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Models for transport and fate of carbon, nutrients and point source released radionuclides to an aquatic ecosystem

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Abstract

In this report three ecosystem models are described in terms of structure, initial data, and results. All models are dynamic, mass-balanced and describe the transport and fate of elements in an open aquatic ecosystem. The models are based on ecologically sound principles, provide model results with high resolution and transparency, and are constrained by the nutrient dynamics of the ecosystem itself. The processes driving the transport in all the models are both the biological processes such as primary production, consumption, respiration and excretion, and abiotic e.g. water exchange and air-sea exchange.

- The first model, the CNP-model, describes the distribution and fluxes of carbon and nutrients for the coastal ecosystem off Forsmark.
- The second model, the C-14 model, is an extension of the CNP-model and describes the transport and distribution of hypothetically released C-14 from the underground repository SFR-1 to the ecosystem above.
- The third model, the RN-model, is a generic radionuclide flow model that models the transport and distribution of radionuclides other than C-14 hypothetically discharged to the ecosystem. The model also analyses the importance of some radionuclide specific mechanisms for the radionuclide flow. The generic radionuclide model is also based on the CNP-model, but has radionuclide specific mechanisms connected to each compartment.

Sammanfattning

I den här rapporten beskrivs struktur, initiella data och resultat av tre olika ekosystem-modeller. Alla modellerna är dynamiska, massbalanserade och beskriver hur ämnen är fördelade och transporteras mellan olika organismer och abiotiska komponenter i ett öppet akvatiskt ekosystem. Modellerna är baserade på välkända generella ekologiska principer, de genererar resultat med god upplösning och tydlighet, och begränsas av ekosystemets egna närsaltstillgångar. De drivande processerna i modellerna är både biologiska processer, såsom primärproduktion (fotosyntes), konsumtion, respiration och exkretion, och abiotiska processer, såsom vattenutbyte och utbyte mellan vatten och luft.

- Den första modellen, CNP-modellen, beskriver fördelning och transport av kol och närsalter i kustekosystemet utanför Forsmark.
- Den andra modellen, C-14 modellen, är en utbyggd CNP-modell som beskriver transporten och fördelningen av hypotetiskt utsläppt C-14 från SFR-1 (slutgiltigt förvar för radioaktivt driftavfall) som ligger i berggrunden under det modellerade ekosystemet.
- Den tredje modellen, RN-modellen, är en generisk radionuklidmodell som modellerar transport och fördelning av andra radionuklider än C-14 hypotetiskt utsläppta till ekosystemet. Den modellen analyserar också vikten av olika radionuklidspecifika mekanismer för flödet genom ekosystemet. Den generiska modellen är också baserad på CNP-modellen men har radionuklidspecifika mekanismer länkade till varje modell-enhet för att kunna hantera skillnaderna mellan kol, kväve och fosfor och andra ämnen.

Contents

1 Introduction

In this report three ecosystem models are described. They were all developed for the purpose to model the transport and fate of carbon, nutrients and radionuclides in the coastal area of Öregrundsgrepen (Baltic Sea). The models are examples of tools to be used in the safety assessment of the deep repository for high level radioactive waste in Sweden. The aim of the safety assessment is to describe and analyse the long-term safety of the repository and to evaluate the environmental consequences of hypothetically radionuclide discharges from the repository. An overview of the complete safety assessment procedure for the biosphere and the interactions between the safety assessment, site investigation program and the research and development group at SKB can be found in SKB-biosphere assessment reports /e.g. Löfgren and Lindborg, 2003; SKB, 2004/.

- The first model described in this report is a carbon and nutrient flow model (CNP-model) for the coastal ecosystem off Forsmark.
- The second model is an extension of the CNP-model that models the transport and distribution of hypothetically released C-14 from an underground repository to the system.
- The third model is a generic radionuclide flow model that models the transport and distribution of radionuclides other than C-14 hypothetically discharged to the system. This model also analyses the importance of some radionuclide specific mechanisms for the radionuclide flow. The generic radionuclide model is based on the CNP-model, but has radionuclide specific mechanisms connected to each compartment.

1.1 Background and aim of the studies

Fate modelling of radioactive waste disposal typically deals with large variations over time and space. Potential releases may occur in the distant future and is expected to occur at low levels and over very long periods of time /e.g. SKB, 1999; SKB, 2004/. Therefore, models that assess both the dispersal of radionuclides in the ecosystem and enable calculation of the associated radiation exposure to biota are required. Although considerable advances have been made in the understanding of the behaviour of radionuclides in the environment, there are still gaps in knowledge and capability of modelling the fate of anthropogenic radionuclides /e.g. Davis et al. 1998; Kryshev et al. 1998; Bird et al. 1999; MacKenzie, 2000/.

With the models described in this report the attempt was to overcome some of the shortcomings of more conventional transfer models for radionuclides by adopting a dynamic ecosystem approach, where both important biological (e.g. photosynthesis, trophic transfer and mineralization) and environmental processes (e.g. sedimentation, air-water exchange and water movement) are included. Contrary to most earlier modelling efforts, radionuclide contamination in these models was treated as occurring in an open system, where flows of matter and energy occur both within the system and across the system boundaries. Such a processes oriented approach can provide a powerful tool for increasing the understanding of fundamental mechanisms controlling the fate of radionuclides through the environment as well as within organisms /sensu Jørgensen, 1995; van Dorp et al. 1998; Whicker et al. 1999; MacKenzie, 2000/.

The reason to focus on C-14 in the first model was because it is a radionuclide of considerable interest in the disposal of nuclear low-level waste because of the quantities often found, its high environmental mobility, high bioavailability and relatively long half-life (5,730 years) /Liepins and Thomas, 1988/. Modelling studies of low-level waste disposal facilities have indicated that C-14 has the major contributions to the radiation dose from the released sources /Merill, 1986; Bandrowski, 1998/. This was also indicated in the safety assessment of SFR-1 /Lindgren et al. 2001/. The main mechanism for this is that C-14 easily becomes incorporated into food webs via photosynthesis by primary producing organisms /Cook et al. 1998/. Another reason to start the radionuclide modelling with C-14 is that it is quite straightforward to model the dynamics of C-14 if the carbon flow of the system is known.

Traditional transfer models for radionuclides are usually element specific, of non-mechanistic nature and developed for steady-state conditions /e.g. Bergström et al. 1999; Thiessen et al. 1999; Whicker et al. 1999/. The uptake of radionuclides by biota or adsorption to particles is typically modelled with bioconcentration factors (TF) and distribution coefficients (K_d) /e.g. Ribbe et al. 1991; Hilton, 1997; Thiessen et al. 1999; Karlsson et al. 2001/. These are empirically derived constants that describe the ratios of radionuclide concentration in the organisms or in the particulate fractions of the water (Bq/kg wet weight or Bq/g dry weight) to the concentration of dissolved radionuclides in the ambient media (Bq/l or Bq/g dry weight) /e.g. Hilton, 1997/.

The bioconcentration factor approach has the advantage of being easy for assessors to use, but several objections have also been raised:

- BCFs do not involve any fundamental understanding of uptake and transport processes in the environment, as they are empirically derived from laboratory studies or field measurements /Sansone et al. 2002/.
- BCFs are only valid if steady-state in the system can be assumed, which is not always the case /Whicker et al. 1999; Thorne, 2003/.
- The relationship between the radionuclide concentrations in the environment and the radionuclide concentration within an organism may not be linear /Brown et al. 2003/.
- BCFs are not available for all organisms and specific environments of interest in assessments for nuclear facilities /Jones et al. 2003/.

Due to the problems with the bioconcentration factor approach a need to develop exposure models based on (i) ecologically sound principles, (ii) that provide high resolution model results, and (iii) that are constrained by the dynamics of the ecosystem itself (e.g. primary production, recycling capacity and the rate of import and export of matter to and from the system) was identified. The aim of the model studies described in this report was to fulfil these criteria. Models built on these principles would for instance easily be based on site-specific data and, due to the inbuilt constraints, only generate data within possible/realistic ranges. The constraints are often possible to measure or estimate fairly accurately and may be scaled for changes in e.g. light intensity, climate, water exchange or bathymetry /Kumblad and Kautsky, 2004/. This also allows prediction of radionuclide fate even after expected environmental changes.

1.2 History of the model development

The chronological order of the model development is not fully consistent with the order of the models presented in this report, which might need to be explained. The first model (chronologically) developed was a carbon flow model /described in Kumblad, 2001/ based on a carbon budget /c.f. the current document and in Kumblad, 1999/. The carbon flow model was then further extended into a C-14 flow model which also included an extrapolation and evaluation of carbon and C-14 flow in the ecosystem in 2,000 years from now /described in Kumblad, 2001/. During the analysis of the carbon mass-balance of the area in 2,000 years, it was evident that the primary production became limited by DIC, which was interpreted as an overestimation of the primary production. To obtain a realistic estimation of the primary production, nutrient dynamics was then introduced in the models which lead to the first version of the CNP-model /c.f. the current document and in Kumblad and Kautsky, 2004/. Analysis of the CNP model lead to calibrations of the C-14 flow model in terms of reduced primary production. The calibrated version of the C-14 model is described in section 4 in this report and in /Kumblad et al. 2003/. Parallel to the second phase of the C-14 modelling, the development of the generic radionuclide model was initiated. This was based on the CNP-model but was as the C-14 model driven by carbon only, that was calibrated against the availability of dissolved nitrogen and phosphorous in the ecosystem.

1.3 Organisation of this report

Initially there is a brief description of the framework used for modelling development, comprehensive assumptions and an overview of the different types of model blocks.

In the following chapters, each of the three models are described in terms of an overview of the model, model assumptions, model structure, model results, verification and conclusions.

2 Modelling framework

Both the C-14 flow model (C14-model) and the generic radionuclide model (RN-model) are driven by a site specific ecosystem model (CNP-model) which was based upon a carbon budget (compilation of ecological data from the area).

The CNP-model identifies and quantifies the circulation of carbon, nitrogen and phosphorous into and between the components of the food web of the ecosystem at the site. The CNP circulation was assumed to regulate and constrain uptake dynamics of other chemical components such as radionuclides. The model compartments represent both abiotic components, e.g. dissolved and particulate matter, and the major functional organism groups in the system, e.g. phytoplankton, zooplankton, fish, benthic plants, grazers and benthos. The main processes included in the CNP-model were primary production (i.e. carbon fixation by photosynthesising organisms), respiration, consumption (grazing and predation) and excretion (production of urinary products and faeces). Processes such as water exchange, sedimentation and gas exchange over the air-sea interface were also included. Both the C14-model and RN-model are driven by the CNP-model in the sense that the uptake- and excretion rates in biota and transport of the radionuclides in the system are linked to the dynamics of carbon and nutrients and thereby also regulated and constrained by these ecological processes (Figure 2-1).

In the C14-model, the flow of C-14 is modelled proportionate to the flow of stable carbon (given by the CNP-model). For example, the uptake of C-14 in primary producers is modelled to be proportionate to the amount of C-14 compared to stable carbon in the compartment for dissolved inorganic carbon (from which the primary producers obtain their carbon) and the rate of primary production.

In the RN-model, three radionuclide specific mechanisms are associated to the compartments in the CNP-model. These mechanisms are radionuclide adsorption to organic surfaces, radionuclide uptake by autotrophic organisms (i.e. primary producers) and radionuclide elimination by heterotrophic organisms (i.e. consumers). These three mechanisms are also calculated in the mentioned order in the model.

2.1 Model implementation

All three models were implemented in Matlab (version 7.0) with Simulink (version 6.0) for PC, simulated with simulation time 100–2,000 years, solution algorithm ode23t and variable time step size.

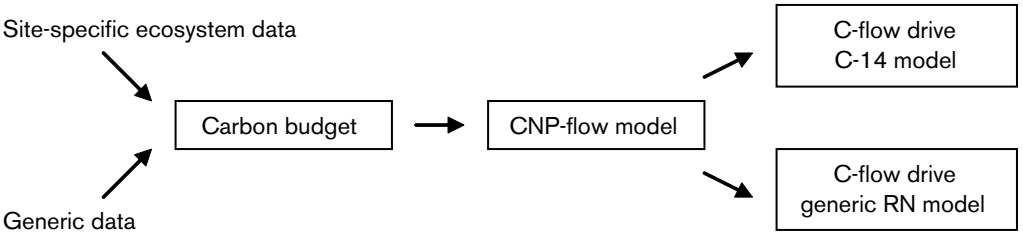

Figure 2-1. *Conceptual description of the three models.*

2.2 Assumptions for the modelling framework

The assumptions that the model framework were based upon could be summarised as follows:

- The structure and function of the ecosystem is of major importance for the fate of radionuclides discharged to aquatic ecosystems.
- The metabolic rates of the organisms in the ecosystem regulate and constrain the rate of uptake and elimination of radionuclides.
- Particle reactive radionuclides adsorb to organic surfaces (including organisms) and adsorb homogeneously to all organic surfaces in the system.
- The availability of radionuclide in the water or in prey items constrains uptake or trophic transfer of radionuclides.
- Diffusion is not a major process compared to uptake in association with metabolic processes, such as primary production and consumption, and adsorption of radionuclides to particles or outflow via water exchange.

2.3 Description of model-blocks

To simplify model development, a set of model-blocks for various ecosystem units and for the computation of the flow of information and matter between these units have been developed. The five different types of model-blocks are reservoirs, primary producers, consumers, directors, exchangers and the surface model-block.

- The reservoirs are model-blocks that describe the state and dynamics of non-living matter. These were used for the compartments dissolved inorganic matter (DIM) and particulate organic matter (POM) in all three models with a slight difference in block structure in the RN-model (which is described in chapter 5).
- The second class of model-blocks, the primary producers, were built to mimic the processes performed by primary producing organisms. Primary producer model-blocks were used for the two compartments phytoplankton and benthic plants in all three models.
- The consumer model-blocks mimics animals, and were used for the compartments zooplankton, macrograzers, fish, benthos, eagle, eider duck and seal in all three models.
- The directors, handle the information of the demand of matter, i.e. CNP, C-14 or RN, according to the model equations, by biota compartments as well as directing the actual flow of matter from the reservoirs to the biota compartments and between the different biota compartments. The C-14 and RN-model also has a point source director, from which the C-14 or RN nuclide discharge to the system is regulated. In addition to this the RN-model has a surface sub-system director that models the sorption and desorption of radionuclides to organic surfaces and the following ingestion of radionuclides associated to the surfaces of preys or POM.
- The exchanger blocks calculate the export of matter due to water exchange. In all three models, the exchangers were connected to DIM, POM, phytoplankton and zooplankton.
- The surface model-block handles the modelling of the surface adsorption of radionuclides on all organic surfaces in the system. The adsorbed radionuclides are taken from the DIM compartment and are redirected to POM or the organism surfaces.

