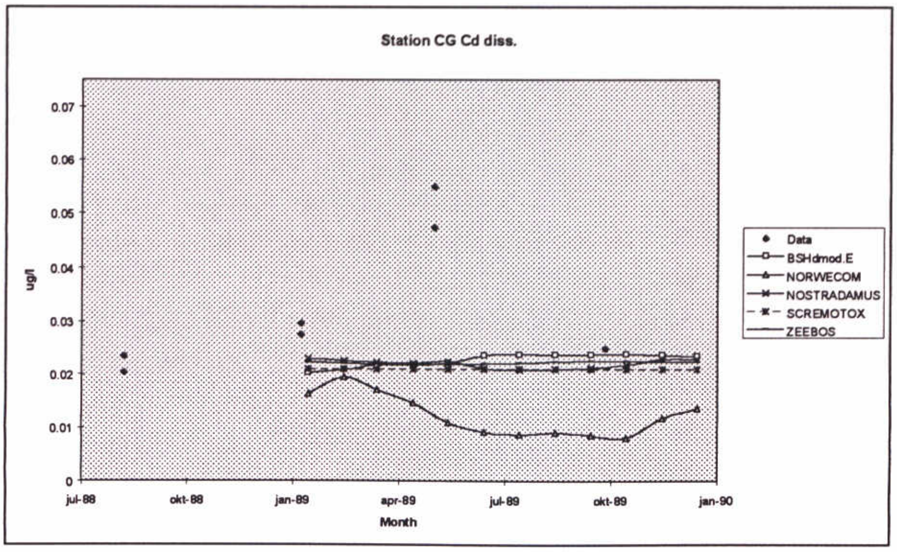

Station AM - Cd diss.
ug/l
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
jul-88
okt-88
jan-89
apr-89
jul-89
okt-89
jan-90
Month
Data
BSHdmod.E
NORWECOM
NOSTRADAMUS
SCREMOTOX
ZEEBOS


Station AG Cd diss.
ug/l
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
jul-88
okt-88
jan-89
apr-89
jul-89
okt-89
jan-90
Month
Data
BSHdmod.E
NORWECOM
NOSTRADAMUS
SCREMOTOX
ZEEBOS


Station BB Cd diss.
ug/l
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
jul-88
okt-88
jan-89
apr-89
jul-89
okt-89
jan-90
Month
Data
BSHdmod.E
NORWECOM
NOSTRADAMUS
SCREMOTOX
ZEEBOS


Station BU Cd diss.
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
ug/l
jul-88
okt-88
jan-89
apr-89
jul-89
okt-89
jan-90
Month
Data
BSHdmod.E
NORWECOM
NOSTRADAMUS
SCREMOTOX
ZEEBOS


Station CP Cd diss.
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
ug/l
jul-88
okt-88
jan-89
apr-89
jul-89
okt-89
jan-90
Month
Data
BSHdmod.E
NORWECOM
NOSTRADAMUS
SCREMOTOX
ZEEBOS


Station CG Cd diss.
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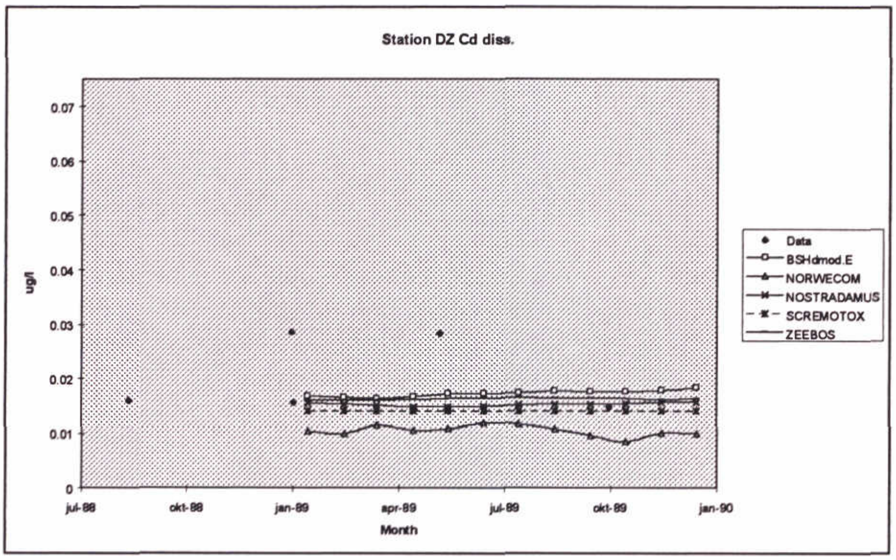
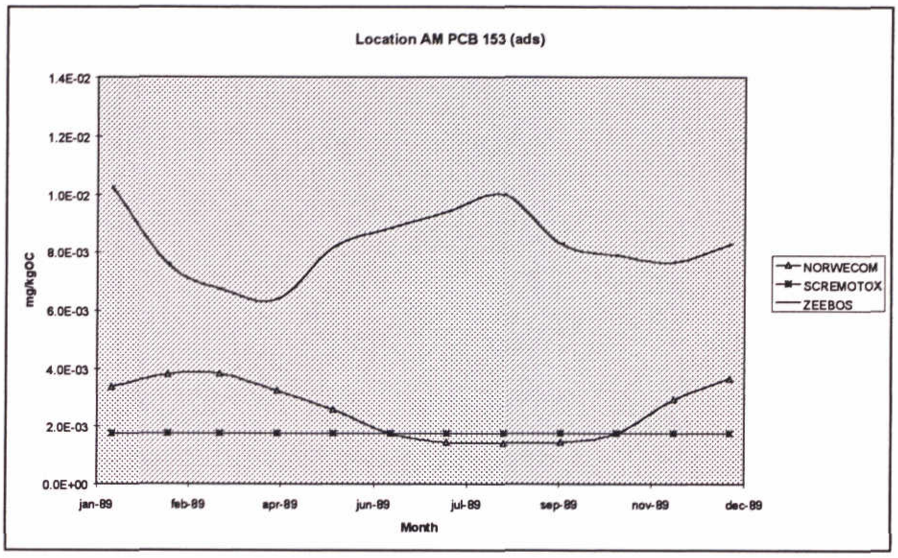
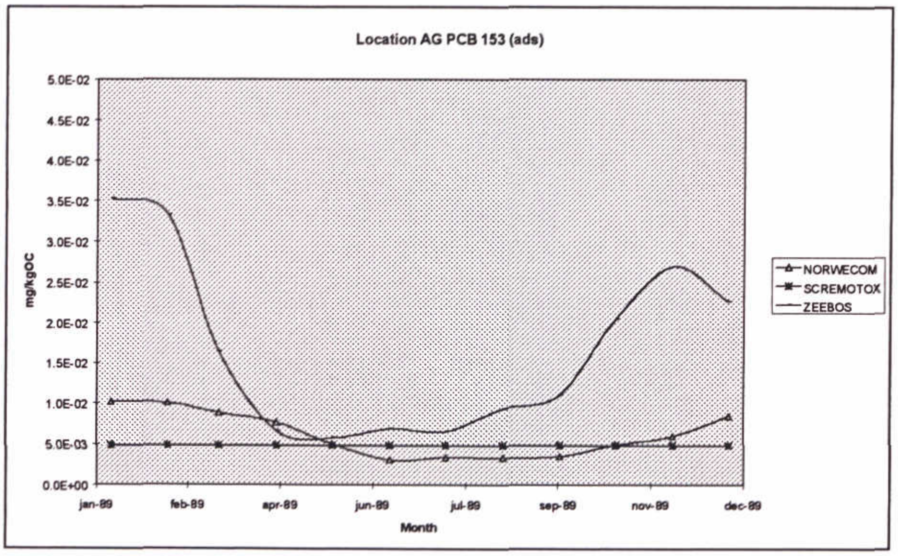
0.06
0.05
0.04
0.03
0.02
0.01
0
ug/l
jul-88
okt-88
jan-89
apr-89
jul-89
okt-89
jan-90
Month
Data
BSHdmod.E
NORWECOM
NOSTRADAMUS
SCREMOTOX
ZEEBOS

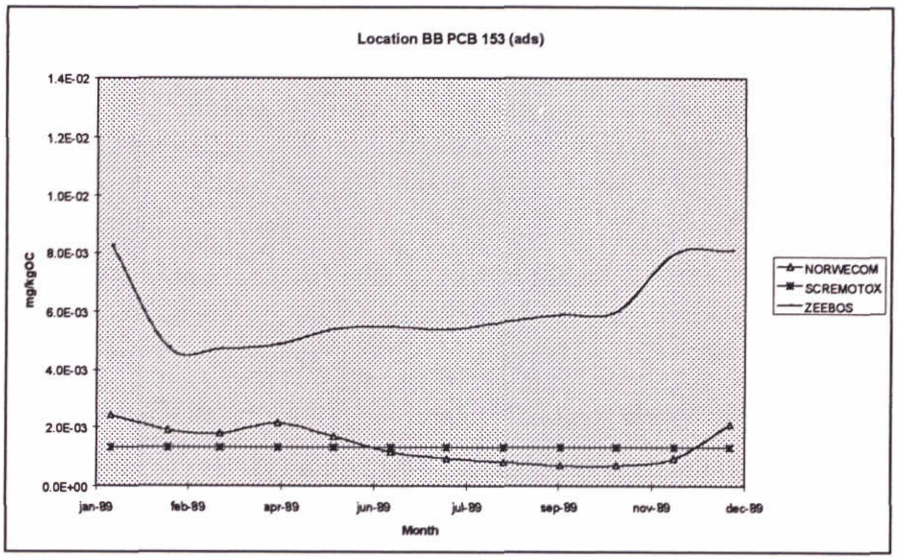

Station DZ Cd diss.
ug/l
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
jul-88
okt-88
jan-89
apr-89
jul-89
okt-89
jan-90
Month
Data
BSHdmod.E
NORWECOM
NOSTRADAMUS
SCREMOTOX
ZEEBOS

Model Results PCB-153

The model results for PCB-153 are plotted for each location in Figure 3.4. There are not sufficient monitoring data of PCB-153 from the North Sea Project or other databases available for a model-data comparison. The North Sea models BSHdmod and NOSTRADAMUS did not calculate PCB concentrations.