3 The CNP-model

3.1 Description of the CNP-model framework

The CNP-model, which describes the flow of carbon, nitrogen and phosphorous in the system, was developed in several steps. First, a carbon budget for the area was established for biomasses and metabolic rates of the major functional organism groups in the ecosystem at the site (i.e. phytoplankton, benthic plants, zooplankton, grazing macrofauna, benthos, fish, seal and eagle) inclusive the reservoirs dissolved inorganic matter (DIM) and particulate organic matter (POM). Then, a mass balance carbon flow model including the same carbon compartments as the carbon budget was constructed. The initial data for the carbon flow model were derived from the carbon budget. DIM was modelled to enter the food web via primary producing organisms and then channelled through the food web according to the food web structure. POM on the other hand was assumed to provide the benthic fauna with organics carbon and gain matter from the production of faeces and other excess products from organisms in the area.

The metabolic processes accounted for in the modelling of primary producers were photo-synthesis, respiration, grazing (predation) and excess production and the corresponding processes for the consumers were consumption, respiration, predation, excess production and faeces production.

The nutrient uptake by primary producers was assumed to be proportional to the stoichiometric relationships between carbon and the nutrients (i.e. the Redfield ratios) in the organisms, and the trophic transfer of the nutrients was assumed to be proportional to respiration and estimated excretion ratios for carbon /Kautsky, 1995/.

3.2 Model assumptions (CNP-model)

The major assumptions made in the CNP-model:

- Carbon, nitrogen and phosphorous are considered to enter the food web mainly via the photosynthesis process by primary producers and then transfer to higher trophic levels over grazers and predators.
- The respiration is assumed to provide a way for re-circulation of dissolved CNP in the system via DIM, as well as the production of faeces provides a re-circulation pathway of particulate CNP via POM.
- An annual average of ecological processes gives a sufficient estimate of their seasonal variation.
- Surplus amount of primary production (ungrazed) is assumed to become a part of POC and is apportioned to detritus feeding benthic fauna or exported form the system via water exchange.
- Fish consumption was estimated from the abundance of fish species in the area /Neuman, 1982/ and their main food sources /Curry-Lindahl, 1985/.

- The nutrient uptake by primary producers was estimated to be proportional to the stoichiometric relationships between carbon and the nutrients (i.e. the Redfield ratios) in the organisms and the trophic transfer of the nutrients to be proportional to respiration and estimated excretion ratios for carbon.
- Initial nutrient concentrations in DIM available for primary production were assumed to be the same as average nutrients concentrations in the area given by /Nitchals, 1985/ and /Lindblad, 1994/.
- The biomass in the compartments is assumed to be constant between years.

3.3 Construction of the carbon budget

The first step in the development of the carbon budget was to identify and group plants and animals present in the area into compartments, representing organisms that have similar ecological functions and live in the same habitat. A description of the compartments used in the carbon budget as well as their assumed occurrence in the ecosystem is reported in Table 3-1.

Table 3-1. Description of the compartments used in the carbon budget and carbon flow model and the source of data for each compartment.

Model compartment	Organism group(s)[source]	Description of the compartment	Occurrence in the ecosystem
Phytoplankton	Phytoplankton[1]	Pelagic microalgae and photosynthesising bacteria	In water column in photic zone
	Bacterioplankton[2]	Pelagic heterotrophic bacteria	In water column in whole system
Benthic plants	Microphytes[3]	Benthic microalgae	On seabed in photic zone
	Macrophytes[4]	Benthic macroalgae, phanerogams, bryophytes	On seabed in photic zone
Zooplankton	Zooplankton[5]	Planktonic animals	In water column in whole system
Macrograzers	Macrograzers[4]	Grazing macrofauna > 500µm	On seabed in photic zone
Benthos	Filter feeders[4]	Filter feeding macrofauna > 500 µm	In/on seabed at all depths
	Benthic microfauna[6]	Benthic bacteria < 3 µm	In/on seabed at all depths
	Benthic meiofauna[7]	Meiofauna 3–500 µm	In/on seabed at all depths
	Benthic macrofauna[4]	Soft bottom dwelling macrofauna > 500 µm	In/on seabed below photic zone
Fish	Fish[8]	Fish, demersal and pelagic	In whole system
Seal	Seal[9]	Grey seal	Modelled on individual level
Eider duck	Eider duck[10]	Diving ducks (mainly eider duck)	Modelled on population level
Eagle	Eagle[11]	White-tailed eagle	Modelled on individual level
Humans	Humans[12]	Average Swedish man	Modelled on individual level
POC	POC[13]	Nonliving particulate organic carbon	In water column in whole system
DIC	DIC[14]	Nonliving dissolved inorganic carbon	In water column in whole system

[1] /Lindahl and Wallström, 1980/, [2] /Kuparinen, 1987/, [3] /Snoeijs, 1985, 1986 /, [4] /Kautsky et al. 1999/
[5] /Eriksson et al. 1977/, [6] /Mohammadi et al. 1993/, [7] /Ankar, 1977/, [8] /Jansson et al. 1985/,
[9] /Roos, 2000 pers comm), [10] /Kautsky et al. 1983; Gilek et al. 1997/, [11] /Helander, 1983/, [12] /Wikberger, 2000/,
[13] /Nitchals, 1985/, [14] /Larsson, 1999 pers comm/

The biomass, primary production, respiration and consumption were established for each compartment from investigations conducted in or close to the area surrounding the repository. All variables were recalculated to be representative for the whole study area on an annual basis (e.g. zooplankton respiration per model area and year). Data expressed in dry weight were converted to carbon weight with the aid of conversion factors /Kautsky, 1995/. The annual primary production was derived in different ways depending on the form of the original data. In studies where the primary production had been measured, an annual average was established from the data. In studies where only the biomass was measured, the primary production was derived from the biomass (Eq 1);

$$PP_{sp} = B_{sp} \times CF_{ppsp} \times 105 \quad (1)$$

where sp was the species or taxa, PP_{sp}, the annual primary production for sp, B_{sp}, the biomass for sp and CF_{ppsp}, the conversion factor for biomass to primary production per light-day for sp /Kautsky, 1995/. The seasonal variability in primary production was compensated for by normalising the primary production per light-day (a day with a minimum insolation of 5 MJ/m^2) and multiplying with the annual number of light-days for this particular area /i.e. 105 days per year, Krezel, 1985/. In the model the net primary production was used, i.e. the difference between the respiration and the gross primary production.

In studies where the respiration was measured, an annual average was established, and in studies where only the biomass was measured, the respiration was derived from the biomass (Eq 2);

$$R_{sp} = B_{sp} \times CF_{rsp} \times 2{,}400 \quad (2)$$

where R_{sp} was the annual respiration for species or taxa sp, B_{sp}, the biomass of sp, and CF_{rsp}, the conversion factor for biomass to respiration per 1°C for sp /Kautsky, 1995/. The respiration was compensated for seasonal changes in temperature by normalising the respiration per 1°C and multiplying by the annual degree-days (annual sum of daily water temperature (°C) at the site, i.e. 2,400°C per year /Kautsky and Kautsky, 1995/. The consumption (C_{sp}) was defined to be three times the respiration for all heterotrophic organisms /Elmgren, 1984/ except microorganisms whose consumption were assumed to be two times the respiration (Eqs 3 and 4);

$$C_{sp} = R_{sp} \times 3 \quad (3)$$

$$C_{sp} = R_{sp} \times 2 \quad (4)$$

The variables in the carbon budget (i.e. biomass, primary production, respiration and consumption) were compiled in agreement with the general energy equation. This equation characterizes consumption as equal to the sum of secondary production, respiration and egestion when the biomass is constant /Crisp, 1971/. Egestion is the portion of ingested material that is not assimilated, and instead is released into the environment as faecal and urinary products /Baird and Ulanowicz, 1993/. Egestion and secondary production were in this study merged to one unit, excess (E_{sp}), and assumed to be the residual of consumption (C_{sp}) and respiration (R_{sp}) (Eq 5);

$$E_{sp} = C_{sp} - R_{sp} \quad (5)$$

The biomass, primary production, respiration and consumption for species or taxa associated to the same compartment were summed up and used as initial data in the carbon flow model.

3.4 Construction of the carbon flow model (a theoretical description)

To facilitate the modelling procedure, some of the compartments used in the carbon budget were fused to larger unities (Table 3-1). For instance, the micro- and macrophyte compartments were fused to one compartment for benthic plants, the phytoplankton compartment was fused with the bacterioplankton compartment and filter feeders, benthic macro-, meio- and microfauna were fused into one compartment, benthos. Then, the fused compartments were connected in agreement with the structure of the food web of the ecosystem at the site to a carbon flow model (Figure 3-1).

3.4.1 Primary production

In the model dissolved inorganic matter (DIM) was defined to enter the food web in the primary production process (Eqs 6 and 7);

$$PP_{phytoplankton\,(t+1)} = \frac{PP_{phytoplankton(t)}}{B_{phytoplankton(t)}} \times B_{phytoplankton(t+1)} \quad (6)$$

$$PP_{benthicplants\,(t+1)} = \frac{PP_{benthicplants(t)}}{B_{benthicplants(t)}} \times B_{benthicplants(t+1)} \quad (7)$$

where the rate of primary production for phytoplankton/benthic plants ($PP_{(t+1)}$) was equal to their annual primary production ($PP_{(t)}$) per biomass ($B_{(t)}$) (derived from the carbon budget) multiplied by their prevailing biomass ($B_{(t+1)}$). The primary production process in the model was constrained by the amount of DIC available in the DIC-compartment.

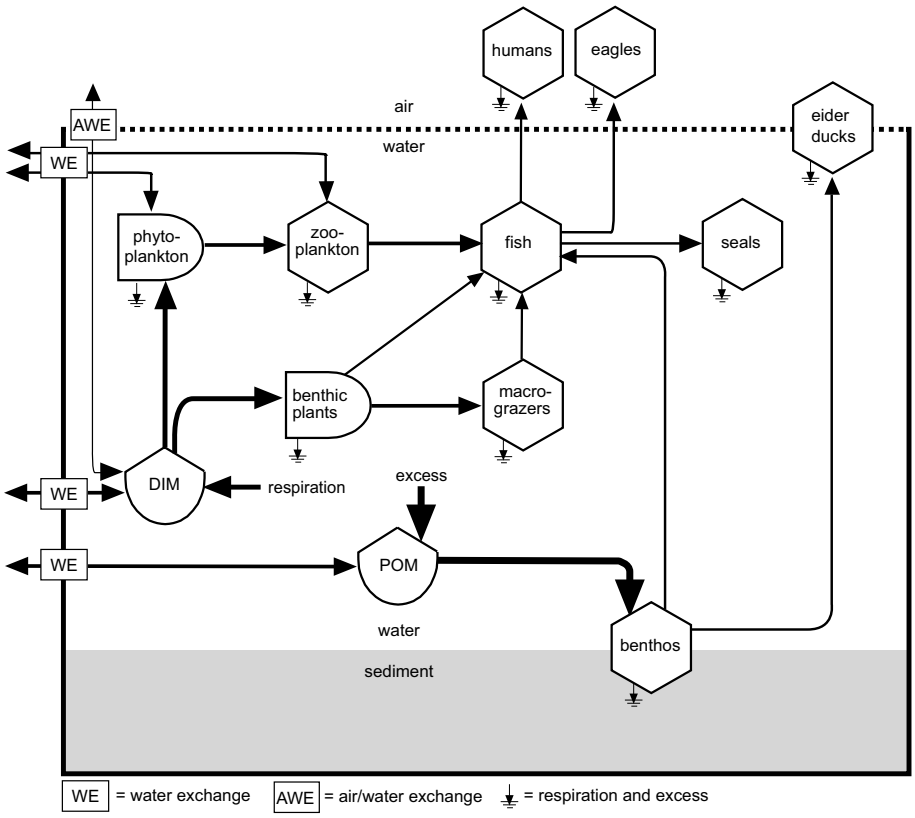

Figure 3-1. *Conceptual structure of the CNP-model.*

3.4.2 Respiration

The rate of animal respiration ($R_{(t+1)}$) was similarly determined as the annual respiration ($R_{(t)}$) per biomass ($B_{(t)}$) (derived from the carbon budget) multiplied by the prevailing biomass ($B_{(t+1)}$) for the compartment (Eq 8, exemplified for zooplankton);

$$R_{zooplankton(t+1)} = \frac{R_{zooplankton(t)}}{B_{zooplankton(t)}} \times B_{zooplankton(t+1)} \quad (8)$$

Carbon dioxide respired in the respiration process was connected to the DIC-compartment, which provided a re-circulation mechanism of carbon in the model.

3.4.3 Consumption

The consumption rate ($C_{(t+1)}$) was in the model determined as in the carbon budget, i.e. a function of the respiration rate (Eqs 9 and 10, exemplified for zooplankton and benthic bacteria);

$$C_{zooplankton(t+1)} = R_{zooplankton(t+1)} \times 3 \quad (9)$$

$$C_{bethicbacteria(t+1)} = R_{benthicbacteria(t+1)} \times 2 \quad (10)$$

In the model the consumption rate was constrained by the availability of the food source.

3.4.4 Excess

The residual of inflow (consumption or primary production) and outflow (respiration and predation/grazing) of carbon to a compartment was defined as the excess ($E_{(t+1)}$) and was determined as in Eqs 11 and 12 (exemplified for phytoplankton and zooplankton);

$$E_{phytoplankton(t+1)} = PP_{phytoplankton(t+1)} - C_{zooplankton(t+1)} \quad (11)$$

$$E_{zooplankton(t+1)} = C_{zooplankton(t+1)} - R_{zooplankton(t+1)} - C_{fish(t+1)} \quad (12)$$

The excess from all compartments was connected to the particulate organic carbon (POC) compartment, which feeds the benthos compartment and thus provided a second route for carbon re-circulation in the model. The carbon content in the DIC- and POC-compartments was, beside the inflow to the compartments (in form of respiration and excess) and the outflows (in form of primary production and benthos consumption) also dependent on the water exchange rate, i.e. water volume and the retention time of the water.

3.5 Modelling of nitrogen and phosphorous flows

The nutrient uptake by primary producing organisms was modelled proportional to the stoichiometric relationships between carbon and nutrients for the various organism groups included in the model (i.e. Redfield ratios). This was in the model calculated with the "Liebig law block" (see section 3.6.1) that calculates an array of coefficients that restricts the uptake to the limiting constituent and thus restricts the CNP requirement from the DIM compartments to be proportional to the required uptake restricted to minor constituent. The CNP-ratios for uptake and trophic transfer of the nutrients was modelled proportional to the mass flow of carbon as well as the nutrient mineralization by consumers which was assumed to be proportional to respiration and estimated excretion ratios /Kautsky, 1995/.