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mg/kgOC
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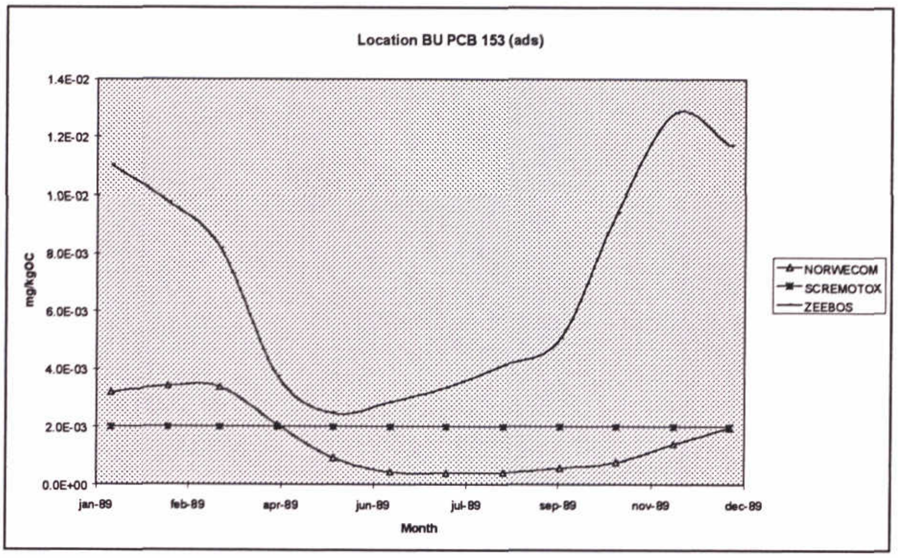
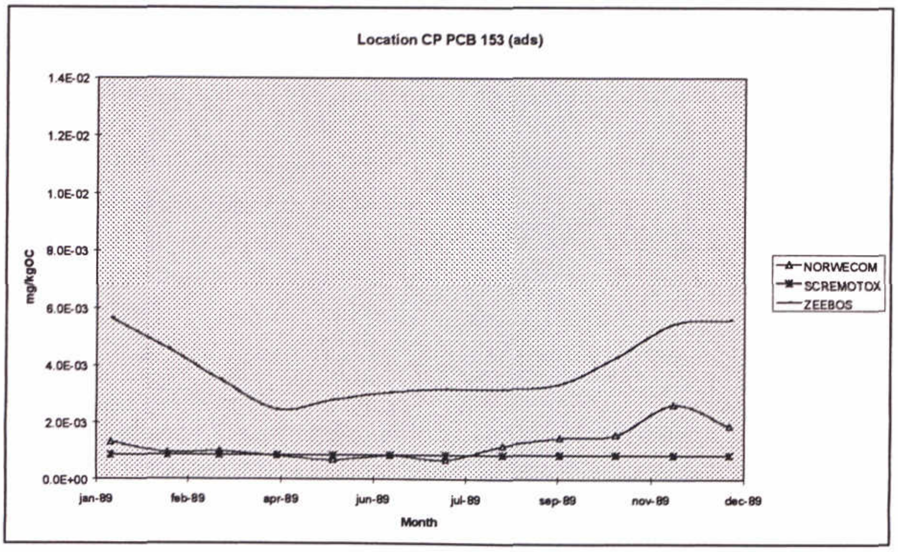
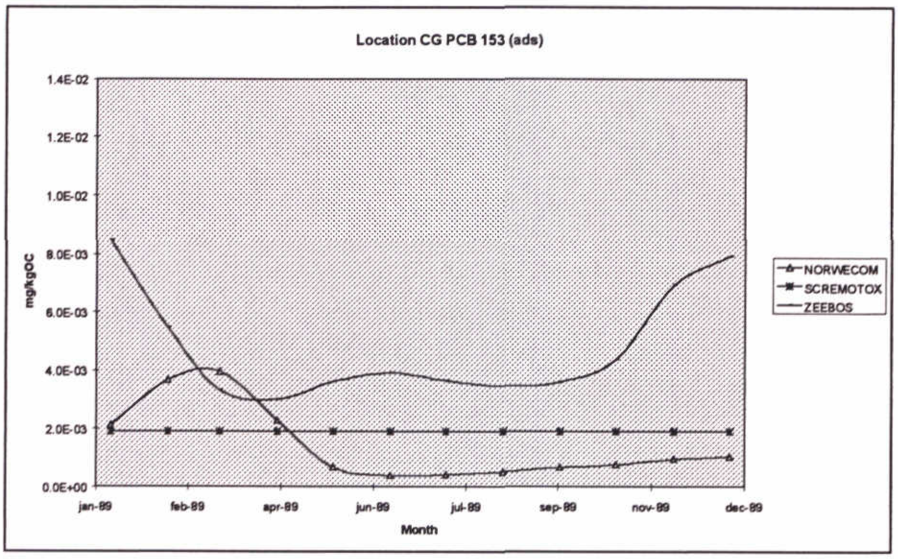
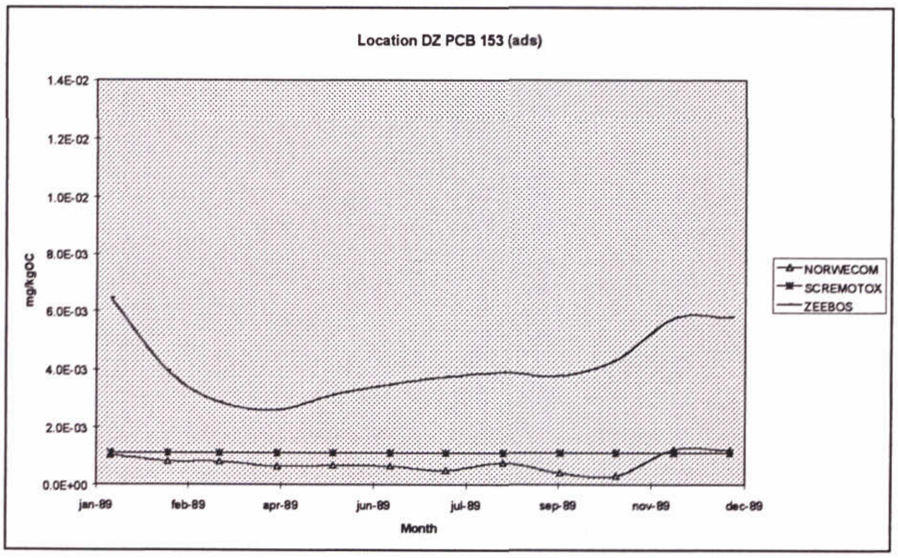
1.2E-02
1.0E-02
8.0E-03
6.0E-03
4.0E-03
2.0E-03
0.0E+00
jan-89
feb-89
apr-89
jun-89
jul-89
sep-89
nov-89
dec-89
Month
NORWECOM
SCREMOTOX
ZEEBOS


Location BU PCB 153 (ads)
mg/kgOC
1.4E-02
1.2E-02
1.0E-02
8.0E-03
6.0E-03
4.0E-03
2.0E-03
0.0E+00
jan-89
feb-89
apr-89
jun-89
jul-89
sep-89
nov-89
dec-89
Month
NORWECOM
SCREMOTOX
ZEEBOS


Location CP PCB 153 (ads)
mg/kgOC
1.4E-02
1.2E-02
1.0E-02
8.0E-03
6.0E-03
4.0E-03
2.0E-03
0.0E+00
jan-89
feb-89
apr-89
jun-89
jul-89
sep-89
nov-89
dec-89
Month
NORWECOM
SCREMOTOX
ZEEBOS


Location CG PCB 153 (ads)
mg/kgOC
1.4E-02
1.2E-02
1.0E-02
8.0E-03
6.0E-03
4.0E-03
2.0E-03
0.0E+00
jan-89
feb-89
apr-89
jun-89
jul-89
sep-89
nov-89
dec-89
Month
NORWECOM
SCREMOTOX
ZEEBOS


Location DZ PCB 153 (ads)
mg/kgOC
1.4E-02
1.2E-02
1.0E-02
8.0E-03
6.0E-03
4.0E-03
2.0E-03
0.0E+00
jan-89
feb-89
apr-89
jun-89
jul-89
sep-89
nov-89
dec-89
Month
NORWECOM
SCREMOTOX
ZEEBOS

3.3 Yearly Average Concentrations

The five North Sea models calculated yearly average concentrations at the seven selected NSP stations for salinity, Total Suspended matter (SPM) and dissolved cadmium. These results are given in Table 3.8 - 3.10.

Graphs for salinity and SPM are presented, showing the mean and standard deviation of concentrations for the data and each of the models.

Salinity

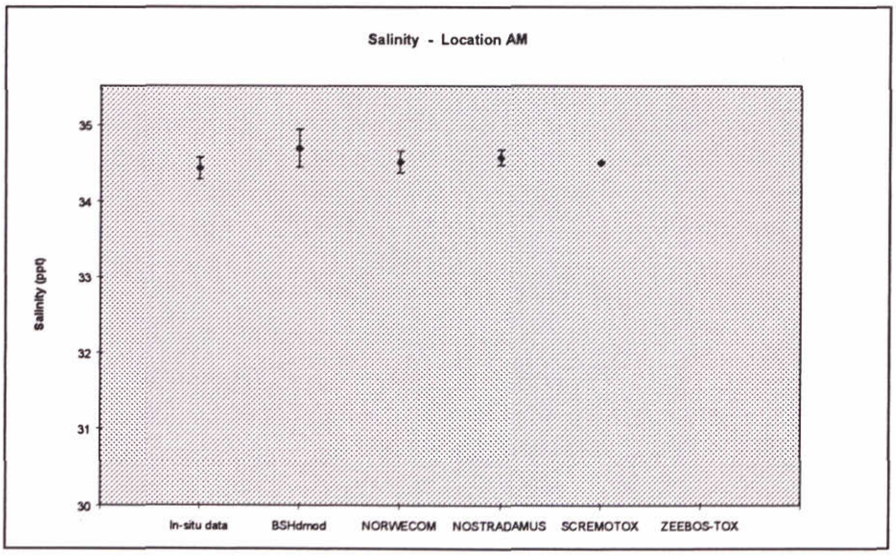
Table 3.8 Yearly averaged model results (salinity ppt)

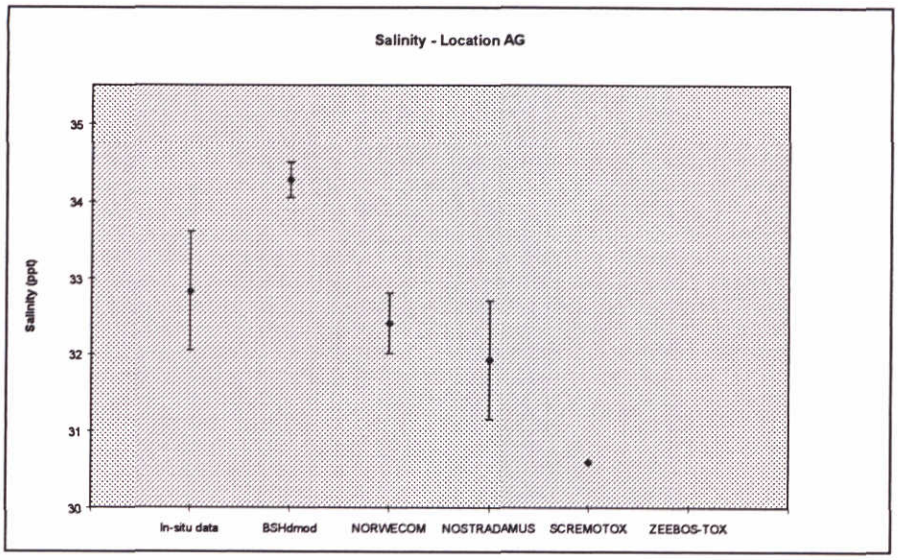
			Model Results of salinity in ppt (mean ± s.d.)				
	NSP location	In-situ data (mean ± s.d.)	BSHcmod[1]	NORWE-COM	NOSTRA-DAMUS	SCREMO-TOX[2]	ZEEBOS-TOX
1.	AM	34.43 ± 0.14	34.69 ± 0.25	34.51 ± .14	34.57 ± 0.10	34.5	-
2.	AG	32.83 ± 0.78	34.28 ± 0.23	32.41 ± .40	31.93 ± 0.78	30.6	-
3.	BB	34.52 ± 0.12	34.71 ± 0.13	34.48 ± .19	34.50 ± 0.04	34.6	-
4.	BU	33.22 ± 0.46	34.17 ± 0.22	33.36 ± .42	34.23 ± 0.05	33.7	-
5.	CP	34.85 ± 0.11	34.92 ± 0.07	34.89 ± .11	34.66 ± 0.11	34.8	-
6.	CG	32.38 ± 0.53	33.55 ± 0.70	32.40 ± .33	33.95 ± 0.14	33.2	-
7.	DZ	34.66 ± 0.10	34.86 ± 0.04	34.66 ± .17	34.55 ± 0.02	34.8	-

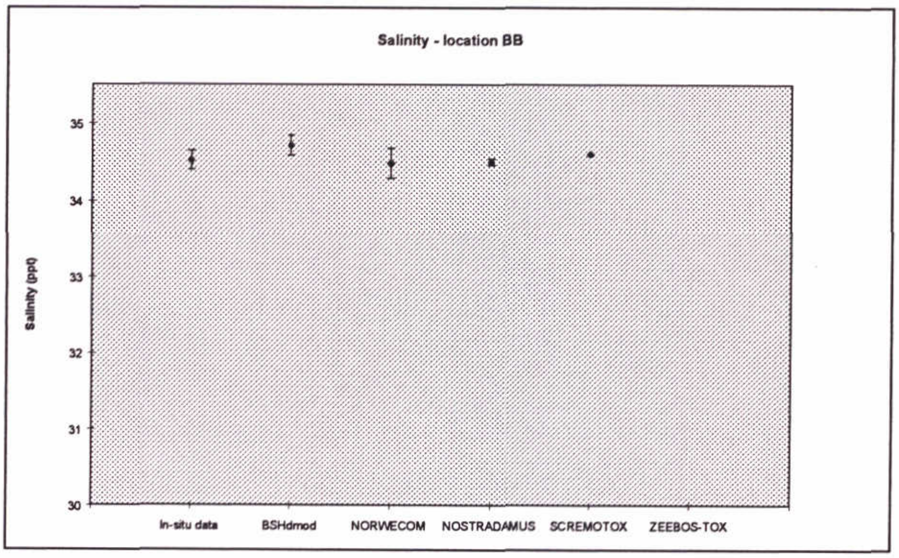
Notes:

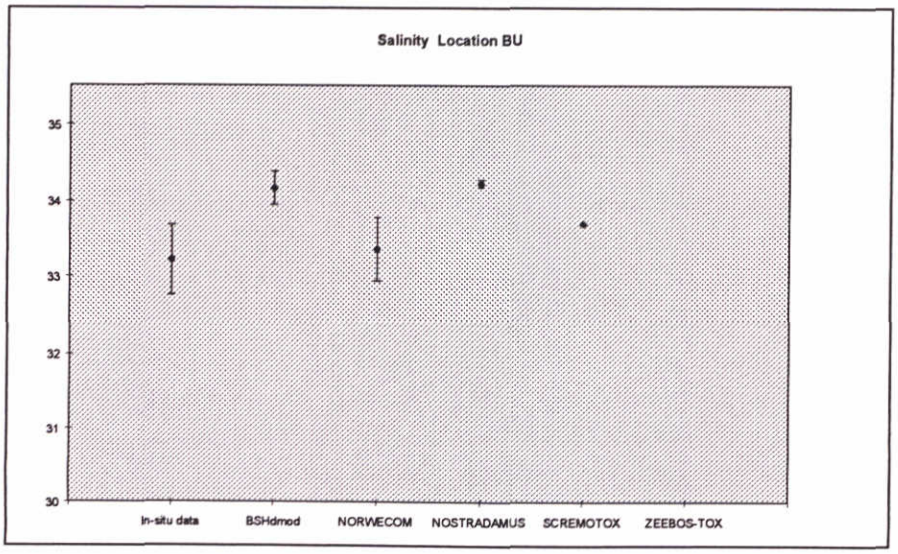
1) In the BSH simulation hydrodynamic data of the year 1995 are used. Also, In the hydrodynamic numerical model (BSHcmod) for the fresh water input by rivers only annual mean values are used

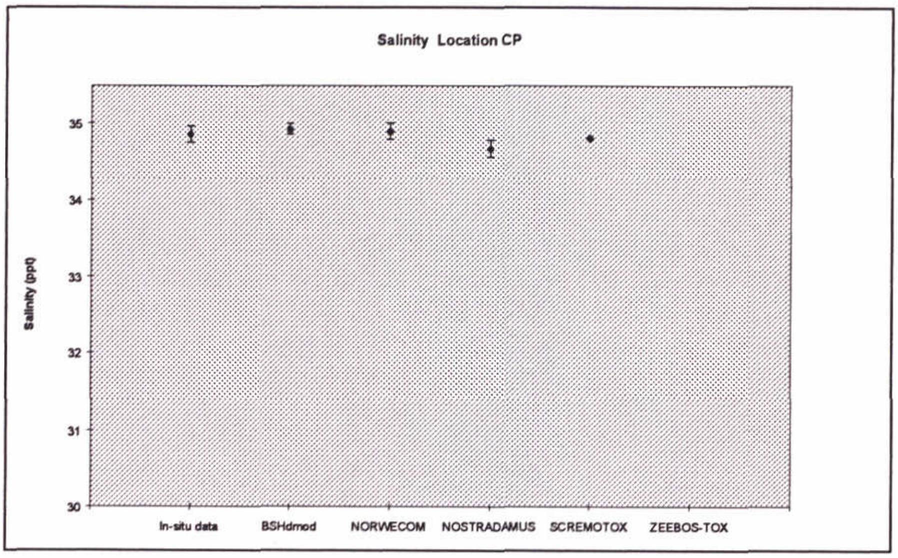
2) For Scremotox, river flow data of 1990 are used. These values are fixed in the model and cannot be changed. Because the model calculates steady state concentrations there is no standard deviation of results.

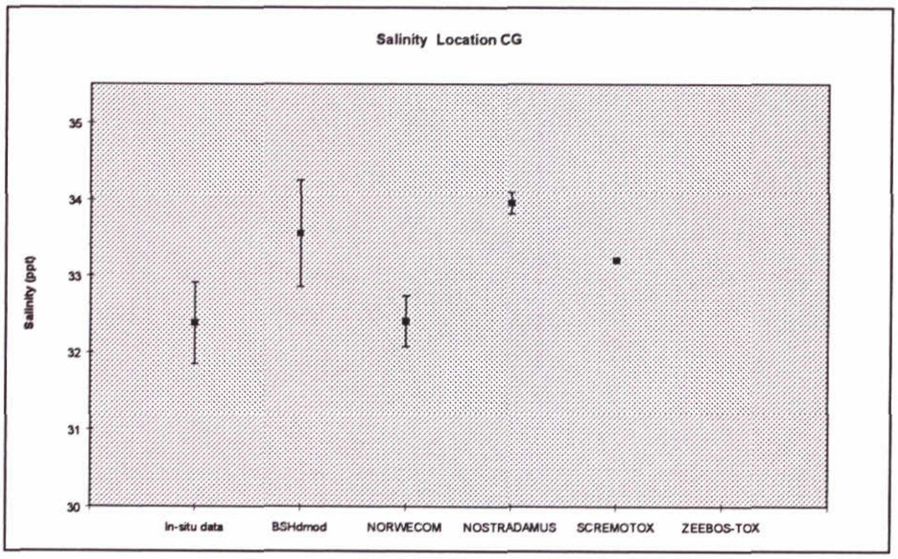


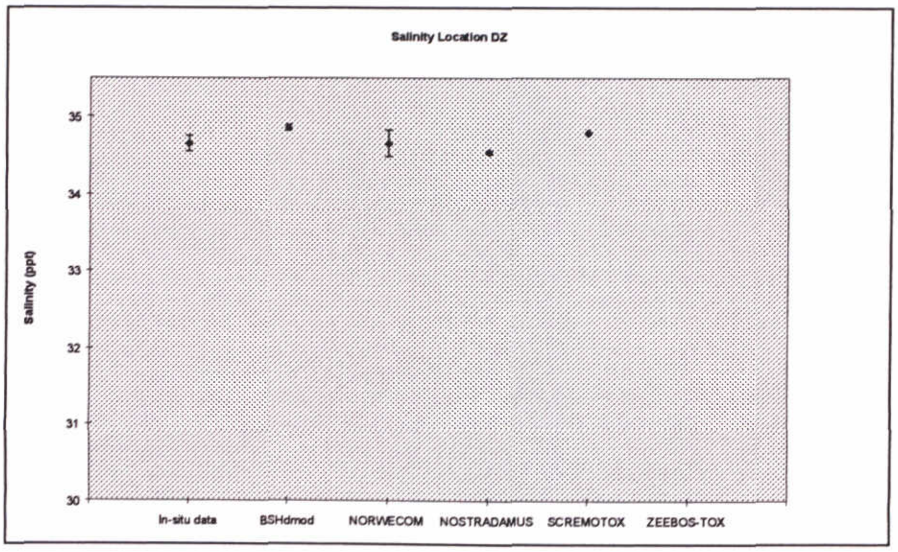

Salinity - Location AG
Salinity (ppt)
35
34
33
32
31
30
In-situ data
BSHdmod
NORWECOM
NOSTRADAMUS
SCREMOTOX
ZEEBOS-TOX


Salinity - location BB
Salinity (ppt)
35
34
33
32
31
30
In-situ data
BSHdmod
NORWECOM
NOSTRADAMUS
SCREMOTOX
ZEEBOS-TOX


Salinity Location BU
35
34
33
32
31
30
In-situ data
BSHdmod
NORWECOM
NOSTRADAMUS
SCREMOTOX
ZEEBOS-TOX


Salinity Location CP
Salinity (ppt)
35
34
33
32
31
30
In-situ data
BSHdmod
NORWECOM
NOSTRADAMUS
SCREMOTOX
ZEEBOS-TOX


Salinity Location CG
Salinity (ppt)
35
34
33
32
31
30
In-situ data
BSHdmod
NORWECOM
NOSTRADAMUS
SCREMOTOX
ZEEBOS-TOX


Salinity Location DZ
Salinity (ppt)
35
34
33
32
31
30
In-situ data
BSHdmod
NORWECOM
NOSTRADAMUS
SCREMOTOX
ZEEBOS-TOX