The CNP-ratios used in the model are shown for each functional group in Table 3-2. The initial nutrient concentrations available for primary production were assumed to be the same as average nutrient concentrations in the area /Nitchals, 1985; Lindblad, 1994/.

Table 3-2. CNP-ratios for the functional groups used in the Liebig law block of the CNP-model /Kautsky, 1995/.

Functional group	C	N	P
Phytoplankton	1.000	0.168	0.013
Benthic plants	1.000	0.168	0.013
Zooplankton	1.000	0.257	0.018
Grazers	1.000	0.257	0.018
Fish	1.000	0.257	0.018
Benthic bacteria	1.000	0.180	0.056
Benthic meiofauna	1.000	0.257	0.018
Benthic macrofauna	1.000	0.257	0.018

3.6 Construction of the CNP-model (a description of the Simulink model)

An overview of the Simulink model with its compartment and connections is shown in Figure 3-2. In the present section all compartments included in the models are described in detail. The description of each compartment contains (1) an illustration of the compartment with its variables and connections, (2) a list and a description of its variables, (3) its equations and (4) its parameters and parameter estimations.

3.6.1 Terminology

The signal in the CNP-model is a vector where the first number represent carbon, the second nitrogen and third phosphorous. In the C-14 model the first number in the vector is carbon and the second C-14. In the RN-model the first number is carbon and the second is the radionuclide chosen in that particular simulation. The expression [1] in the equations that are presented in this section, refer to the first number in the vector, while [2] to the second and [3] to the third. Abs refers to the absolute value of the following expression and min or max refers to the minimum or maximum value of the following expressions. Mux is the expression used to describe that several signals are fused into a vector.

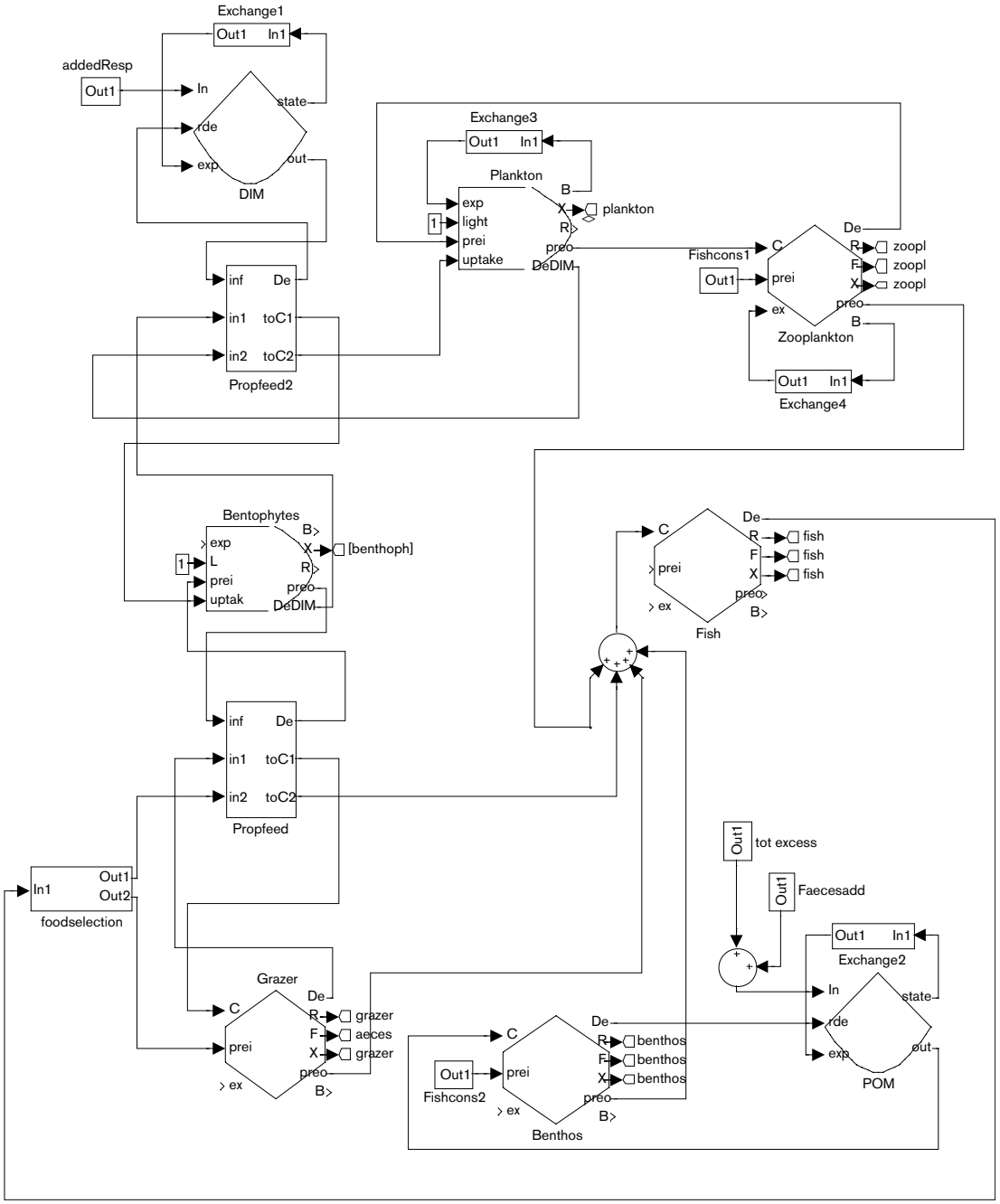

Figure 3-2. *Structure of the CNP-model.*

3.6.2 Dissolved inorganic matter (DIM)

Variables

Inflow: inflow of matter to DIM from the respiration process from all consumers (connected from the director total respiration).

Demand by producers: demand of DIM by all primary producers, i.e. benthic plants and phytoplankton (connected from the director food proportions II).

Import/export: inflow/export of matter to DIM due to water exchange (connected from the exchanger DIM-exchange).

Mass: content of matter in the DIM compartment (= state).

Outflow: the outflow of matter from the DIM compartment (connected to the director food proportions II).

Equations

Content of matter in DIM

mass = import/export + inflow – outflow – decay

Outflow from DIM (the Liebig law function)

outflow = available × min (availableCNP/requestedCNP)/(available/requested)

- available = abs(min(mass + in); requested)
- requested = demand by producers
- the Liebig-function sorts out the minimum value from: $C_{available}/C_{requested}$, $N_{available}/N_{requested}$, $P_{available}/P_{requested}$ and calculates an array with coefficients that restricts the uptake to the limiting constituent (C, N or P).

Radionuclide decay

decay = mass × decay constant

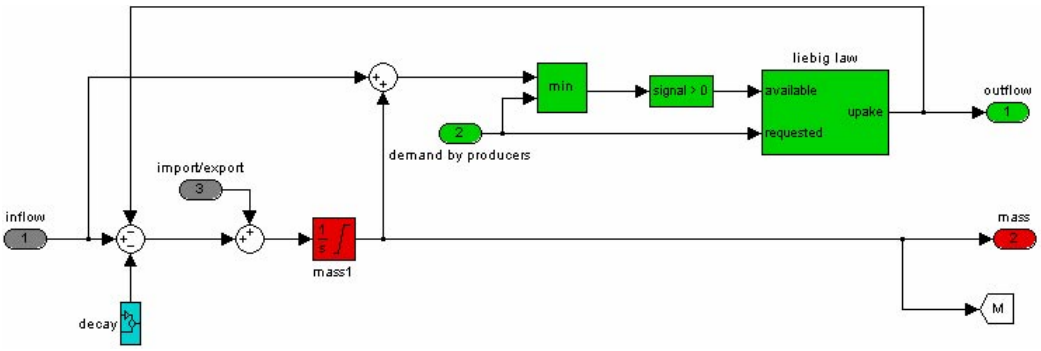

Figure 3-3. *Structure of model compartment for DIM (dissolved inorganic matter).*

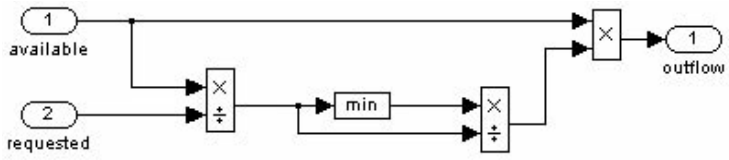

Figure 3-4. *The Liebig Law function.*

Table 3-3. Input parameters for the DIM-compartment.

Parameter	Value	Unit
Initial mass of DIC	1.78×10^{9}	gC
Initial mass of DIN	2.22×10^{6}	gN
Initial mass of DIP	1.11×10^{6}	gP
Decay constant for C, N and P	0	$year^{-1}$

3.6.3 Particulate organic matter (POM)

Variables

Inflow: inflow of matter to POM via the defecation process and excess from all biota compartments (connected from the director food proportions I).

Demand by decomposers: demand of POM by benthos.

Import/export: inflow of matter to POM due to water exchange (connected from the exchanger POM-exchange).

Mass: content of matter in the POM compartment.

Outflow: the outflow of matter from the POM compartment (connected to benthos).

Equations

Content of matter in POM

mass = import/export + inflow – outflow – decay

Concentration

c = mass/mass [1]

Outflow from POM

outflow = min ((inflow [1] + mass [1]), demand by decomposers [1]) × c

- inflow [1] is the first value (i.e. carbon) in the vector in and has an initial start value of 10^{11} (needed for the model to start and stabilise)

Radionuclide decay

decay = mass × decay constant

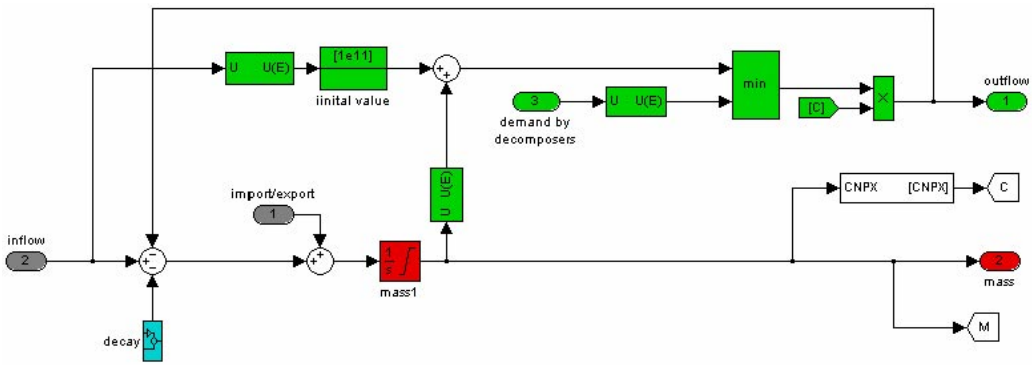

Figure 3-5. *Model compartment fort POM (particulate organic matter).*

Table 3-4. Input parameters for the POM compartment.

Parameter	Value	Unit
Initial mass of POC	1.06×10^{7}	gC
Initial mass of PON	1.77×10^{6}	gN
Initial mass of POP	1.37×10^{5}	gP
Decay constant for C, N and P	0	$year^{-1}$

3.6.4 Phytoplankton

Variables

Import/export: flow of matter to/from the phytoplankton compartment due to water exchange (connected to the director phytoplankton exchange). This variable reports the exchange of phytoplankton with the environment outside the system boundaries. The import/export-variable can be positive or negative depending on the biomass concentrations outside the system and thus influence the biomass of the phytoplankton compartment.

Light: light insolation. The light-variable is connected to phytoplankton from a constant (light insolation) and is multiplied by a productivity constant (phytoplankton productivity coefficient) resulting in a potential maximum productivity, which is a signal of the demand for DIM from the DIM compartment via demand of dim (see below). The light-variable in this model could be modified and associated with light intensity curves and the productivity constant which would provide a more dynamic model than what is it in its present state.

Demand by grazers: demand of phytoplankton by zooplankton (connected to the zooplankton compartment and delivers information of the desired demand of phyto-plankton from zooplankton).

Uptake: uptake of matter in phytoplankton from the DIM compartment (connected to phytoplankton from food proportions II).

Biomass: biomass content in the phytoplankton compartment and the phytoplankton exchange with the environment outside the system boundaries (connected to the director phytoplankton exchange). The biomass variable can be positive or negative depending on the biomass concentrations outside the system.

Excess: outflow of excess matter from phytoplankton to POM (connected to POM via the director total excess).

Respiration: outflow of matter from phytoplankton to DIM due to respiration (connected to DIM via the director total respiration). The phytoplankton respiration is in the present model included in the production (net production), thus the respiration is zero.

Grazing: outflow of matter from phytoplankton to zooplankton (connected to zooplankton)

Demand of DIM: demand of DIM by phytoplankton (connected to food proportions II). Demand of DIM is related to the light-variable.

Equations

Demand of DIM by phytoplankton

demand of DIM = light × kprod × biomass × ((phytoplankton CNP/phytoplankton CNP[1])/c

- kprod = phytoplankton productivity

Concentration

c = biomass/biomass[1]

Biomass

biomass = import/export – excess + uptake – respiration – decay – grazing

Grazing on phytoplankton by zooplankton

grazing = min (demand by grazer[1], abs (uptake[1] – respiration[1] – decay[1])) × c

Excess

excess = ((uptake – respiration – decay – grazing + biomass)[1] – maximum biomass) × c

Respiration

respiration = biomass × kresp

- kresp = phytoplankton respiration coefficient

Radionuclide decay

decay = biomass × decay constant

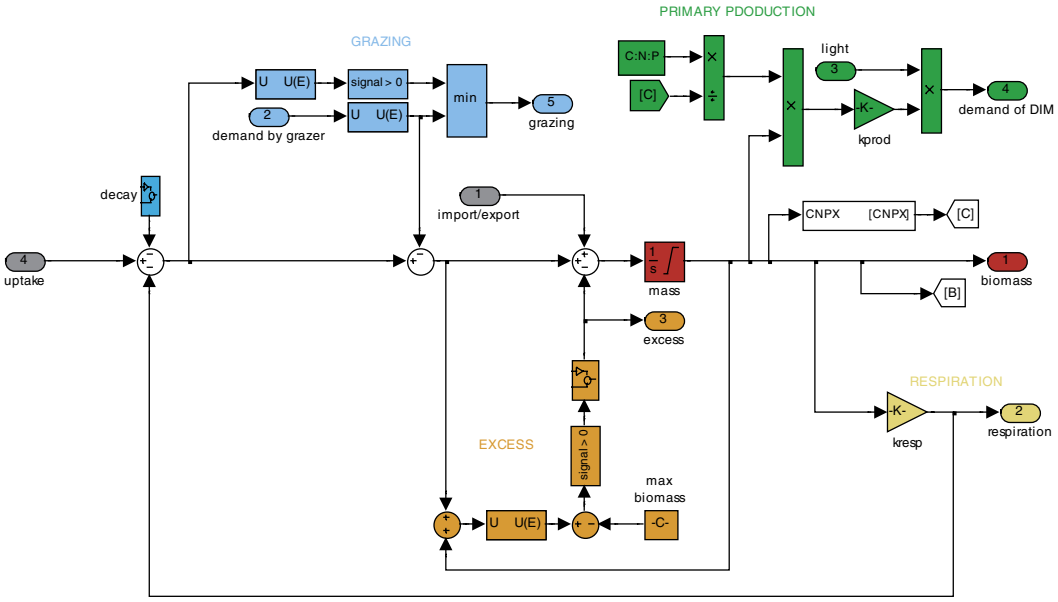

Figure 3-6. *Model compartment for phytoplankton.*

Table 3-5. Input parameters for phytoplankton compartment.