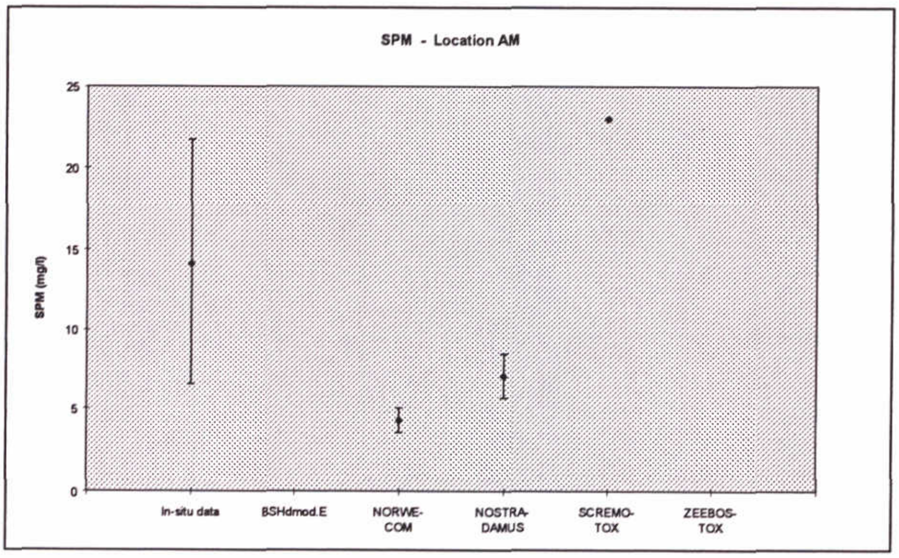
Suspended Particulate Matter

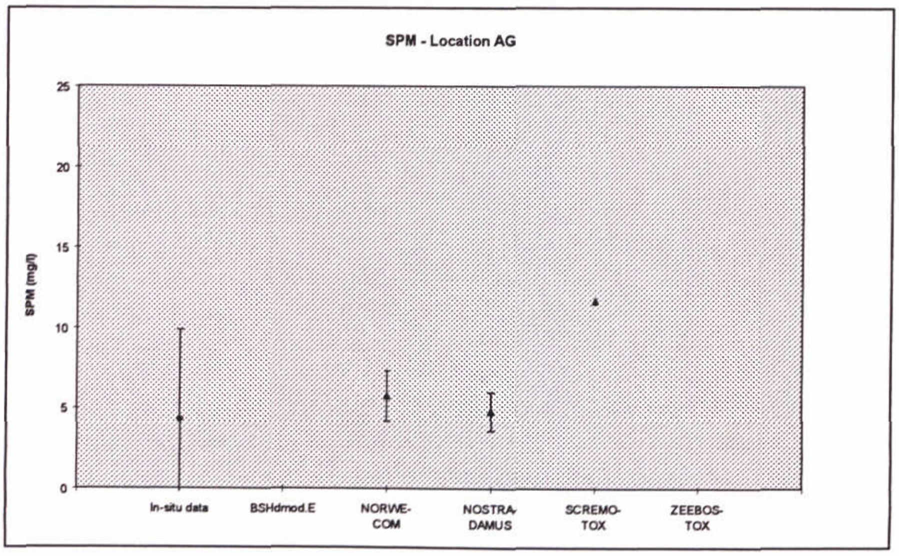
Table 3.9 Yearly averaged model results (Total SPM mg/l)

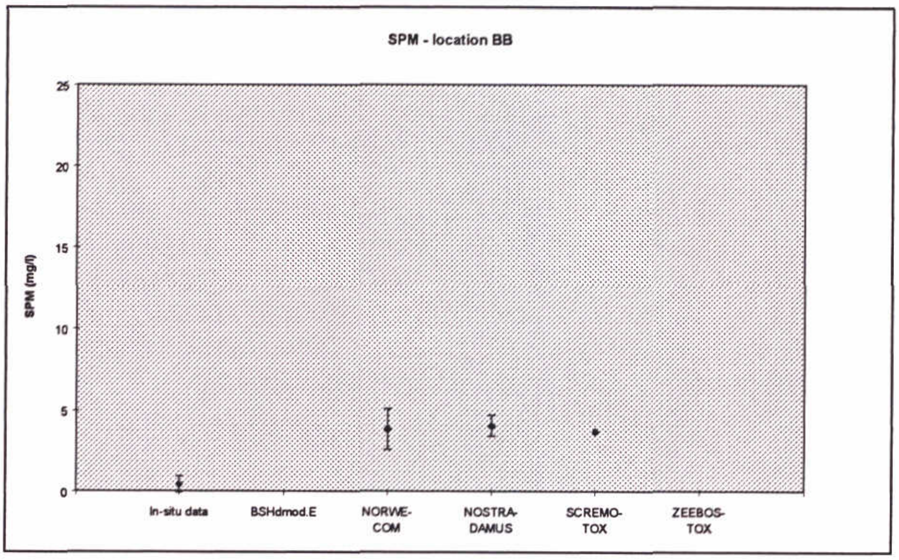
			Model Results of Total SPM in mg/l (mean ± s.d.)				
	NSP location	In-situ data (mean ± s.d.)	BSHdmod.E	NORWE-COM	NOSTRA-DAMUS	SCREMO-TOX[1]	ZEEBOS-TOX
1.	AM	14.1 ± 7.6	-	4.26 ± 0.74	7.04 ± 1.40	23.0	-
2.	AG	4.3 ± 5.6	-	5.76 ± 1.57	4.80 ± 1.19	11.7	-
3.	BB	0.43 ± 0.48	-	3.85 ± 1.27	4.05 ± 0.64	3.7	-
4.	BU	0.65 ± 0.73	-	2.87 ± 0.73	6.30 ± 1.22	4.1	-
5.	CP	0.05 ± 0.04	-	0.67 ± 0.24	0.78 ± 0.44	1.7	-
6.	CG	2.3 ± 3.2	-	2.90 ± 0.79	4.94 ± 1.40	4.4	-
7.	DZ	0.70 ± 0.28	-	1.84 ± 1.04	1.44 ± 0.63	1.5	-

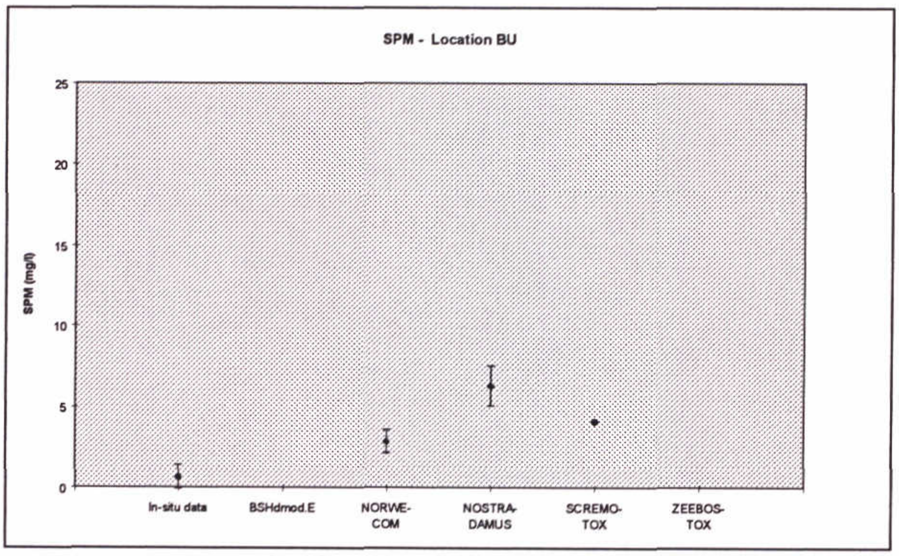
Notes:

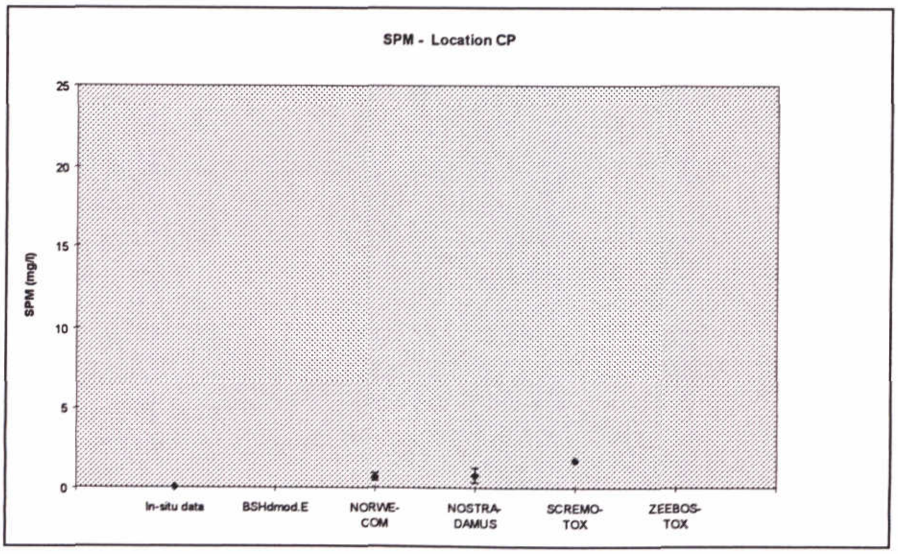
1) For Scremotox, river flow data of 1990 are used. These values are fixed in the model and cannot be changed. Because the model calculates steady state concentrations there is no standard deviation of results.

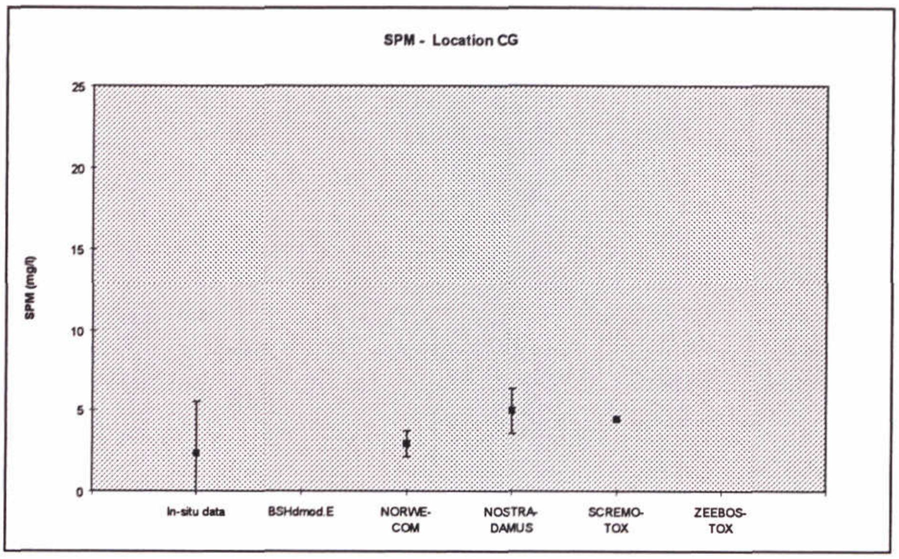


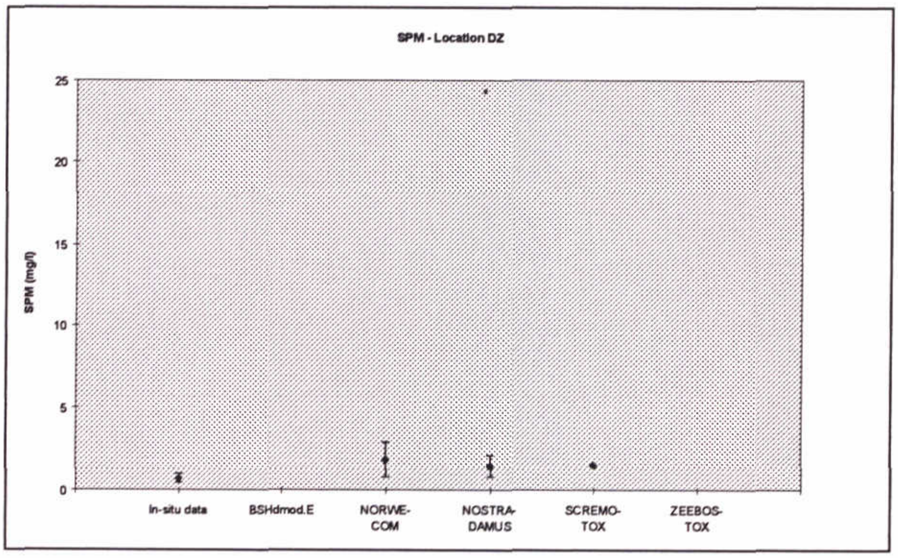



SPM - location BB
SPM (mg/l)
25
20
15
10
5
0
In-situ data
BSHdmod.E
NORWE-COM
NOSTRA-DAMUS
SCREMO-TOX
ZEEBOS-TOX


SPM - Location BU
SPM (mg/l)
25
20
15
10
5
0
In-situ data
BSHdmod.E
NORWE-COM
NOSTRA-DAMUS
SCREMO-TOX
ZEEBOS-TOX


SPM - Location CP
SPM (mg/l)
25
20
15
10
5
0
In-situ data
BSHdmod.E
NORWE-COM
NOSTRA-DAMUS
SCREMO-TOX
ZEEBOS-TOX


SPM - Location CG
SPM (mg/l)
25
20
15
10
5
0
In-situ data
BSHdmod.E
NORWE-COM
NOSTRA-DAMUS
SCREMO-TOX
ZEEBOS-TOX


SPM - Location DZ
SPM (mg/l)
25
20
15
10
5
0
In-situ data
BSHdmod.E
NORWE-COM
NOSTRA-DAMUS
SCREMO-TOX
ZEEBOS-TOX

Cadmium

The cadmium results are presented not as concentrations but in terms of a 'cost function'. The cost function is a simple equation which give quantitative measures of deviation between model and field data, normalized in units of standard deviation. The cost function is:

$$C_{x,t} = \frac{M_{x,t} - D_{x,t}}{sd_{x,t}}$$

with

$C_{x,t}$	Cost Function (normalised deviation per station)
$M_{x,t}$	mean value of the model results per station over the whole year
$D_{x,t}$	mean value of the in situ data per station over the whole year
$sd_{x,t}$	standard deviation of the in situ data per station over the whole year

Table 3.10 Yearly averaged model results (Cost Function for cadmium dissolved, µg/l)

			Cost Function				
	NSP location	In-situ data (mean ± s.d.)	BSHdmod.E[1]	NORWE-COM	NOSTRA-DAMUS	SCREMO-TOX	ZEEBOS-TOX
1.	AM	0.039±0.020	-0.74	-0.93	-1.02	-0.81	-0.92
2.	AG	0.030±0.013	-0.50	-0.67	-0.06	-0.33	-0.22
3.	BB	0.030±0.013	-0.77	-1.21	-0.92	-1.15	-0.81
4.	BU	0.034±0.015	-0.73	-1.38	-0.83	-1.0	-0.67
5.	CP	0.011±0.003	+2.0	-0.23	+1.09	+1.0	+2.0
6.	CG	0.033±0.015	-0.68	-1.38	-0.73	-0.8	-0.63
7.	DZ	0.022±0.008	-0.62	-1.52	-0.84	-1.0	-0.77

Note:
1) in the BSH simulation, hydrodynamic data of the year 1995 are used

3.4 Mass Balance Calculations

Mass balance calculations were made to compare the models in terms of hydrodynamic transport (inflow and outflow of the whole North Sea), and internal processes (e.g. sedimentation, volatilization, degradation, evaporation) and to help understand differences in model predictions for a specific area. In the mass balance calculation, the inflows (mass in) and outflows (mass out) of the system are quantified. Mass changes within the system (due to e.g. sedimentation or volatilization) are also quantified. Mass balance calculations have been made for water, suspended particulate matter, cadmium and PCB. Results are presented in Tables 3.11 - 3.14. Net inflows and outflows for the Straight of Dover and the North Atlantic are given. Complete mass balances showing inflow and outflow over each boundary are given in Appendix D.

Table 3.11 Modelled Mass Balance Water (tons/year = m^3/yr)

	BSHcmod[1]	NORWE-COM	NOSTRA-DAMUS	ZEEBOS-TOX	SCREMO-TOX
MASS IN					
Straight of Dover (net)	2.2×10^{12}	4.0×10^{12}	2.5×10^{12}	no mass balance calculation of water	3.4×10^{12}
Rivers	0.1×10^{12}	0.13×10^{12}	0.09×10^{12}		0.17×10^{12}
Offshore	$.0002 \times 10^{12}$	0	0		0
Total Mass In	2.3×10^{12}	4.1×10^{12}	2.6×10^{12}		3.6×10^{12}
MASS OUT					
North Bound (net)(56°N)	2.2×10^{12}	3.1×10^{12}	2.5×10^{12}	no mass balance calculation of water	3.4×10^{12}
Net evaporation	0	0	0.005×10^{12}		0
Total Mass out	2.2×10^{12}	3.1×10^{12}	2.5×10^{12}		3.4×10^{12}
NET (in-out)	0.1×10^{12}	1.0×10^{12}	0.1×10^{12}		0.2×10^{12}

[1] Note: in the BSH simulation, hydrodynamic data of the year 1995 are used

Table 3.12 Modelled Mass Balance SPM (Mtons/year)

	BSHdmod.E[1]	NORWE-COM	NOSTRA-DAMUS	ZEEBOS-TOX	SCREMO-TOX
MASS IN	no calculation (SPM not in model)				
Straight of Dover (net)		14.8	17.2	no mass balance calculation of SPM	5.7
Rivers		1.6	1.6		14.8
Atmos. Depos.		0	0		0
Offshore		0	12.6		0
Erosion[1]		3.4	57.4		8.8
Total Mass In		19.8	88.8		29.3
MASS OUT	no calculation (SPM not in model)				
North Boundary (56°N)		26.5	18.8	no mass balance calculation of SPM	10.8
Sedimentation		negligible	69.8		18.4
Total Mass out		26.5	88.6		29.2
NET (in-out)		-6.7	0.2		0.1

Table 3.13 Modelled Mass Balance Cadmium (tons/year)

	BSHdmod.E[1]	NORWE-COM	NOSTRA-DAMUS	ZEEBOS-TOX	SCREMO-TOX
MASS IN					
Straight of Dover (net)	52	100	66	85	83
Rivers	12	16	17	27	13
Atmos. Depos.	20	10	13	9	10
Offshore	20	0	0	0	2
Total Mass In	104	126	96	121	108
MASS OUT					
N. Boundary (net) (56°N)	70	40	90	119	93
Sedimentation (net)	0	83	9	19	14
Total Mass out	70	123	99	138	106
NET (in-out)	34	3	-3	-17	1

[1] Note: in the BSH simulation, hydrodynamic data of the year 1995 are used

Table 3.14 Modelled Mass Balance PCB (kg/year)

	NORWECOM	ZEEBOSTOX	SCREMOTOX
MASS IN			
Straight of Dover (net)	11.5	7.1	11
Rivers	38.4	51	23.5
Atmos. Depos.	29.3	26	28.8
Offshore	0	0	0
Erosion	0	0	0
Total Mass In	79.2	84.1	63.3
MASS OUT			
North Bound (net) (56°N)	3.7	9.7	16.3
Sedimentation	56.2	36.7	23.7
Volatilization	0	42.3	25.4
Degradation	0	0.0023	0
Total Mass out	59.9	88.7	65.4
NET (in-out)	19.3	-4.6	-2.1

3.5 Validation of estuary and bioaccumulation models (regional data sets)

Several models were presented in the ASMO workshop which could not participate in the comparative validation exercise. These models were for substances other than cadmium and PCB and/or modelled geographic areas other than the North Sea:

1. PROVANN (North Sea model for oil dispersion)
2. SAWES (Western Scheldt estuary model for heavy metals and organic contaminants)
3. PCB bioaccumulation model (foodchain uptake model)
4. TELEMAC/SUBIEF (Bay of Seine model for radionuclides)

As these models are completely unrelated, it was not possible to define any comparative exercises. Instead, the conceptual background and relevant validation results were presented for each model during the workshop.

3.6 Interpretation of model validation results

3.6.1 Monthly time scale

The validation on the monthly time scale is intended to indicate how well the models perform at specific locations over a yearly cycle.

When the data are reviewed with these criteria, some general comments can be made:

1. For dissolved cadmium, the modelled concentrations are all very similar (in the range of 0.01 -0.03 ug/l) but are consistently *lower* than the measured concentrations. This can be seen in the plots of model predictions together with the data (Figure 3.2) as well as in the calculated cost function results (Table 3.10).
2. For cadmium, none of the models predict the seasonal variation in concentrations that is shown by the data. The data show maximum spring time concentrations as high as 0.07 ug/l.

3. For PCB-153 there is no field data with which to make a comparison. However, model results (NORWECOM and ZEEBOS-TOX) show that chemical processes result in much more seasonal dynamics in calculated concentrations than for cadmium.

From (1), it can be concluded that there must be (an) additional source(s) of cadmium in the North Sea which all the models are missing. Sources may include cadmium flowing into the North Sea from outside the region as well as sources within the North Sea. Cold deep water flowing in from the North Atlantic can have higher concentrations than the surface water. As boundary concentrations used for modelling are primarily taken from surface water measurements, this extra mass entering the North Sea is not accounted for. Also, the 2-dimensional models (depth-averaged) cannot account for different water masses of different quality flowing into the region.

Another possibility that was presented during the workshop is that offshore drilling activities are contributing significantly to loads. While available data are still very preliminary, it seems that the discharge of large volumes of production water could be adding cadmium at a level comparable to the combined loads of all the rivers.

The model input data did include an offshore load of 20 tons/yr cadmium (though this was not included in all the models), but even including this, the model results were below the measured values. There is still some uncertainty as to the magnitude of this source. Other potential sources of contaminants must also be considered, such as dumping of contaminated dredged sediments along the Belgian, Dutch and UK coasts (which was not included in the model exercises).

From (2) it can be concluded that there is most likely a (chemical fate) process taking place which the models do not include. One hypothesis is that the higher spring concentrations are due to seasonally variable benthic exchange of dissolved cadmium (there is some evidence for this) coupled to longer term desorption of cadmium from particles derived from river inputs (Tappin et al., 1995). Since none of the models incorporates these processes, it is not surprising that the spring distributions are not simulated. The concentration patterns illustrates the potential importance of benthic exchange for cadmium (and other metals too). In terms of understanding of the North Sea system, very little is known about the recycling capabilities of the seafloor sediments for contaminants. Potentially there is also a seasonal influence from external sources which is not included in the model (i.e. time varying boundary concentrations, sediment dumping, or atmospheric deposition). Variations of the distribution coefficient Kd over the season are quite possible, but this would not explain the observed concentration pattern. Kd values would likely increase in the spring due to changes in pH caused by algae growth. An increased Kd would result in a decreased concentration of dissolved cadmium, not an increase as is seen. A final possibility lies in a systematic error in the measurements. Of all the models, NORWECOM shows the most seasonal dynamics in dissolved concentration, but this is not always consistent with the patterns shown in the data.