Parameter	Value	Unit
Initial phytoplankton biomass C	1.06×10^{7}	gC
Initial phytoplankton biomass N	1.77×10^{6}	gN
Initial phytoplankton biomass P	1.37×10^{5}	gP
Phytoplankton productivity coefficient	28.4	$g/g/m^3$
Phytoplankton CNP	[1; 0.168; 0.013]	–
Phytoplankton respiration coefficient*	0	$g/g/m^3$
Maximum biomass	Initial biomass	
Decay constant for C, N and P	0	$year^{-1}$

* The respiration constant is zero becasue the productivity coefficient was based on net primary production.

3.6.5 Benthic plants

Variables

Light: light insolation. The light-variable is connected to benthic plants from a constant (light insolation) and is multiplied by a productivity constant (benthic plant productivity coefficient) resulting in a potential maximum productivity, which is a signal of the demand for DIM from the DIM compartment via demand of dim (see below). The light-variable in this model could be modified and associated with light intensity curves and the productivity constant which would provide a more dynamic model than what is it in its present state.

Demand by producer: demand of benthic plants by grazers and fish (connected to the director food proportions I) delivers information of the desired demand of benthic plants from grazers and fish.

Uptake: uptake of matter in benthic plants from the DIM compartment (connected to director food proportions II).

Excess: outflow of excess matter from benthic plants to POM (connected to POM via the director total excess).

Biomass: biomass content in the benthic plant compartment

Respiration: outflow of matter from benthic plants to DIM due to respiration (connected to DIM via the director total respiration). The benthic plant respiration is in the present model included in the production (net production), thus the respiration is zero.

Grazing: outflow of matter from benthic plants to grazers and fish (connected to the director food proportions I).

Demand of DIM: demand of DIM by benthic plants (connected to food proportions II). Demand of DIM is related to the light-variable.

Equations

Demand of DIM by benthic plants

demand of DIM = light × kprod × biomass × ((benthic plant CNP/benthic plant CNP[1])/c)

- kprod = benthic plant productivity

Concentration

c = biomass/biomass[1]

Biomass

biomass = import/export – excess + uptake – respiration – decay – grazing

Grazing on benthic plants by grazers and fish

grazing = min(demand by grazers[1], abs(uptake[1] – respiration[1] – decay[1])) × c

Excess

excess = ((uptake – respiration – decay – grazing + biomass)[1] – maximum biomass) × c

Respiration

respiration = biomass × kresp

- kresp = benthic plant respiration coefficient

Radionuclide decay

decay = biomass × decay constant

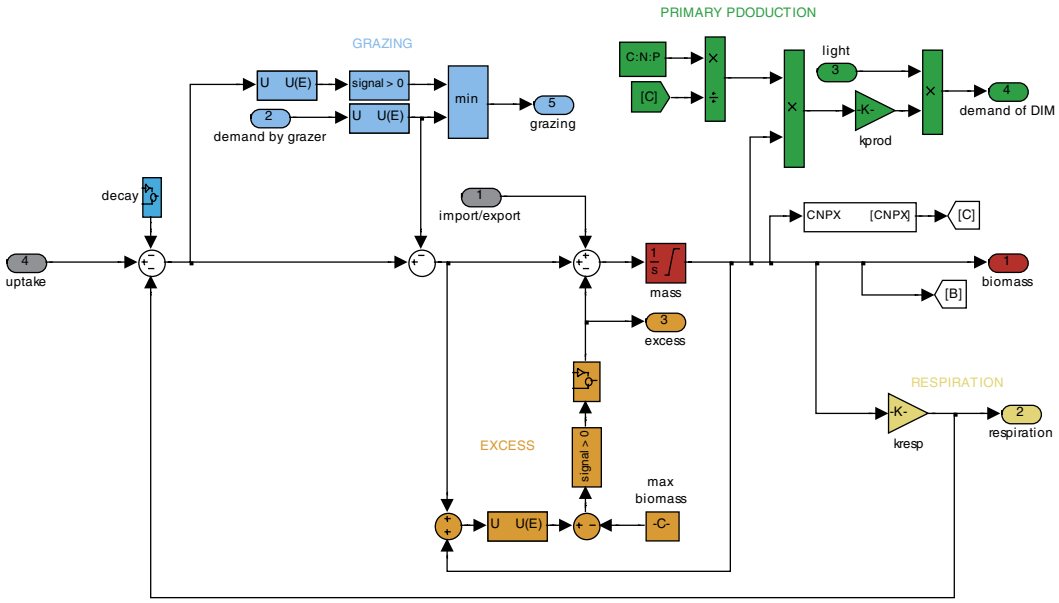

Figure 3-7. *Model compartment for benthic plants.*

Table 3-6. Input parameters for benthic plants.

Parameter	Value	Unit
Initial benthic plant biomass C	1.34×10^{8}	gC
Initial benthic plant biomass N	6.72×10^{6}	gN
Initial benthic plant biomass P	1.07×10^{6}	gP
Benthic plant productivity coefficient	5.97	$g/g/m^2$
Benthic plant CNP#	[1; 0.168; 0.013]	–
Benthic plant respiration coefficient*	0	$g/g/m^2$
Maximum biomass	Initial biomass	
Decay constant for C, N and P	0	$year^{-1}$

Average of *Fucus vesicolosus* and *Cladocera* spp.

* The respiration constant is zero becasue the productivity coefficient was based on net primary production.

3.6.6 Zooplankton

Variables

Consumption: consumption of phytoplankton by zooplankton

Demand by predator: demand of zooplankton by fish (connected to the director fish food selection II) and reports the demand of zooplankton according to the ratio fish zooplankton consumption to total fish consumption.

Import/export: flow of matter to/from the zooplankton compartment due to water exchange (connected to zooplankton from the director zooplankton exchange). This variable reports the exchange of zooplankton with the environment outside the system boundaries. The ex-variable can be positive or negative depending on the biomass concentrations outside the system and thus influence the biomass of the zooplankton compartment.

Demand of food: demand of phytoplankton by zooplankton.

Respiration: outflow of matter from zooplankton to DIM due to respiration (connected to DIM via the director total respiration).

Faeces: outflow of matter to POM from zooplankton due to defecation (connected to the director total faeces production).

Excess: outflow of matter to POM from zooplankton to POM (connected to the director total excess production).

Predation: outflow of matter from zooplankton to fish.

Biomass: biomass content in the zooplankton compartment and the zooplankton exchange with the environment outside the system boundaries (connected to the director zooplankton exchange). The biomass variable can be positive or negative depending on the biomass concentrations outside the system.

Equations

Demand of phytoplankton by zooplankton

demand of food = biomass × kresp × resex × kdemand

- kresp = zooplankton respiration coefficient
- kdemand = respiration to consumption coefficient for zooplankton

Respiration

respiration = biomass × kresp × resex

- kresp = zooplankton respiration coefficient

Faeces

faeces = consumption × kfaeces

- kfaeces = 1 – zooplankton assimilation efficiency

Concentration

c = biomass/biomass[1]

Biomass

biomass = consumption – faeces – respiration – decay – predation + import/export – excess

Predation on zooplankton by fish (food proportion I)

predation = min(demand by predator[1], abs(consumption[1] – faeces[1] – respiration[1] – decay[1])) × c

Resex

resex = c/(max biomass/max biomass [1])

Excess

excess = abs(consumption – faeces – respiration – decay – predation + biomass – max biomass) × c

Radionuclide decay

decay = biomass × decay constant

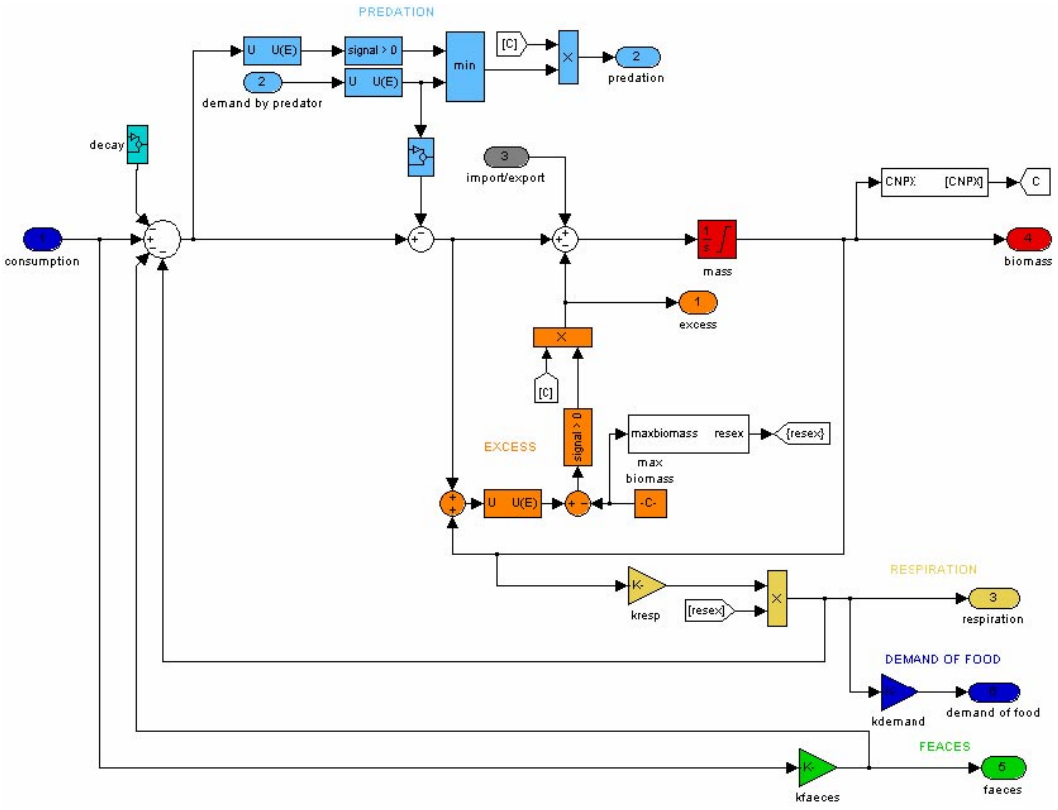

Figure 3-8. *Model compartment for zooplankton.*

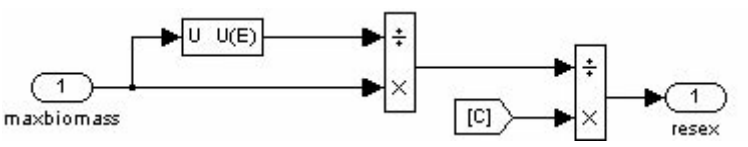

Figure 3-9. *Resex sub-model.*

Table 3-7. Input parameters for zooplankton.

Parameter	Value	Unit
Initial zooplankton biomass C	1.25×10^{6}	gC
Initial zooplankton biomass N	3.21×10^{5}	gN
Initial zooplankton biomass P	2.25×10^{4}	gP
Respiration to consumption coefficient	3	$g/g/m^2$
Zooplankton CNP	[1; 0.257; 0.018]	–
Zooplankton respiration coefficient	[13.84; 3.56; 0.25]	$g/g/m^2$
Zooplankton excretion coefficient	[1; 0.095; 0.03]	–
Zooplankton assimilation coefficient	0.8	–
Maximum biomass	Initial biomass	

3.6.7 Grazers

Variables

Consumption: consumption of benthic plants by grazers (connected for food proportion I).

Demand by predator: demand of grazer by fish (connected to the director fish food selection I) and reports the demand of grazer according to the ratio fish grazer consumption to total fish consumption.

Demand of food: demand of benthic plants by grazers (connected to food proportion I).

Respiration: outflow of matter to DIM from grazer due to respiration (connected to the director total respiration).

Faeces: outflow of matter to POM from grazer due to the defecation process (connected to director total faeces production).

Excess: outflow of matter to POM from grazer (connected to the director total excess production).

Predation: outflow of matter from grazer to fish.

Biomass: biomass content in the grazer compartment.