For PCB-153 and other organic pollutants there is no data set with which to make comparisons between models and field measurements. As such, model results can only be compared against each other. It can be seen from the models NOWECOM and ZEEBOS that there is a more dynamic variation in concentration over the year. The model SCREMOTOX calculates only a steady-state (constant) concentration. The data presented are for adsorbed PCB (onto organic carbon), and thus the concentration dynamics can be due to a large extent to the variation in the organic carbon concentration over the year. Specifically, the typically lower concentrations of adsorbed PCB in the summer are due to the higher POC concentrations, as calculated by a eutrophication module.

3.6.2 Yearly time scale

The North Sea models calculated yearly average concentrations at the seven selected NSP stations for salinity, Suspended Particulate Matter (SPM) and dissolved cadmium.

Four of the models calculated salinity and SPM and results are generally in good agreement with the measurements. For salinity, the largest range in data and the most differences in models are for the coastal locations in the Dutch coastal zone and the German Bight. For SPM, the largest range in the data is near the UK coast, most likely due to cliff erosion, and in the Dutch coastal zone and German Bight. None of the models have the same extent of variation as seen in the data.

Five of the models calculated dissolved cadmium concentrations and the results were presented as a cost function value. Almost all the cost functions were negative, indicating that the modelled results were lower than the data. This is also consistent with the comparison of model results and data on a seasonal time scale.

3.6.3 Mass balance

The mass balances of the different models help to explain some of the different results that are calculated. From the water mass balance, it can be seen that there are different net flows in the North Sea area, i.e. different amounts of water entering and exiting the area over the boundaries. This is consistent with the different focus of time scales, spatial scales and especially meteorological forcings used in each model.

Differences are also seen in the fluxes of SPM in the models, due to large conceptual differences in the way sediment matter is modelled. SPM is defined differently in most models, in some cases consisting of only inorganic material, while in others including organic and detrital material as calculated by an ecological model. In some models, SPM is input as a forcing function, while in others it is calculated dynamically. One model has no SPM. Sources and sinks of SPM are also variable, with cliff erosion included in some models as an important source. Significant differences are seen in the sedimentation fluxes in the models, due to large conceptual differences in the interaction between the water column and bottom sediment and the manner in which the sediment bottom is included in the model.

The differences in water balance and sediment flux are reflected in the calculated mass balances for cadmium and PCB. The inflow from the Straight of Dover and outflow to the North are noticeably different, as are fluxes due to sedimentation. For PCB, the loss due to volatilisation can be important, but not all of the models include this process.

It can be noted that although the river and atmospheric input data were defined for the comparison exercise, the models still show differences in these values in the mass balance. This reflects the differences in how models are set up to accept external data. For example, the specific rivers included in a model can be fixed, or their discharges may be fixed. Although the boundary concentrations were defined for the comparison exercise, differences in mass inflow and outflow reflect the different hydrodynamics of the models.

Although there are noted differences in the mass balances given by the different models, the net transport over the boundaries for water, SPM, cadmium and PCB are in general agreement with the range of values found in literature (NSTF, 1993). Residual flows through the Dover Straight as calculated by different model studies have been reported in the PROMISE study as given in Table 3.15 (Boon et al., 1997).

Table 3.15: Residual flows through Dover Strait (in 10^{12} m^3/yr) from literature.

Source	*Tide only*	*Tide+Ave. wind*	*Remarks*
Prandle 1978	3.6	4.9	M2-tide Proc.R.Soc.Lond.A.,359,(1978),189
Prandle 1984	1.6	2.8	based on Cs-tracer data Phil.Trans.R.Soc.Lond.A,310(1984),407,tau=0.07 Pa
Salomon 1993a	1.2	4.7	Averaged wind is SW 8 m/s tau wind=0.13 Pa Ocean.Acta,16,(1993),439\
Salomon 1993b	1.2	3.6	Averaged wind over period 1983-1991 Ocean. Acta, 16,1993,449
Prandle, 1996	1.1	3.0	Based on HF radar and ADCP field data Cont Shelf Research , vol 16, no 2, 237-257

Flows through the Northern Boundary of the North Sea were calculated by three different models as part of the NOWESP study (Smith et al., 1998). Here the calculated range varied over an order of magnitude from 2.5 to 20.5 (x 10^{12} m^3/yr).

3.7 Summary

Despite all the conceptual differences in the models, as reflected in the mass balances, the models show much agreement in calculated concentrations, as seen for conservative substances or those not significantly affected by processes (e.g. salinity, and dissolved cadmium). This can reflect the similarity in general transport pathways. Salinity and dissolved cadmium concentrations are determined to a large extent by boundary concentrations and large scale transport patterns. The river inputs are quite well known, and it is now the boundary concentrations which are more in question.

Differences in SPM fluxes between the models are noticeable. It was agreed during the workshop that the SPM fluxes are still largely unknown and that these are of high importance to pollutant transport (especially for substances which are significantly adsorbed to particulate matter).

Field measurements for model validation are sparse. The ICES data set was first reviewed and did have some data for cadmium. However, this was only in the form of yearly average values, and was primarily at coastal locations, not 'open sea' areas. The NERC NSP data proved to be the most complete in spatial and temporal coverage for the validation of dissolved cadmium concentrations. Field data for PCBs and other organics such as atrazine and PAHs was even more scarce. Insufficient data was found for model validation.

4 Model Responsiveness

Model responsiveness exercises involved simulating reduction scenarios for riverine contaminant loads. A base case for contaminant loads was defined (year 1989), as well as two reduction scenarios (50% Cadmium reduction and 50% PCB reduction). The responses of the different models to these reductions were then compared. Such an exercise gives an indication of the changes that can be expected in the natural system due to a realistic policy decision, and illustrates the role that predictive models can play in marine management. Additionally, the responsiveness illustrates many of the characteristics of the models.

4.1 Importance of model responsiveness to contaminant loads

One important goal of contaminant fate and transport models is to illustrate effects of potential or proposed management strategies.

The types of questions that posed from a management perspective may be as follows:

- Which pollutants need to be reduced ?
- By how much (10%, 50%, 80%)?
- Where do reductions have to take place for improvements to occur? (Within a specific country? In all countries?)
- What will we consider an improvement?
- When can an improvement be expected?

Additionally, the social-economic factors must be considered, namely whether the societal cost of reducing pollutant inputs will be worth the (expected) benefits.

Models can play an active role in discussions about these issues. The models are ideally suited to calculate some of the cause and effect relationships between given contaminant input conditions and resulting water quality. Various scenarios of anthropogenic reductions can be simulated, and resulting water quality results can then be evaluated and used for the further discussion on socio-economic costs and benefits.

As a first step to using models to support such management discussions and decisions, an evaluation of model responsiveness to defined load reduction scenarios, and comparison of responsiveness of different models to given scenarios is illustrative of the capabilities of the models.

4.2 Defined Reduction Scenarios

An analysis of the responsiveness of models to defined load reduction scenarios has been made, and the responsiveness of the different models has been (directly) compared. The responsiveness of the models to load reductions was calculated for cadmium and PCB at seven selected locations within the North Sea.

Two reduction scenarios were considered in the exercise, namely:

- 50% reduction scenario cadmium
- 50% reduction scenario PCB-153

The base situation was for cadmium and PCB inputs from 1989 as these are well documented. Load reductions have been made for the riverine and atmospheric loads. Boundary concentrations (and thus mass flowing in from outside the model area) were not changed.

Ideally, the models were annually reinitialized (i.e. final timestep results were reused as initial conditions for the following run) as often as necessary so that a dynamic steady state was reached. For some of the models with long run times this was not possible. For the models which were reinitialized to reach a dynamic steady state situation, the results of the exercise represent the maximum change that the reductions can have on the ocean/coastal system. For the models which are not reinitialized, and are run for e.g. only 1 year, the results of the exercise represent the effect of a 1 year reduction in loadings.

Summary tables showing the range of predictions of the different models are presented below. The tables show the reduction in the environmental concentrations for dissolved cadmium and adsorbed PCB-153 which result from a 50% reduction in river and atmospheric loads.

Table 4.1 Results of reduction scenario for cadmium

		Reduction relative to 1989 (%)				
	NSP location	BSHdmod.E[1]	NORWE-COM	NOSTRA-DAMUS	SCREMO-TOX	ZEEBOS-TOX
1.	AM	6	1	4	1	6
2.	AG	8	8	12	16	13
3.	BB	6	3	6	3	9
4.	BU	9	4	8	6	8
5.	CP	1	2	1	1	4
6.	CG	9	5	8	7	10
7.	DZ	3	4	4	1	4

[1] Note: in the BSH simulation hydrodynamic data of the year 1995 are used

Table 4.2 Results of reduction scenario PCB-153

		Reduction relative to 1989 (%)				
	NSP location	BSHdmod.E	NORWE-COM	NOSTRA-DAMUS	SCREMO-TOX	ZEEBOS-TOX
1.	AM	-	21	-	15	43
2.	AG	-	41	-	47	49
3.	BB	-	33	-	7	48
4.	BU	-	35	-	33	47
5.	CP	-	43	-	0.2	45
6.	CG	-	39	-	35	48
7.	DZ	-	46	-	1	46

4.3 A comparison of model responsiveness

For PCB and cadmium, the model responsiveness to anthropogenic load reductions from rivers and atmosphere is fairly consistent. For cadmium, a 50% reduction in loads generally has an effect of less than 15% in environmental concentrations at the seven selected locations. The largest concentration decreases are seen in the coastal zones where river discharges are the largest contributing source of contaminants. The largest decreases are predicted in the Dutch coastal zone (maximum 16%) where the influence of the decreased Rhine River inputs is the highest. The smallest decreases (1-4%) are seen in the central North Sea, where river influence is small, and inflow over the boundaries is the largest contributing source of contaminants. In general, water flowing into the North Sea from the English Channel and Atlantic has a large contribution to the amount of cadmium in the North Sea. The river and atmospheric load reductions will not change this source.

It should be noted that some data from the Dutch coastal zone for the period 1980-1990 do show that there has been a significant decrease in environmental concentrations of cadmium corresponding to 50% reduction in the Rhine river inputs (Scholten et al., 1998). However, an additional factor is the reduction in loads from dredged material dumping. The dredged materials were not included in the model simulations.

For PCB, the models predict a larger impact of river and atmospheric loads reduction, as high as 40-49% at some locations. This is primarily an indication of the relative importance of rivers as the contributing source of PCB to the North Sea, compared to inflow from the boundaries. As with cadmium, the largest reductions were generally in the coastal regions, where the influence of rivers is largest.

At this point in time, the responsiveness cannot be validated against field data.

The differences in responsiveness for reductions between the models can be differences in model concepts as well as factors such as:

- duration of simulations (whether models have reached steady state)
- forcing
- boundary conditions (and location of the model boundaries - particularly the Northern boundary is quite different in the models)

Ideally, these listed differences should be minimized, and this was done as much as possible for these exercises. However, some differences do remain. As previously mentioned, some of the models simulations are made repeatedly until they reach a dynamic steady state (i.e. the results of a one year simulation are used as the starting point of the following simulation, and a series of simulations is run until they reach a steady state). Other models, particularly those with long run times, are run just once (i.e. 1 year of simulation) and then results are presented. Obviously, these models may show less response to the load reduction scenarios, especially in regions further from the coastal zone.

Because the boundary in different models is at different locations, the relative influence of boundary concentrations (external inflow) compared to rivers and atmosphere can be different.

5 Conclusions and Recommendations

While most of the models presented and discussed at the workshop were focused on the region of the North Sea (Convention region II), the conclusions drawn and recommendations made are considered to be relevant to all the waters of the Convention area.

5.1 Conclusions

The workshop has had a significant output with respect to:

- an update of available models and data for marine contaminant issues in the Convention area
- validation and comparison of model results
- Answers to JAMP questions on contaminant transport and fate issues in the Convention area, in particular the responses of the various models to anthropogenic input reduction scenarios
- Common strategy for cooperation, on further model development and application, also with the aim of contributing to the Quality Status Report (QSR) 2000.

1. Update of available models and data

Models compared and evaluated at this workshop included models for:

- greater North Sea: BSHdmod.E, NORWECOM, SCREMOTOX, ZEEBOS-TOX, PROVANN
- southern North Sea: NOSTRADAMUS
- Bay of Seine: Telemac/SUBIEF
- estuaries: SAWES and PCB bioaccumulation model

General descriptions, main characteristics, strengths and weaknesses, references and a list of contact persons/institutes are available for all of these models. These models are all for application within OSPAR region II. No models for other regions were presented, and it is not certain if such models are available.

The models have different strengths in physical (hydrodynamics) and biological/chemical processes which reflect the different goals for which they were developed. In terms of hydrodynamics, some models have detailed 3-dimensional computations of flow while others are 2-dimensional (depth averaged), 1-dimensional or even 0-dimensional (no hydrology). For the biological/chemical processes, models incorporate very different degrees of complexity in processes relating to chemical fate. The simplest models (chemically) treat contaminants as conservative substances which are transported through the system according to the large scale flow pattern. The more chemically complex models include a wide range of processes which can affect pollutant fate. A few models go beyond the calculation of environmental concentrations, and include uptake within the food chain and assessment of environmental risk. Given the wide range of models, the choice of which model to use for assessment of pollutant transport and fate depends on the specific questions being posed.

Important exchange and use of common datasets, was made, namely:

- riverine input data on a monthly basis
- atmospheric deposition data
- estuarine retention information
- North Sea Project and ICES data

2. Validation and comparison of model results

The exercises show that the cost function is a valuable method for performing model validation and model comparison, and can be widely used in the future. Overall results as to the goodness-of-fit can be summarized:

- water transport: mass balances show different fluxes into/out of North Sea.
- SPM: large scale fluxes are still poorly understood, and are calculated very differently with the different models. However, the SPM flux is crucial for determining the fate of many contaminants, especially those which are largely adsorbed to particulate matter.
- cadmium: Despite differences in the models, calculated concentrations are similar and the general distribution pattern of dissolved cadmium over the North Sea is similar (as is the salt pattern). This reflects the fact that cadmium is mostly dissolved in water, and its fate is determined largely by large scale water transport. Models results are low and do not reflect the seasonal variability as shown in NSP field measurements.
- PCB and other organic pollutants: the data for model validation is not available. Because PCB (in contrast with cadmium) is largely adsorbed to particulate matter, its fate is controlled by a combination of large scale water transport and processes such as sedimentation, resuspension and volatilization.

The relative responses of the models to riverine and atmospheric load reductions are similar. The response to load reduction of cadmium are small (<16%) compared to PCB-153 (up to 49%). This indicates the that rivers and atmosphere are a large contributing source of PCB to the North Sea. For cadmium, much of the source is coming from outside the region via the boundaries.

Although there are differences in the mass balances given by the different models, the net transport over the boundaries for water, SPM, cadmium and PCB are in general agreement with the range of values found in literature.

There is an important need for model comparisons, especially given the wide range of existing models. Model intercomparison is one aspect of model validation, which must be an ongoing process. Aspects of validation include not only the comparison of model results with field data, but also the comparison of models with each other. During the workshop it was stated that the process of model intercomparison and exchange of knowledge and experiences, contribute significantly to a further development and upgrading of this kind of modelling.

3. Answers to JAMP questions

Despite the differences between models and some of the limitations of the models which have been presented, the models show much agreement in calculated concentrations, and predictions of relative decreases in environmental concentrations due to load reductions. The models in their current state can offer significant insight into contaminant fates in the North Sea, including links between inputs and concentrations, and can thus be used to address the issues which are raised by the JAMP questions.

5.2 Recommendations

Further development and improvement of models can still be achieved. Specifically, further development for other Convention areas (outside of the North Sea Region II) is important.

One enhancement of the operational use of the models would be a more complete validation of the responsiveness of the models based on actual field data. Such a validation could improve the reliability of the models. Currently, field data on contaminants is very limited.

International coordination and cooperation should facilitate further validation of the models, including comparison exercises. OSPARCOM, ASMO or Regional Task Teams could provide the platform for such further developments.

Data on loads from offshore drilling activities are not generally available, and existing data as used in the model exercises still have some uncertainties. Efforts should be made to further quantify this potentially significant source of contaminants to the North Sea.

5.3 Follow-up

While no specific appointments for continuing comparison exercises or a follow-up workshop have been made, there was a general consensus that such a follow-up would be desirable for continuing with the method of model validation and comparison that has been started within ASMO.

The workshop participants aim to prepare the workshop results for publication in a peer-reviewed scientific journal for broader publication.

Relation to QSR 2000

The models presented and the exercises conducted during the ASMO workshop can in principle make important contributions to the Quality Status Report (QSR) 2000 and the regional QSRs. In order for the models to be used within this framework, modelling studies will need to be defined. For this purpose, general questions pertaining to relevant issues will have to be posed by policy makers and their organizations. These questions will then need to be 'translated' into the specific questions which can be answered by models.

From the workshop, a good overview of the available models as well as a network of people working in the field has been established. This network can be activated to respond to the questions raised, in terms of assessing how and to what extent the questions can be answered, as well as performing the calculations necessary to answer the questions.

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Relevant references for each of the presented models is given below.

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Appendix A

Workshop Terms of Reference

OSLO AND PARIS CONVENTIONS FOR THE PREVENTION OF MARINE POLLUTION
ENVIRONMENTAL ASSESSMENT AND MONITORING COMMISSION (ASMO)

Terms of reference
for an ASMO (OSPAR)
modelling workshop on transport and fate of contaminants
Within the JAMP
(Joint Assessment and Monitoring Programme)

Presented by the Netherlands

Introduction

At the second meeting of ASMO, Arc et Senans, 24-28 April 1995, a draft working programme for the modelling coordination was presented by the Netherlands, and approved by the meeting. Three modelling areas were identified, and for each of these areas it was agreed that a workshop should be organised:

1. risk assessment of accidents in shipping and offshore industry (workshop held 15-17 November 1995)
2. eutrophication issues (workshop held 5-8 November 1996)
3. transport routes and fate of contaminants (workshop on 4-7 November 1997)

This document contains the terms of reference for the workshop on 'Transport Routes and Fate of Contaminants', to be held 4-7 November 1997.

The ASMO modelling workshop considered here will in principle address the entire OSPAR Convention area and not only the North Sea, though this depends on the participants and the models made available. Moreover, the issues to be addressed will be related to the Joint Assessment and Monitoring Programme.

Contaminant transport and fate issues for modelling in JAMP

The need for modelling activities in the entire convention area has been identified for pollutant issues mentioned in Section II ('Issues to be taken into account in development and implementation of the Joint Assessment and Monitoring Programme') and Annex 5 ('Issues for inclusion in the regional assessment for region II: Greater North Sea') of the OSPARCOM ASMO 1995 Summary Record. These JAMP issues with reference to modelling are:

JAMP (Issues to be taken into account; No. 1.16):

- What are the fluxes and environmental pathways?
- Where do persistent pollutants end up?

JAMP (Annex 5, No. I.17):

- Where do persistent pollutants ultimately end up?
- Which quantities of pollutants enter the Region (i.e. region II) from outside?
- What is the time lag between input reductions and reductions in field concentrations?
- Which fluxes occur in the marine environment?

As models are developed to analyze causal relationships, i.e. the processes behind the above issues, we propose to test the model output on the JAMP issues mentioned above by focusing on the following main modelling topics:

1. Large scale pollutant transport and fate in order to link sources to concentrations throughout the modelled area. For the large scale models (e.g. North Sea), comparisons of concentrations can be made (dissolved and adsorbed concentrations) given input loads from the rivers, atmosphere and other sources (dumping of dredged materials). Also, fluxes between the different regions in the Convention area could be addressed (e.g. mass flows and exchanges).

2. The role of estuarine processes (e.g. sedimentation/retention) in determining fluxes into the coastal and marine areas. With estuary models, the amount of pollutant retention can be calculated due to sedimentation and other physical/chemical processes. Comparisons can be made as the amount of retention occurring in different estuaries, and the main processes which account for the retention.

3. Links of pollutant concentrations to biological effects (JAMP, Issues to be taken into account, No. 1.17). The models to be used for 1. and 2. above calculate only pollutant *concentrations* in the environment, while an important aspect of marine pollution is the effect of pollutants to the marine ecosystem. To this end, additional analyses of the calculated concentrations must be made to evaluate the effect on the environment of the pollutants. Comparison of calculated concentrations with effect concentrations (e.g. Ecotoxicological Assessment Criteria) can be made. Alternatively, additional model analysis (e.g. accumulation and effect modelling) can be performed.

Objectives of the model workshop on contaminant fate and transport

The main objectives of the model intercomparison for Pollutant Transport and Fate models can be specified by the following items:

1. To exchange information on and to evaluate the conceptual basis of the models in relation to the objectives for their development and application (e.g. research, retrospective assessments and predictions), and in relation to the pollutant transport and fate issues in JAMP and basic pollutant variables.
2. To evaluate the agreement between model results and regional in situ data and to evaluate the justification of the model concept for the original domain of application, (based on individual presentation of validation results).
3. To compare the results of model applications for common regions and periods, in view of available in situ data, (based on model-model intercomparison).
4. To compare and to evaluate the response of the model to changes in environmental conditions such as meteorological forcing and pollutant inputs from various sources.
5. To elaborate further cooperation and exchange of model-concepts, data-sets and model-results to harmonize future developments and applications of pollutant transport and fate models.
6. To discuss and provide an answer to the question: "What kind of variables relating to pollutant transport and fate can be modelled realistically and what kind of variables are less likely to be modelled realistically given the-state-of-the-art in physical and chemical numerical modelling?"

7. To provide ASMO with harmonized and accurate (including uncertainty estimates) information on model results on the JAMP issues and on the assessment of causes and effects of marine pollution, in both a retrospective and a predictive way, as a contribution to the QSR2000 for the OSPARCOM Convention area and its subregions like the North Sea.
8. To describe clearly the applicability and limitations of the modelling approaches.
9. To perform a sensitivity analysis on the physical, chemical and biological process parameters and their relative contributions on the overall results.
10. To focus with priority on the chemical part of the pollutant transport and fate model and its significance for real environmental conditions.
11. To provide a connection between pollutant fate processes in the open sea, the coastal zone and estuaries. Particular attention will be given to retention processes which occur in estuaries (e.g. sedimentation), and the contributions of atmospheric deposition.

Comparison methodology

Because most of the models are developed for different regions and different purposes, it should not be the intention of this ASMO modelling workshop to prescribe detailed test cases. Instead, a more general means of intercomparison is foreseen. Quantitative 'Cost Functions' as developed and applied for the ASMO eutrophication workshop will be discussed and evaluated for their use in follow-up intercomparison activities. The cost function is an equation for quantifying differences between two different data sets, and can thus be used for validating model results against regional data as well as common data sets (e.g. ICES).