Equations

Demand of benthic plants by grazers

demand of food = biomass × kresp × resex × kdemand

- kresp = grazer respiration coefficient
- kdemand = respiration to consumption coefficient for grazer

Respiration

respiration = biomass × kresp × resex

- kresp = grazer respiration coefficient

Faeces

faeces = consumption × kfaeces

- kfaeces = 1 – grazer assimilation efficiency

Concentration

c = biomass/biomass[1]

Biomass

biomass = consumption – faeces – respiration – decay – predation– excess

Predation on grazer by fish (food proportion I)

predation = min(demand by predator[1], abs(consumption[1] – faeces[1] – respiration[1] – decay[1])) × c

Resex

resex = c/(max biomass/max biomass [1)]

Excess

excess = abs(consumption – faeces – respiration – decay – predation + biomass – max biomass) × c

Radionuclide decay

decay = biomass × decay constant

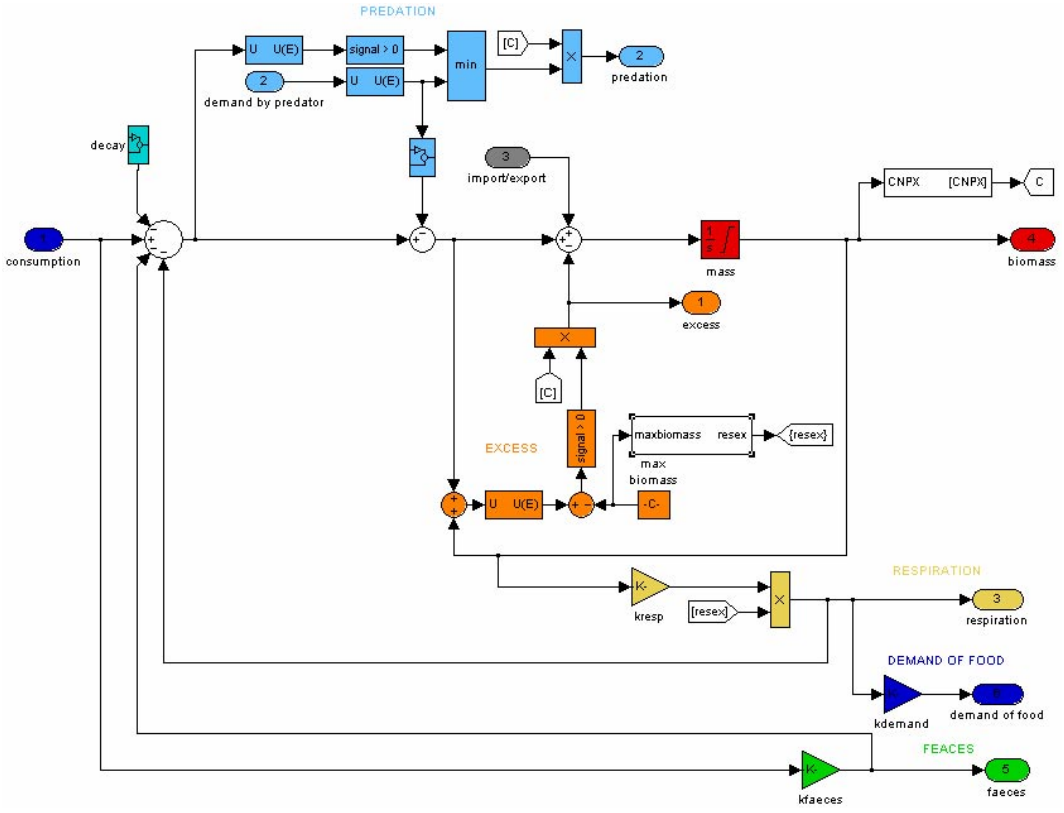

Figure 3-10. *Model compartment for grazers.*

Table 3-8. Input parameters for grazers.

Parameter	Value	Unit
Initial grazer biomass C	4.50×10^{6}	gC
Initial grazer biomass N	1.16×10^{6}	gN
Initial grazer biomass P	8.10×10^{4}	gP
Respiration to consumption coefficient	3	$g/g/m^2$
Grazer CNP	[1; 0.257; 0.018]	–
Grazer respiration coefficient	[4.13; 1.06; 0.074]	$g/g/m^2$
Grazer excretion coefficient	[1; 0.105; 0.024]	–
Grazer assimilation coefficient	0.8	–
Maximum biomass	Initial biomass	

3.6.8 Fish

Variables

Consumption: consumption of benthic plants, grazer, zooplankton and benthos by fish (connected to the director food proportions I).

Demand by predator: is not included in the model.

Demand of food: demand of benthic plants and grazers by fish (connected to the director fish food selection).

Respiration: outflow of matter to DIM from fish due to respiration (connected to the director total respiration).

Faeces: outflow of matter to POM from fish due to the defecation process (connected to director total faeces production).

Excess: outflow of matter to POM from fish (connected to the director total excess production).

Predation: This variable was not calculated by the model but separately from the modelling results.

Biomass: biomass content in the fish compartment.

Equations

Demand of food by fish

demand of food = biomass × kresp × resex × kdemand

- kresp = fish respiration coefficient
- kdemand = respiration to consumption coefficient for fish

Respiration

respiration = biomass × kresp × resex

- kresp = fish respiration coefficient

Faeces

faeces = consumption × kfaeces

- kfaeces = 1 – fish assimilation efficiency

Concentration

c = biomass/biomass[1]

Biomass

biomass = consumption – faeces – respiration – decay – predation– excess

Resex

resex = c/(max biomass/max biomass [1)]

Excess

excess = abs(consumption – faeces – respiration – decay – predation + biomass – max biomass) × c

Radionuclide decay

decay = biomass × decay constant

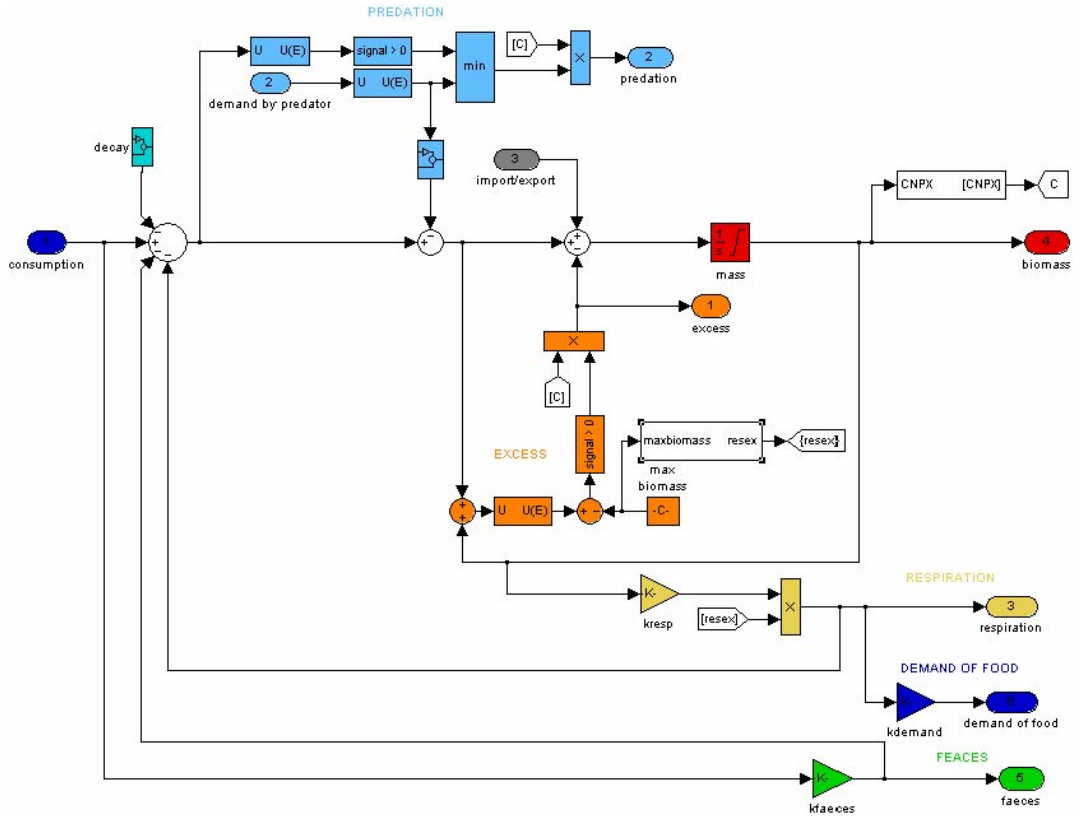

Figure 3-11. *Model compartment for fish.*

Table 3-9. Input parameters for fish.

Parameter	Value	Unit
Initial fish biomass C	8.28×10^{6}	gC
Initial fish biomass N	2.13×10^{6}	gN
Initial fish biomass P	1.49×10^{5}	gP
Respiration to consumption coefficient	1.73	$g/g/m^2$
Fish CNP	[1; 0.257; 0.018]	–
Fish respiration coefficient	[1.73; 0.16; 0.052]	$g/g/m^2$
Fish excretion coefficient	[1; 0.095; 0.030]	–
Fish assimilation coefficient	0.8	–
Maximum biomass	Initial biomass	gC

3.6.9 Benthos

Variables

Consumption: consumption of POM by benthos.

Demand by predator: demand of benthos from fish (connected to fish consumption III) and reports the demand of benthos according to a ratio fish benthos consumption to total fish consumption.

Demand of food: demand of POM by benthos.

Respiration: outflow of matter to DIM from benthos due to respiration (connected to the director total respiration).

Faeces: outflow of matter to POM from benthos due to the defecation process (connected to the director total faeces production).

Excess: outflow of matter to POM from benthos (connected to the director total excess production).

Predation: outflow of matter from benthos to fish.

Equations

Demand of POM by benthos

demand of food = biomass × kresp × resex × kdemand

- kresp = benthos respiration coefficient (respiration per biomass)
- kdemand = respiration to consumption coefficient for benthos (consumption per biomass)

Respiration

respiration = biomass × kresp × resex

- kresp = benthos respiration coefficient (respiration per biomass)

Faeces

faeces = consumption × kfaeces

- kfaeces = 1 – benthos assimilation efficiency

Concentration

c = biomass/biomass[1]

Biomass

biomass = consumption – faeces – respiration – decay – predation– excess

Predation on benthos by fish (food proportion I)

predation = min(demand by predator[1], abs(consumption[1] – faeces[1] – respiration[1] – decay[1])) × c

Resex

resex = c/(max biomass/max biomass [1)]

Excess

excess = abs(consumption – faeces – respiration – decay – predation + biomass – max biomass) × c

Radionuclide decay

decay = biomass × decay constant

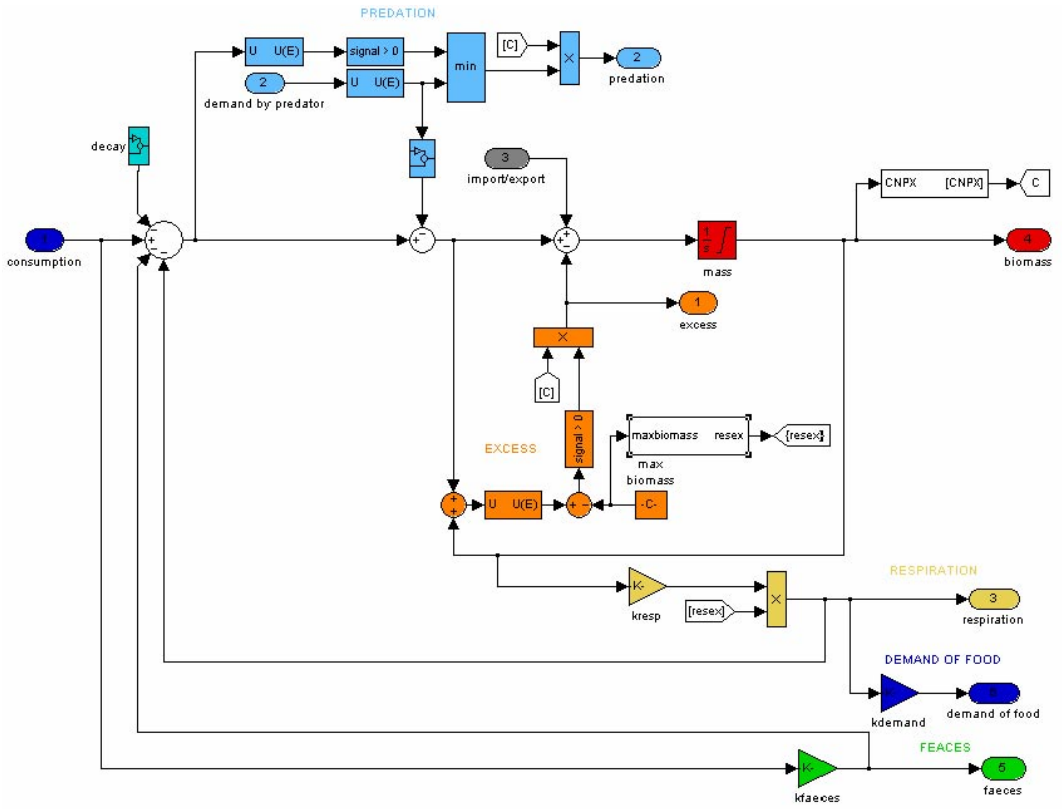

Figure 3-12. *Model compartment for benthos.*

Table 3-10. Input parameters for benthos.

Parameter	Value	Unit
Initial benthos biomass C	1.17×10^{8}	gC
Initial benthos biomass N	2.92×10^{7}	gN
Initial benthos biomass P	2.57×10^{6}	gP
Respiration to consumption coefficient	2.86	$g/g/m^2$
Benthos CNP	[1; 0.249; 0.022]	–
Benthos respiration coefficient	[3.56; 0.89; 0.078]	$g/g/m^2$
Benthos excretion coefficient	[1; 0.249; 0,018]	–
Benthos assimilation coefficient	0.8	–
Maximum biomass	Initial biomass	

3.6.10 Food proportions I (director)

Food proportions I handles the demand and distribution of matter between benthic plants, grazers and fish.

Variables

inf: inflow of matter from benthic plants.

in1: demand of matter from benthic plants by grazers.

in2: demand of matter from benthic plants by fish.

de: demand of matter from benthic plants by grazers and fish.

toC1: outflow of matter from food proportion I to grazer.

toC2: outflow of matter from food proportion I to fish.

Equations

Consumption by grazers

$$toC1 = c \times ((inf[1] \times in1[1])/(in1[1] + in2[1]))$$

Consumption by fish

$$toC2 = c \times ((inf[1] \times in2[1])/(in1[1] + in2[1]))$$

Demand of benthic plants by grazers and fish

$$de = in1[1] + in2[1]$$

Concentration

$$c = inf/inf[1]$$

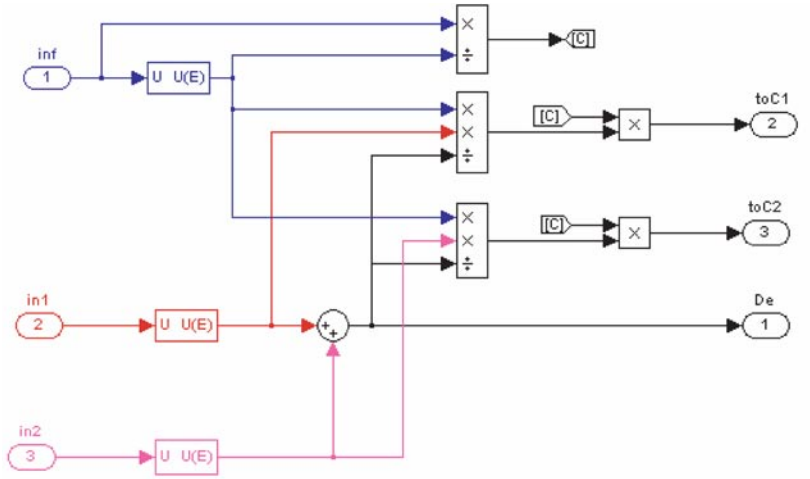

Figure 3-13. *Model compartment for food proportions I.*

3.6.11 Food proportions II (director)

Food proportions II direct the demand and the distribution of matter between DIM, phytoplankton and the benthic plants.