The ability to meet the workshop objectives as specified above will depend on the status of the models and the available data sets.

The methodology for intercomparison will therefore include:

1. The set up and distribution of a summarized overview of available models, their concepts, their purpose and their domain of application, and their status of development and validation.
2. The set up and distribution of a common data-sets for pollutant inputs, meteorological forcing and relevant in-situ data, which can be used to test (calibrate, validate) the models against field data and allows a more direct intercomparison between the models for retrospective periods (e.g. 1990-1995). Both large scale transport models and estuarine models will be evaluated. A data set for the North Sea, and if possible for other regions (e.g. ICES), will be compiled for this purpose. Data from RIKZ is available for inputs.
3. Description of output parameters and formats (files, graphs etc.), to allow a direct comparison between model results and in situ data.
4. Description of desired model tests and applications to quantify the response of the models to changes in environmental conditions such as pollutant inputs, meteorological forcing etc. Model tests could focus on questions like:
    - do models provide realistic results in their original /intended domain of application?
    - are models applicable for a wide range of reduction measures?
    - what sort of data is required for parameterisation and forcing?

Output

The workshop aims at the following significant output:

1. An updated overview of available models for marine pollutant transport and fate issues in the convention area.
2. Answers to the JAMP questions on pollutant transport and fate issues.
3. Recommendations for co-operation on further model development and application.

Timeframe, participants and finance

timeframe:
A four day meeting, 4 (14.00 hour) - 7 (15.00 hour) November 1997, The Hague, The Netherlands.

participants:
Contracting Parties will be invited, via national focal points, to nominate participants for the workshop. Representatives of relevant international fora will also be invited.

finance:
Costs of workshop preparation, logistics and reporting will be covered by the Netherlands. No workshop fee will be charged. Contracting parties are responsible for their own expenses, i.e. preparatory costs such as model simulations to be presented at the workshop as well as travel and accommodation costs. **ASMO expects that national agencies will provide or assist with financial support for the participants nominated to represent their country.**

Actions

This schedule of activities is based on the assumption that the modelling workshop on pollutant transport and fate issues will be held in November 1997 (proposed period: 4-7 November 1997). The tentative timing is given for each activity, based on experience from the previous 2 ASMO modelling workshops. If possible, the schedule can be shifted forward so that participants have more time to prepare model simulations for the workshop. This will depend to a large extent on the active involvement of the ASMO focal points in appointing participants in a timely manner.

1. The Netherlands to submit this t.o.r. to the focal points of each country as a draft announcement. The submittal includes a request for comment on the t.o.r. and nomination of participants. Comments received before 28 February 1997 will be taken into account in the text to be submitted to the ASMO meeting in April 1997. If no comments are supplied, it will be assumed that the focal points are in agreement with this t.o.r.

2. The Netherlands to submit this t.o.r. by 14 March to ASMO 1997 for discussion and approval, together with a preliminary list of nominated participants (received from focal points).

3. ASMO 1997 (7-11 April) to decide whether this t.o.r. justifies holding the proposed workshop in November 1997.

4. The Netherlands to distribute a request to the focal points for final selection and appointment of participants (April 1997).

5. Contracting Parties / focal points to confirm their participants (May 1997).

6. The Netherlands to distribute directly to nominated participants a request for information on models to be applied, using the available inquiry form (May 1997).

   Participants to fill out the inquiry form for pollutant transport and fate models, informing about the models to be applied for the workshop, and contribute to regional an/or common data sets for model comparison (May - September 1997).

7. The Netherlands to update the inventory of models applicable to pollutant transport and fate issues (November 1997).

8. The Netherlands to prepare a guidance document containing among others:
    - a common database for model input (and forcing)
    - common databases for validation
    - proposed common quantifiable parameters for model-model output intercomparison

    (draft May 1997, final version September 1997).

9. Participants to prepare model simulations to be presented at the workshop (May - Oct 1997)

10. The Netherlands to organise the workshop proper (November 1997).

11. The Netherlands to prepare a report of the workshop results including reworking comments of participants and experts (February 1998), and to submit results and recommendations to the ASMO 1998.

Appendix B

List of Participants

"Modelling of Contaminant Transport and Fate Issues"
ASMO International Workshop
The Hague, The Netherlands, November 4 - 7, 1997.

List of Participants:

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	Arie de Vries	RIKZ
	Rik Sonneveldt	RIKZ
	Jo Suijlen	RIKZ
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	Lisette Enserink	RIKZ
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	Maarten Ouboter	Delft Hydraulics
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Appendix C

Workshop Programme

ASMO Contaminant Transport and Fate Workshop Programme

Tuesday 4 November

13.00-14.00	Arrival and lunch
14.00-14.30	Welcome and Introduction to the workshop: context and scope (R. Laane)
14.30-15.00	Introduction to ASMO/OSPARCOM and the QSR process (J. Visser and L. Enserink)
15.00-15.15	Coffe Break
15.15- 16.15	**Session I: Intro. to Models and Validation in Common Domain** 1. Stolwijk from RIKZ/NL 2. Huber/Dick from BSH
16.15-16.30	Refreshment Break
16.30-17.30	**Session I: (cont'd)** 3. Ouboter from Delft Hydraulics/NL 4. Tappin from SOC/UK

Wednesday 5 November

9.00	Coffee
9.15-11.00	**Session I: (cont'd)** 5. Soiland from IMR/NO 6. Reed/Rye from Sintef/NO 7. Normant from EDF/FR
11.00-11.15	Coffee Break
11.15-13.00	**Session I: (cont'd)** 8. Loizeau from IFREMER/France 9. Baart from Delft Hydraulics/NL
13.00-14.00	Lunch
14.00-15.00	**Discussion I:** **Overview of models and Comparison of Cost Function Results** **chaired by: E. Svendsen/IMR**
15.00-15.15	Coffee Break
15.15-16.00	**Discussion I (cont'd)**
16.00-16.15	Refreshment Break
16.15-17.30	**Discussion I (wrap-up)** **Conclusions over model validation exercise** **chaired by E. Svendsen and R. Laane**

Thursday 6 November

9.00	Coffee	
9.15- 11.00		**Session II. Response to anthropogenic input reduction** 1. Stolwijk from RIKZ/NL 2. Tappin from SOC/UK 3. Soiland from IMR/NO 4. Reed/Rye from Sintef/NO
11.00-11.15	Coffee Break	
11.15-13.00		5. Ouboter from Delft Hydraulics/NL 6. Baart from Delft Hydraulics/NL **Discussion (II)** **Similarities and differences in model responsiveness chaired by R. Laane/RIKZ** **Presentation of Aquapol Database - A. deVries/RIKZ**
13.00-14.00	Lunch	
14.00-15.00		**Workgroups on model input data, offshore platforms, mass balances , estuarine retention, bioaccumulation**
15.00-15.15	Coffee Break	
15.15-16.15		**Results of Workgroups**
16.15 - 16.30	Refreshment Break	
16.30-17.30		**Appointments for further work to be completed**
19.00		*Dinner at Scheveningen Pier*

Friday 7 November

9.00	Coffee	
9.15-11.00		**Discussion (III):** **Review of model comparisons and recommendations for monitoring - Chaired by R. Laane/RIKZ**
11.00-11.15	Coffee Break	
11.15-13.00		**Discussion (IV): Development of conclusions on contaminant transport and fate models for ASMO; chaired by R. Laane/RIKZ** Closing of workshop
13.00-14.00	Lunch	

Appendix D

Complete Mass Balance Results

Complete Mass Balance Results:

Table D1 Modelled Mass Balance Water (tons/year = m^3/yr)

	BSHcmod[1]	NORWE-COM	NOSTRA-DAMUS	ZEEBOS-TOX	SCREMO-TOX
MASS IN					
Straight of Dover	16.4×10^{12}	5.4×10^{12}	2.5×10^{12}	no calculation	3.4×10^{12}
North Boundary (56°N)	79.5×10^{12}	31.9×10^{12}	6.4×10^{12}		8.5×10^{12}
Rivers	0.1×10^{12}	0.13×10^{12}	0.09×10^{12}		0.17×10^{12}
Offshore	$.0002 \times 10^{12}$	0	0		0
Total Mass In	96.0×10^{12}	37.4×10^{12}	9.0×10^{12}		12.1×10^{12}
MASS OUT					
Straight of Dover	14.2×10^{12}	1.4×10^{12}	0		0
North Boundary (56°N)	81.7×10^{12}	35.0×10^{12}	8.9×10^{12}		11.9×10^{12}
Net evaporation	0	0	0.005×10^{12}		0
Total Mass out	95.9×10^{12}	36.4×10^{12}	8.9×10^{12}		11.9×10^{12}
NET (in-out)	0.1×10^{12}	1.0×10^{12}	0.1×10^{12}		0.2×10^{12}

Table D2 Modelled Mass Balance SPM (Mtons/year)

	BSHdmod.E[1]	NORWE-COM	NOSTRA-DAMUS	ZEEBOS-TOX	SCREMO-TOX
MASS IN	no calculation			no calculation	
Straight of Dover		20.3	17.2		5.7
North Boundary (56°N)		33.6	5.3		15.0
Rivers		1.6	1.6		14.8
Atmos. Depos.		0	0		0
Offshore		0	12.6		0
Erosion		3.4	57.4		8.8
Total Mass In		58.9	94.1		44.3
MASS OUT	no calculation			no calculation	
Straight of Dover		5.5	0		0
North Boundary (56°N)		60.1	24.1		25.8
Sedimentation		negligible	69.8		18.4
Total Mass out		65.6	93.9		44.2
NET (in-out)		-6.7	0.2		0.1

Table D3 Modelled Mass Balance Cadmium (tons/year)

	BSHdmod.E[1]	NORWE-COM	NOSTRA-DAMUS	ZEEBOS-TOX	SCREMO-TOX
MASS IN					
Straight of Dover	409	132	66	87	83
North Boundary (56°N)	1333	421	93	112	130
Rivers	12	16	17	27	13
Atmos. Depos.	20	10	13	9	10
Offshore	20	0	0	0	2
Erosion	0	0	35	37	0
Total Mass In	1794	579	224	272	238
MASS OUT					
Straight of Dover	357	32	0	2	0
North Boundary (56°N)	1403	461	183	231	223
Sedimentation	0	83	44	56	14
Volatilization	0	0	0	0	0
Degradation	0	0	0	0	0
Total Mass out	1760	576	227	289	237
NET (in-out)	34	3	-3	-17	1

[1] Note: in the BSH simulation, hydrodynamic data of the year 1995 are used

Table D4 Modelled Mass Balance PCB (kg/year)

	NORWE-COM	ZEEBOS-TOX	SCREMO-TOX
MASS IN			
Straight of Dover	15.2	7.3	11
North Boundary (56°N)	29.5	12.0	17.9
Rivers	38.4	51	23.5
Atmos. Depos.	29.3	26	28.8
Offshore	0	0	0
Erosion	0	0	0
Total Mass In	112.4	96.3	81.2
MASS OUT			
Straight of Dover	3.7	0.2	0
North Boundary (56°N)	33.2	21.7	34.2
Sedimentation	56.2	36.7	23.7
Volatilization	0	42.3	25.4
Degradation	0	0.0023	0
Total Mass out	93.1	100.9	83.3
NET (in-out)	19.3	-4.6	-2.1

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