Variables

inf: inflow of matter from DIM.

in1: demand of matter from DIM by benthic plants.

in2: demand of matter from DIM by phytoplankton.

de: demand of matter from DIM by benthic plants and phytoplankton.

toC1: outflow of matter from food proportions II to benthic plants.

toC2: outflow of matter from food proportions II to phytoplankton.

Equations

Uptake of DIM by benthic plants

$$toC1 = (inf \times in1)/(in1 + in2)$$

Uptake of DIM by phytoplankton

$$toC2 = (inf \times in2)/(in1 + in2)$$

Demand of DIM by benthic plants and phytoplankton

$$de = in1 + in2$$

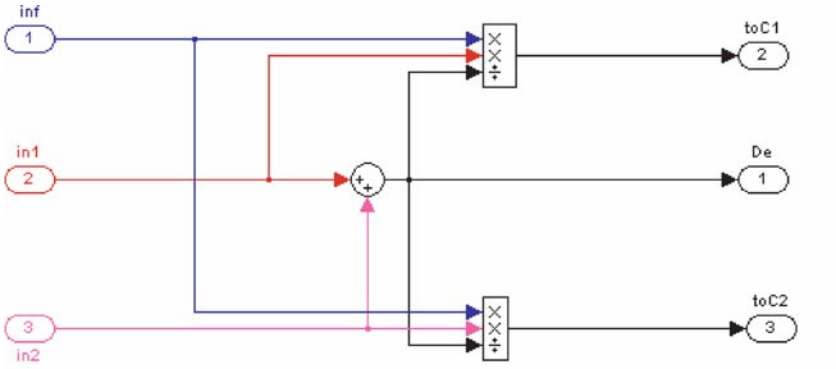

Figure 3-14. *Model compartment for food proportions II.*

3.6.12 Fish food selection I (director)

Fish food selection I handles the demand of benthic plants and grazers by fish.

Variables

in1: demand of matter from benthic plants and grazers by fish.

out1: demand of matter from benthic plants by fish.

out2: demand of matter from grazers by fish.

Equations

Demand of matter from benthic plants

out1 = in1 × foodprop

- foodprod = fish share of benthic plant predation

Demand of matter from grazers

out2 = in1 × foodprop1

- foodprod1 = fish share of grazers predation

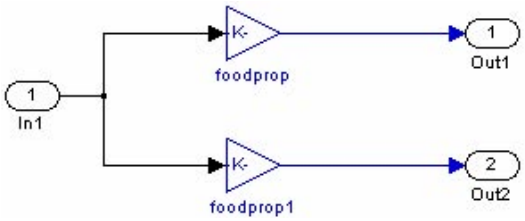

Figure 3-15. *Model compartment for fish food selection I.*

Table 3-11. Input parameters for fish food selection I.

Parameter	Value	Unit
share of benthic plant predation	0.1	–
fish share of grazers predation	0.05	–

3.6.13 Fish food selection II (director)

Fish food selection II handles the demand of benthos by fish.

Variables

out1: demand of matter from benthos by fish.

Equations

Demand of matter from benthos

out1 = in1 × foodprop2

- foodprod2 = fish share of benthos predation
- in1 comes from food selection I

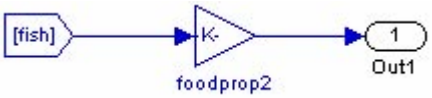

Figure 3-16. *Model compartment for fish food selection II.*

Table 3-12. Input parameters for fish food selection II.

Parameter	Value	Unit
fish share of benthos predation	0.05	–

3.6.14 Food selection III (director)

Fish food selection III handles the demand of zooplankton by fish.

Variables

out1: demand of matter from zooplankton by fish.

Equations

Demand of matter from zooplankton

out1 = in1 × foodprop3

- foodprod3 = fish share of zooplankton predation
- in1 comes from food selection I

Figure 3-17. *Model compartment for fish food selection III.*

Table 3-13. Input parameters for fish food selection III.

Parameter	Value	Unit
fish share of zooplankton predation	0.8	–

3.6.15 Total respiration (director)

Total respiration was used as a director for collecting and re-directing respired material from biota to DIM.

Variables

Total respiration: total respiration by all organisms in the area.

Equations

Total respiration

$$\text{total respiration} = \text{respiration}_{\text{fish}} + \text{respiration}_{\text{grazer}} + \text{respiration}_{\text{benthos}} + \text{respiration}_{\text{zooplankton}} + \text{respiration}_{\text{phytoplankton}} + \text{respiration}_{\text{bentic plants}}$$

3.6.16 Total excess (director)

The total excess director collects excess from all organism compartments and re-directs it to the POM compartment.

Variables

Total excess: total excess produced by all organisms in the area.

Equations

Total excess

$$\text{total excess} = \text{excess}_{\text{fish}} + \text{excess}_{\text{grazer}} + \text{excess}_{\text{benthos}} + \text{excess}_{\text{zooplankton}} + \text{excess}_{\text{benthic plants}} + \text{excess}_{\text{phytoplankton}}$$

3.6.17 Total faeces (director)

This director collects and re-directs faeces produced by consumer compartments to the POM compartment.

Variables

Total faeces: total faeces production by all consumers in the area.

Equations

Total faeces

total faeces = $faeces_{fish} + faeces_{grazers} + faeces_{benthos} + faeces_{zooplankton}$

3.6.18 DIM-exchange (exchanger)

Variables

Mass: mass of DIM.

Import/export: import/export of DIM.

Equations

Import/export:

import/export = (external DIM – mass) × water exchange

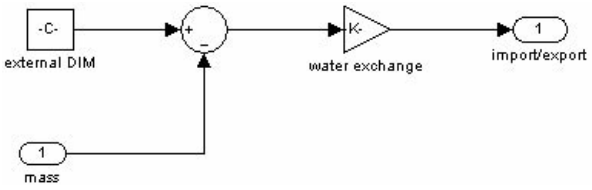

Figure 3-18. *Model compartment for DIM-exchange.*

Table 3-14. Input parameters for DIM-exchanger.

Parameter	Value	Unit
External DIM = initial mass of DIC	1.78×10^{9}	gC
External DIM = Initial mass of DIN	2.22×10^{6}	gN
External DIM = Initial mass of DIP	1.11×10^{6}	gP
Water exchange	365	$year^{-1}$

3.6.19 POM-exchange (exchanger)

Variables

Mass: mass of POM

Import/export: import/export of POM

Equations

Import/export:

import/export = water volume × a × b × water exchange

a = external POM[1] – (mass/water volume)[1]

b = switch (1, 2, 3)

1 = external POM/external POM[1]

2 = external POM[1] – (mass/water volume)[1]

3 = (mass/water volume)/(mass/water volume)[1]

- switch: Pass through input 1 when input 2 is ≥ 0; otherwise, pass through input 3. The input 1 pass-through criterion are input 2 greater than or equal, greater than, or not equal to the threshold. The first and third input ports are data ports, and the second input port is the control port. The threshold is ≥ 0.

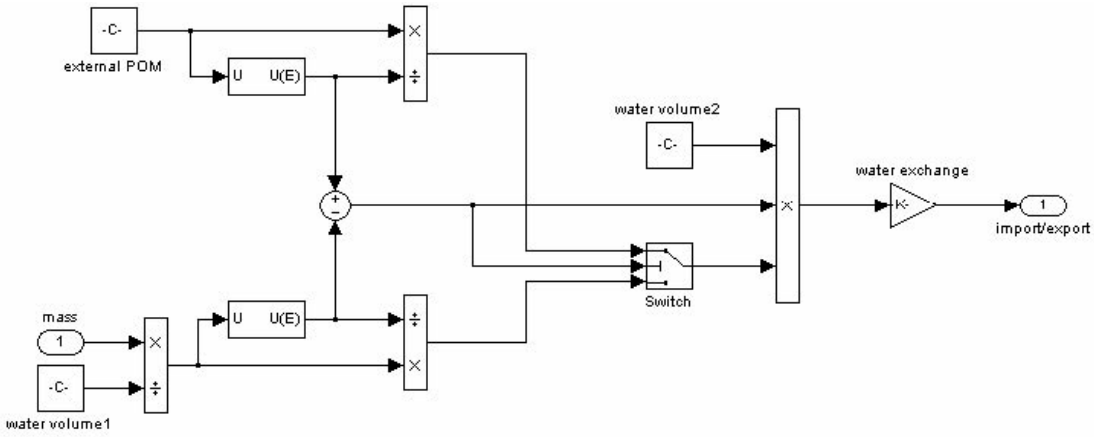

Figure 3-19. *Model compartment for POM exchange.*

Table 3-15. Input parameters fro POM-exchanger.

Parameter	Value	Unit
External level = Initial mass of POC	1.06×10^{7}	gC
External level = Initial mass of PON	1.77×10^{6}	gN
External level = Initial mass of POP	1.37×10^{5}	gP
Water volume	1.11×10^{8}	m^3
Water exchange	365	$year^{-1}$

3.6.20 Phytoplankton exchange (exchanger)

Variables

Biomass: biomass of phytoplankton.

Import/export: export of phytoplankton.

Equations

Import/export:

import/export = water volume × a × b × water exchange

a = external biomass[1] – (biomass/water volume)[1]

b = switch (1, 2, 3)

1 = external biomass/external biomass[1]

2 = external biomass[1] – (biomass/water volume)[1]

3 = (biomass/water volume)/(biomass/water volume)[1]

- switch: Pass through input 1 when input 2 is ≥ 0; otherwise, pass through input 3. The input 1 pass-through criterion are input 2 greater than or equal, greater than, or not equal to the threshold. The first and third input ports are data ports, and the second input port is the control port. The threshold is ≥ 0.

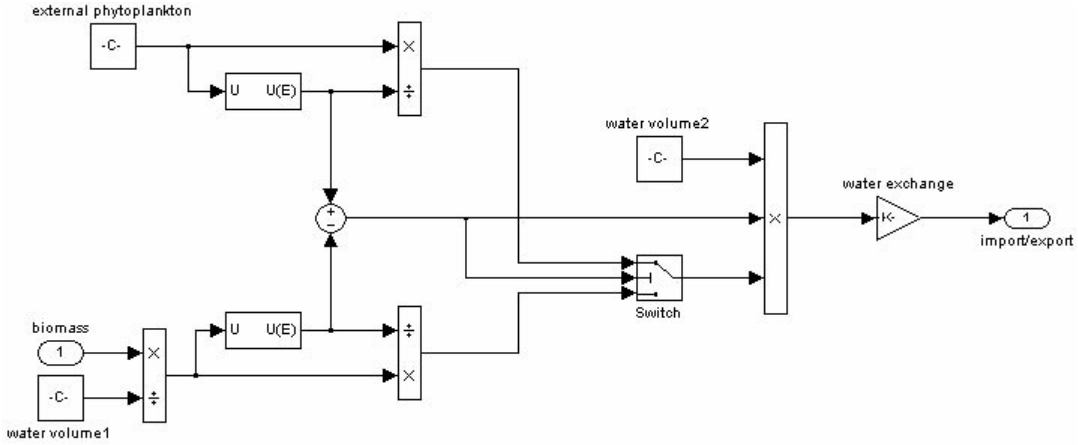

Figure 3-20. *Model compartment for phytoplankton-exchange.*

Table 3-16. Input parameters fro phytoplankton-exchange.

Parameter	Value	Unit
External biomass = Initial mass of phytoplankton	1.06×10^{7}	gC
External biomass = Initial mass of phytoplankton	1.77×10^{6}	gN
External biomass = Initial mass of phytoplankton	1.37×10^{5}	gP
Water volume	1.11×10^{8}	m^3
Water exchange	365	$year^{-1}$

3.6.21 Zooplankton exchange (exchanger)

Variables

Biomass: biomass of zooplankton

Import/export: export of zooplankton

Equations

Import/export:

import/export = water volume × a × b × water exchange

a = external biomass[1] – (biomass/water volume)[1]

b = switch (1, 2, 3)

1 = external biomass/external biomass[1]

2 = external biomass[1] – (biomass/water volume)[1]

3 = (biomass/water volume)/(biomass/water volume)[1]

- switch: Pass through input 1 when input 2 is ≥ 0; otherwise, pass through input 3. The input 1 pass-through criterion are input 2 greater than or equal, greater than, or not equal to the threshold. The first and third input ports are data ports, and the second input port is the control port. The threshold is ≥ 0.

Table 3-17. Input parameters for zooplankton exchange.

Parameter	Value	Unit
External biomass = Initial mass of zooplankton	1.25×10^{6}	gC
External biomass = Initial mass of zooplankton	$3{,}21\times10^{5}$	gN
External biomass = Initial mass of zooplankton	$2{,}25\times10^{4}$	gP
Water volume	1.11×10^{8}	m^3
Water exchange	365	$year^{-1}$

3.7 Modelling results

3.7.1 Carbon dynamics

As a consequence of the shallow hypsography in the analysed area more than half of the total biomass (53%) is found in the phytobenthic community, 39% in the soft bottom community and 8% in the pelagic community (Figure 3-21). The distribution of biomass between producers and consumers, i.e. flora and fauna is equal. A comparison of the biomass present in the various modelled compartments reveals large differences. Macrophytes and benthic macrofauna dominate the biomass and make up almost 40% each and the microphytes approximately 10% of the total biomass (Figure 3-22).

The storages and flows of carbon in the system at steady-state are shown in Figure 3-23. The system is self-sufficient with regard to carbon since the total production of biomass is larger than the total consumption. The excess of produced carbon causes a net export of organic carbon from the area corresponding to almost 10% of the annual primary production. It is the phytobenthic community that contributes to the major part of the production (73%) but only 21% of the consumption. The main part of the consumption is taken care of by organisms in the soft bottom community (72%) and the rest by pelagic organisms (7%). The most significant carbon flow in the system is the export of biomass produced in the phytobenthic and pelagic communities down to the soft bottom and away from the area.

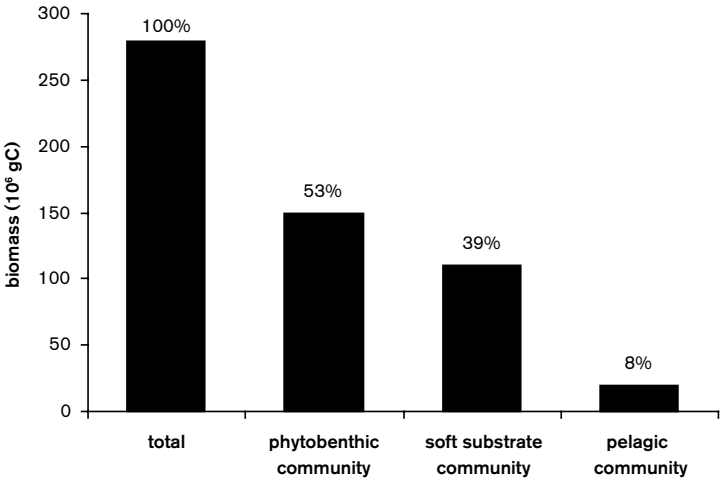

Figure 3-21. *Amount (10^6 gC) and proportion (%) of total biomass between communities in the study area above the final repository of radioactive operational waste (SFR) in Öregrundsgrepen (Baltic Sea). The phytobenthic community comprises benthic plants, grazers, filter feeders, benthic micro- and meiofauna, the soft substrate community filter feeders, benthic macro-, meio- and microfauna, and the pelagic community phytoplankton, zooplankton and fish.*

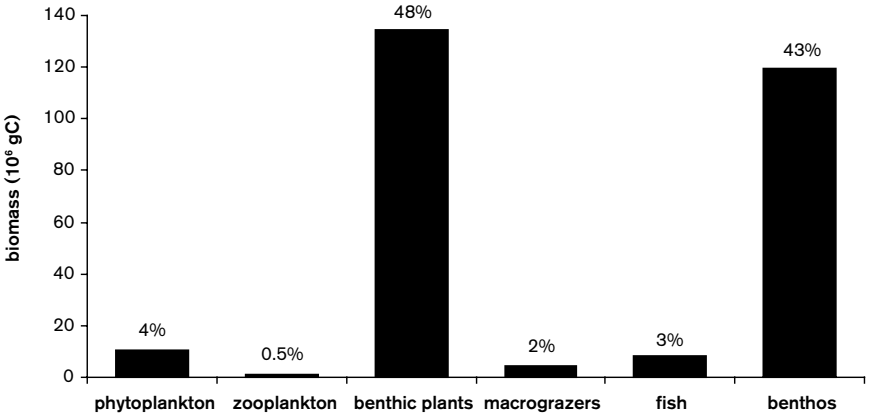

Figure 3-22. *Amount (10^6 gC) and proportion (%) of total biomass between compartments in the study area above the final repository of radioactive operational waste (SFR) in Öregrundsgrepen (Baltic Sea).*

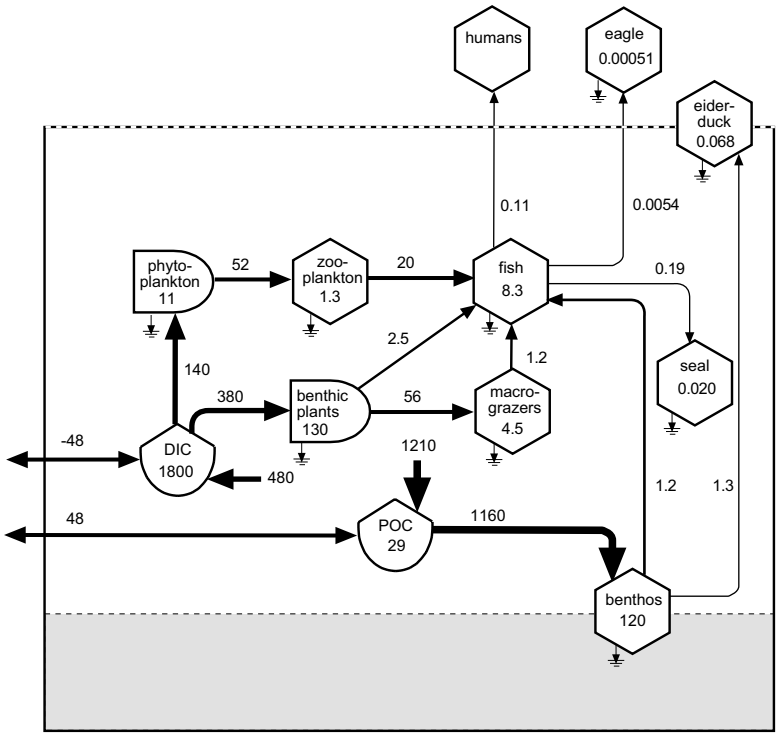

Figure 3-23. *Distribution (10^6 gC) and annual flux (10^6 gC/year) of carbon in the study area above the final repository of radioactive operational waste (SFR) in Öregrundsgrepen (Baltic Sea).*

3.8 Model verification

The Baltic Sea is a thoroughly investigated area and therefore, a considerable amount of information on the structure and function of food webs and ecosystem dynamics exists /e.g. Elmgren and Hill, 1997; Jansson, 1997; Kautsky and Kautsky, 2000; Wulff et al. 2001/. Moreover, the brackish Baltic Sea is poor in species compared to fully marine areas (owing to the low saline conditions, 2–10 PSU) /Elmgren and Hill, 1997/, which enabled the establishment of a carbon budget that provided good quality initial data for the model. The carbon budget established in this study was compared with budgets for adjacent areas /McKellar and Hobro, 1976; Jansson and Wulff, 1977; Ankar and Elmgren, 1978; Jansson et al. 1982; Larsson et al. 1986; Kautsky, 1995; Sandberg et al. 2000/ and showed mostly good compliance with the magnitudes of storages and flows. Deviations were found for benthic macrofauna, where biomasses were five times lower in this budget, and the compartments of the pelagic system, which also were lower in this budget. The observed differences in the pelagic compartment between this study and the budgets assembled by /McKellar and Hobro, 1976/ and /Larsson et al. 1986/ can probably be explained by differences in the time scale. The studies used for validation focused on the pelagic dynamics during the spring bloom, while this budget is an annual mean of biomass and metabolic rates. All other compartments showed good agreement with the compared studies, with respect to both storages and flows of carbon.

3.9 Conclusions

The carbon dynamics is in this area constrained by the amount of nitrogen and phosphorous available for primary production. These results originate form the development phase of the CNP-model which not was described in this report, but elsewhere /Kumblad and Kautsky, 2004/. However, since constraints of ecological processes probably are of major importance for the fate of potentially released radionuclides to the ecosystem this is stated in this section anyway.

The distribution and fluxes of the carbon in the ecosystem estimated from the CNP-model shows that the phytobenthic community dominate both the biomass and primary production of the modelled ecosystem, whereas the major part of the consumption takes place in the soft bottom (50%) and pelagic community (40%). The most significant carbon flows in the system was found to be the export of excess carbon produced in the phytobenthic community to the soft bottom community and away from the area through water movements.

4 The C14-model

4.1 Overview of the C14-model

The C14-model is based on the CNP-model to which a hypothetical point source discharge of C-14 to the system was added. The C-14 transport in the system was modelled to follow the flow of stable carbon isotopes in the ecosystem, i.e. as C in the CNP-model.

4.2 Model assumptions (C14-model)

- The discharged C-14 was assumed to enter the ecosystem via groundwater flow through the sediment and to be bioavailable and inorganic, i.e. as $^{14}CO_2$, $H^{14}CO_3^-$ or $^{14}CO_3^{2-}$.
- The C-14 isotope was assumed to have the same chemical properties as other carbon isotopes and thus assimilated and circulated in the ecosystem as other carbon isotopes do, i.e. no fractionation.

4.3 Construction of the C14-model

The C-14 source was linked both to the DIM-compartment (which in this model is referred to as the DIC compartment) and directly to the benthic plants (to enable simulations of different uptake pathways). The uptake of C-14 in the primary producers (U_{C-14}) was modelled to be in proportion of the amount of C-14 compared to stable carbon in the DIM-compartment (DIC-14/DIC) and the rate of primary production (PP) (Eq 13).

$$U_{C-14} = \left(\frac{C_{DIC-14}}{C_{DIC}} \right) \times PP \tag{13}$$

The transfer of C-14 further up in the food web was modelled to be equivalent to the carbon flow, i.e. C-14-concentrations in the compartments were a function of the consumption rate and the ratio of C-14 to carbon in their food source. The respiration of C-14 was determined by the respiration rate of the compartment and its C-14-concentration. Consumption of C-14 containing food by eagles, eider ducks and seals was also modelled assuming that eagles and seals presumably eat fish and that eider ducks consume benthos. Eagles and seals were modelled for only one individual for the area while eider ducks were modelled at the level of population. Estimations of the C-14 intake by humans consuming contaminated fish from the area were also performed for simulation A. C-14 in water (DIC-14 and POC-14) and the phyto- and zooplankton compartments were also connected to the water exchange to model the C-14 export. The C-14-concentration in these compartments was thus dependent on the total water volume and the retention time of the water.

4.3.1 $^{14}CO_2$ exchange over the air-sea interface

The air-sea exchange of carbon dioxide in the model area was estimated to an annual uptake of 1.2×10^8 gC per year for the whole area, which is an amount that corresponds to approximately 9% of the annual primary production. This estimation was based on

calculations of the carbon dioxide exchange over the air-sea interface of the Baltic proper /Thomas and Schneider, 1999/. The uptake of carbon dioxide was considered in the modelling of C-14.

4.3.2 Water exchange

The continuous water exchange in the area was modelled by subtracting the amount of C-14 in the compartments that are affected by the water exchange (DIC, POC, phytoplankton and zooplankton), and adding the same amount of carbon as many times as the water was exchanged per year.

4.3.3 Calculations of concentrations in biota

Results both from the carbon flow model and the C-14 flow model were used to calculate carbon-normalised C-14-concentrations (Bq/gC) of the compartments. To transform the amount of C-14 from mass to radioactivity, the conversion factor 1.29×10^{10} Bq/gC-14 was used.

4.4 Model simulations; analyses of uptake pathways and water exchange rates

The implications of changes in uptake pathway for C-14 and water exchange rate on the C-14 fate in the ecosystem were explored in four different model simulations (A to D, Table 4-1).

The influence of uptake pathway was analysed by comparing simulation A and B which have different uptake pathways but constant water exchange rate. In simulation A, C-14 was assumed to enter the system in the aphotic zone and thus be taken up homogenously by all plants in proportion to their primary production rate and the C-14 content in the DIC-compartment. In simulation B, C-14 entered the system in the photic zone and was therefore taken up by benthic plants directly from the discharge (and not diluted in the DIC-compartment).

The influence of water exchange rate was examined by comparing simulation A, C and D, which have constant uptake pathway but varying water exchange rates. In simulation A, normal water exchange was used 365 times per year /Engqvist and Andrejev, 1999/, while in simulation C and D, the normal water exchange rate was reduced by a factor of 10 and 100.

Table 4-1. Description of the model simulations made for analyses of the influence of uptake pathway and water exchange rates on the C-14 dynamics in the system.

	Simulation A	Simulation B	Simulation C	Simulation D
Discharge zone	aphotic	photic	aphotic	aphotic
C-14 uptake by	all plants	by benthic plants	all plants	all plants
Water exchange	normal	normal	reduced by 10	reduced by 100

The motivation to examine the uptake pathway is that the relative importance of benthic versus pelagic primary production as the vector for C-14 entry into the food web may vary. It is known that incorporation of carbon into the marine food web mainly occurs via photosynthetic uptake, by the primary producers of free CO_2 and bound CO_2 (in the form of bicarbonate and carbonate) /Lalli and Parsons, 1993/ and that macro algae (e.g. *Fucus vesiculosus*) and benthic micro algae (e.g. diatoms) are important primary producers in shallow areas of the Baltic Sea /e.g. Kautsky and Kautsky, 1995/. However, the importance of the benthic primary producers for C-14 assimilation in the food web will depend on where the discharge of C-14 occurs (e.g. in or below the photic zone). C-14 discharges in the photic zone were in the model imposed to be assimilated by benthic primary producers (since discharges enter the system through the sea bed where benthic plants are located) whereas discharges elsewhere in the system were imposed to be assimilated by both benthic and pelagic primary producers.

The effect of water exchange was analysed because this process may greatly affect the export of C-14 from the area, and since post-glacial land-rise is expected to dramatically change water movements in the area within the 2,000-year modelling period /Engqvist and Andrejev, 2000/. In fact, the modelled area is expected to evolve from being located in a sound to a bay and finally after about 3,000 years in a lake /Brydsten, 1999/.

All four simulations were run for a period of 2,000 years with a constant annual C-14 discharge of 51.3 MBq per year during the first 1,000 years. The discharge rate was the best estimate of the average annual discharge from the repository in case of a leakage /Lindgren et al. 2001/.

4.5 Modelling results

4.5.1 Time course and fate of ^{14}C-contamination

When open dynamic systems are contaminated at a constant rate it will take some time before the concentration of the system components and the whole ecosystem reaches steady-state. Similarly, if the contamination input ceases, the ecological half-life of the contaminant may differ among compartments. Knowledge of the kinetics of pollutants in ecosystems can be used to improve design and interpretation of monitoring studies, environmental assessment etc., e.g. by identifying compartments where the magnitude of the contamination first can be assessed and if the system has reached steady-state. In Table 4-2, estimations of the uptake and elimination kinetics of C-14 in the compartments and the whole ecosystem for all simulations are showed.

In all simulations, both the ecosystem half-life of C-14 and the steady-state in the ecosystem was reached within a year. The overall pattern was that all compartments except benthic plants, fish, seal and eider ducks exhibited prolonged times to reach steady-state in B compared to A. This time lag was caused by the need for re-circulation of C-14 (uptake followed by transfer of excess of C-14 to the DIC-14 compartment) in the benthic food chain prior to uptake in the pelagic compartments. The ecological half-life of C-14 in the ecosystem also increased for many compartments at benthic uptake. Decreased water exchange by a factor ten (simulation C) did not lengthen the ecological half-life of the system although benthic plants and POC were slightly affected. However, when the water exchange was reduced by a factor hundred (simulation D) the time to reach steady-state for the system was longer than in simulation A. Most compartments reached steady-state within a year in simulation A. Pelagic compartments, such as DIC, phytoplankton and zooplankton were quickest, while for instance fish and fish consuming organisms needed longer time.

The same pattern of variation of the ecological half-life as for time to reach steady-state for the compartments can be seen among all simulations.

Table 4-2. Time to reach steady-state concentrations of C-14 (year) and ecological half-life of C-14 (year) in the compartments and the ecosystem for simulation A, B, C and D (defined above).

	Simulation A (year)	Simulation B (year)	Simulation C (year)	Simulation D (year)
Time to reach steady-state concentrations				
Phytoplankton	< 1	~ 1	< 1	< 1
Benthic plants	< 1	< 1	< 1	> 1
Zooplankton	< 1	~ 1	< 1	< 1
Macrograzers	< 1	~ 1	< 1	> 1
Benthos	~ 1	~ 1	~ 1	> 1
Fish	> 1	> 1	> 1	> 1
Seal	> 1	> 1	> 1	> 1
Eider duck	~ 1	~ 1	~ 1	> 1
Eagle	> 1	> 1	> 1	> 1
POC	< 1	< 1	< 1	> 1
DIC	< 1	~ 1	< 1	< 1
Ecosystem	< 1	< 1	< 1	< 1
Ecological half-life				
Phytoplankton	< 1	~ 1	< 1	< 1
Benthic plants	< 1	< 1	~ 1	~ 1
Zooplankton	< 1	~ 1	< 1	< 1
Macrograzers	~ 1	~ 1	~ 1	> 1
Benthos	~ 1	~ 1	~ 1	> 1
Fish	~ 1	~ 1	~ 1	> 1
Seal	~ 1	~ 1	~ 1	> 1
Eider duck	~ 1	~ 1	~ 1	> 1
Eagle	~ 1	~ 1	~ 1	> 1
POC	< 1	< 1	~ 1	> 1
DIC	< 1	~ 1	< 1	< 1
Ecosystem	< 1	< 1	< 1	< 1

Since the developed model was of mass balance type, where the dynamics of both carbon and C-14 was modelled, it was possible to analyse the distribution and flow of the discharged C-14 in the whole system. Figure 4-1 shows the steady-state distribution of C-14 between the compartments and the transfer in the food web for simulation A. Since the modelled area is characterized by a high water exchange rate (less than one day), more than 99% of the discharged C-14 was flushed out of the system immediately. The loss of C-14 to the atmosphere is negligible due to the net uptake of carbon at the air-sea interface. About 0.05% of the C-14 was also assimilated by primary producers, which enabled subsequent transfer of C-14 to organisms at higher trophic levels (e.g. zooplankton, fish and seals). Approximately 10% of the assimilated C-14 was annually re-circulated within the system via the respiration route and 74% was retrieved in excess from biota of which almost 90% was exported from the system via exchange of POC. About 12% of the C-14 inflow to POC was consumed annually by benthos. The exported matter is expected to dilute to much lower concentrations in the larger recipient outside /Karlsson et al. 2001/.

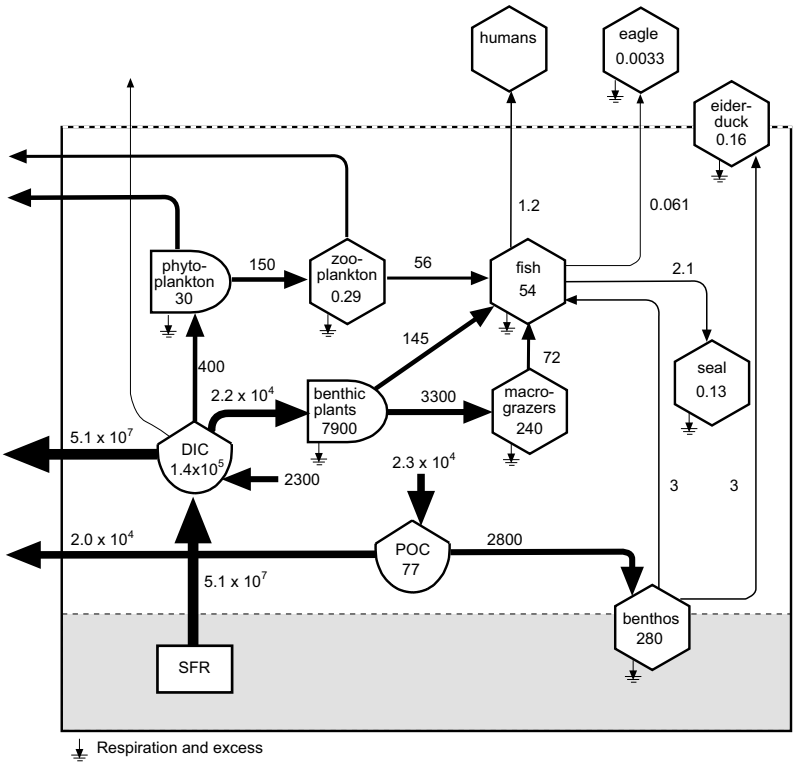

Figure 4-1. *Distribution (Bq) and annual flux of C-14 (Bq/year) of an annual discharge of 51.3 MBq C-14 per year into the study area above the final repository of radioactive operational waste (SFR) in Öregrundsgrepen (Baltic Sea), according to simulation A (uptake by all primary producers from the DIC compartment, normal water exchange).*

4.5.2 C-14-concentrations in biota: Influence of biological and environmental factors

As a first step of evaluating the importance of the route of C-14 entry the homogenous uptake by all plants from the DIC-compartment (simulation A) and uptake by benthic plants only (simulation B) were compared. The uptake pathway in simulation A, caused both the lowest and most homogenous concentrations in biota since the isotope was taken up in proportion to the amount of C-14 to carbon in the DIC-compartment (the largest carbon pool in the system) and because the DIC-compartment was affected by the water exchange (Table 4-3). The lowest concentrations were found in phytoplankton and zooplankton because the water exchange both affects the C-14 in the DIC-compartment and the plankton compartments by continuously adding uncontaminated DIC and plankton to the area. The highest C-14 concentrations were found in organisms that were less affected by the water exchange rate, such as benthic plants and macrograzers. All organisms except the plankton compartments received highest concentrations in the simulation with the benthic uptake pathway (simulation B). Benthic compartments (and the compartments consuming benthic organisms) received approximately twice as high concentration when the C-14 was accumulated via the benthic pathway compared to the other uptake pathway, while phytoplankton and zooplankton obtained approximately 10,000 times lower concentrations (Table 4-3). Hence, the route of C-14 entry into the food web can significantly influence the radionuclide exposure of organisms in the coastal zone. This source of uncertainty will need to be considered when assessing C-14 contamination of aquatic ecosystems.

Table 4-3. C-14 concentrations of the compartments (µBq/gC; mBq/gC) and in the water (µBq/l; mBq/l) for simulation A, B, C and D (defined above).

	Simulation A (µBq/gC (l))	Simulation B (mBq/gC (l))	Simulation C (mBq/gC (l))	Simulation D (mBq/gC (l))
Phytoplankton	2.8	1.9×10^{-4}	0.21	6.1
Benthic plants	58	100	0.58	5.5
Zooplankton	0.23	1.6×10^{-5}	0.10	5.3
Macrograzers	53	90	0.53	5.0
Benthos	2.4	4.0	0.19	5.9
Fish	6.5	11	0.13	3.9
Seal	6.5	11	0.13	3.9
Eider duck	2.4	4.0	0.19	5.9
Eagle	6.5	11	0.13	3.9
DIC	79	5.5×10^{-3}	0.79	7.7
POC	2.7	4.5	0.21	6.7
Water	1.3	1.3×10^{-3}	0.013	0.13

When it comes to influence of water exchange rate, the model simulations A, C and D showed that the larger the water exchange in the area is, the quicker C-14 is removed. The concentrations in the modelled compartments were affected to various extents by the water exchange (Table 4-3). Zooplankton was the most affected compartment since water exchange both contributes to a dilution of C-14 in the zooplankton compartment itself as well as in its food source (phytoplankton). Benthic plants and macrograzers were least affected by the water exchange since they are associated to the seabed. The extent the water exchange influenced the remaining compartments mirrored their location in the ecosystem (habitat), their trophic level and how their food sources were affected by water exchange. Reduced water exchange also extended the time needed for the compartments to reach steady-state as well as slowed down the elimination rate of the isotope (Table 4-3). This is because the amount of C-14 available for re-uptake was larger at reduced rates of water exchange due to a slower DIC transport from the area. Disparities in the C-14-concentrations in bottom dwelling and pelagic compartments increased when the water exchange decreased (Table 4-3). For instance, the concentration in benthic plants was 13% higher than in fish at normal water exchange and 31% higher when the water exchange was reduced by a factor ten. Changes in water exchange will profoundly influence the C-14 dynamics in the studied aquatic ecosystem.

There are several other biological and environmental variables than water exchange rate and uptake pathway that may influence the structure and function of the studied ecosystem and the dynamics of radionuclides, especially over the long time perspective considered in this study. For instance, only since the turn of the last century, the carbon flows of the Baltic Sea has been influenced by human activities such as eutrophication, increased exploitation of the resources of the sea and release of pollutants /Elmgren, 1989; 2001/. Furthermore, human-aided introductions of new species to the Baltic Sea have significantly altered the ecosystems of some Baltic coastal lagoons in terms of e.g. changes in physical and functional diversity, increases in bentho-pelagic linkages, and broadening of the food base for fish and retaining of river input /Olenin and Leppäkoski, 1999/. Probably, environmental changes in e.g. salinity or temperature would shift the ecosystem structure of the bay described in our model. For instance, an increase in salinity would favour the occurrence of the filter-feeding blue mussel, Mytilus edulis, which is almost absent in the area today /Kautsky et al. 1999/. An increased blue mussel population would significantly alter the function of the system by consumption of phytoplankton, which would compete with the pelagic grazing food chain.

The variables examined in this study, i.e. uptake pathway and water exchange rate, are chosen because they are considered as two of the most important in the time-perspective of 2,000 years. Within the long time-period during which contamination from the waste repository may occur (1,000 years or longer), the largest source of environmental change for the modelled site is likely to be the shoreline displacement due to land-rise /Kautsky, 2001/, which significantly will influence the water retention time /Engqvist and Andrejev, 2000/. The entry pathway was analysed because it is crucial for the subsequent fate of the radionuclide in the system.

4.6 Model verification

Validation is a process that tests selected parameters with an independent set of data /Jørgensen, 1994/. Since this model is a predictive long-term assessment model of a nuclear waste it cannot be strictly validated. However, the distribution of C-14 in the compartments according to the model was compared with field measurements of C-14 in biota and water around the Sellafield reprocessing plant in Great Britain /Cook et al. 1998/. When comparing ratios of concentrations in biota and water to the annual amount of discharged C-14 to the water, this C14-model generates slightly lower ratios for fish and benthic organisms as well as in the water (DIC), but higher in seaweed (Table 3-3). This might be due to the high water exchange rate in the study area or the high abundance of benthic primary producers, which are able to accumulate an extensive amount of discharged C-14 /Lalli and Parsons, 1993; Cook et al. 1998/.

4.7 Conclusions

The C-14 model analysed and numerically described the transport and fate of discharged C-14 in the whole ecosystem, i.e. both in the physical environment and in the food web. For example, the established model generated (i) estimates of the time required to reach steady-state and the ecological half-life, (ii) estimates of the rates of C-14 transport (between compartments, re-circulated within the system, sedimentation, and across the system boundaries), and (iii) estimates of the amounts and concentrations of C-14 found in the modelled environmental and biological compartments. Apart from generating estimates of the fate and persistence of hypothetical C-14 releases, the developed model also evaluated the implications of changes in environmental and ecological factors on ecosystem behaviour of C-14.

Steady-state conditions of C-14 were reached in the system after about 4 to 9 months at normal water exchange conditions, depending on which zone in the system C-14 was discharged to and the uptake pathway. The ecological half-life of C-14 in the compartments/ ecosystem was approximately 20 days for the aphotic discharge zone and uptake by all plants and about three times as long due to the opposite release situation. Reduced water exchange lead both to longer periods to reach steady state concentrations and to an extended ecological half-life.

During normal water exchange conditions and C-14 discharge to the apothic zone, more than 99% of the discharged C-14 was flushed out from the system immediately and only 0.2% was assimilated into plants. Approximately 5% of the assimilated C-14 was annually re-circulated within the system via respiration and 74% was retrieved in excess from biota. Almost 90% of this was exported from the system via POC-exchange, while the rest was consumed by benthos or buried into the sediment.

The maximum C-14 concentrations were found in organisms that were less affected by the water exchange rate, such as benthic plants and macrograzers. All organisms except plankton received highest concentrations in simulations with the benthic uptake pathway. The concentrations increased with reduced water exchange. Even in the most pessimistic simulation the concentrations in the most exposed organisms (100 mBq/gC – benthic plants) were far below the background levels.

The implications of route of C-14 entry into the food web significantly influenced the modelled radionuclide exposure of the organisms. The water exchange rate had also a very large influence of the fate of C-14 in the system. The modelling analysis showed that this process had the largest influence on the C-14 fate. The extent, to which the water exchange influenced different organisms, mirrored their location in the food web and how their food sources were affected by the water exchange.

5 The generic radionuclide model

The RN-model is driven by carbon in the CNP-model to which a hypothetical point source of radionuclides was connected. The RN-flow was modelled to follow the flow of organic matter but radionuclide specific mechanisms such as radionuclide uptake by plants, excretion of radionuclides by animals and adsorption of radionuclides to organic surfaces are connected to the CNP-model that handles the differences between the dynamics of carbon and the radionuclides.

5.1 Model assumptions (RN-model)

- The uptake of radionuclides by plants was assumed to be proportional to their photosynthetic rate, but the plants were assumed to have the ability to actively discriminate or enhance the uptake of the radionuclides compared to the carbon uptake.
- The main radionuclide uptake by animals was assumed to be via ingestion of contaminated food (and not by diffusion).
- It was assumed that all consumers could actively excrete or store radionuclides after uptake via consumption.
- It was assumed that radionuclides could adsorb to organic surfaces and that the adsorption was equal to all organic surfaces (e.g. same on organism surfaces and particulate material).
- The surfaces of particles and organisms were estimated by assuming that they had spherical or cylindrical form with radiuses according to Table 5-4. (These calculations were made to enable estimations of consumption of radionuclides adsorbed to organic surfaces.)

5.2 Construction of the RN-model (a theoretical description)

The uptake and excretion of radionuclides to biota and particulate matter was driven by carbon from the CNP-model (section 3). To the carbon flow four radionuclide specific mechanisms were added.

5.2.1 Radionuclide uptake in primary producers

The radionuclide uptake by plants, X_{in} (Bq/yr), was modelled with plant uptake coefficients that were defined to be proportional to bioconcentration factors (BCF) for plants according to:

$$X_{in} = C_{in} \times \frac{C_{DIM}}{V} \times \frac{X_{DIM}}{C_{DIM}} \times K_{BCF} \qquad (14)$$

where,

C_{in} was the rate of primary production (gC/yr),

C_{DIM} was the amount of carbon in the water (gC),

V was the volume of the water (m^3),

X_{DIM} was the amount of dissolved radionuclides in the water (Bq), and

K_{BCF} was the plant uptake coefficient (m^3/gC).

Calculation of K_{BCF}

Bioconcentration factors (BCFs) found in the literature are often defined as the ratio of the concentration of radionuclide in the organism (Bq/kg wet weight) to the concentration of the radionuclide in the water (Bq/l), i.e. l/kg wet weight. Consequently, the BCF values for plants include radionuclides in the organism obtained from diffusion, absorption and adsorption. To obtain BCFs for plant uptake applicable for this system, BCFs from the literature /IAEA, 1985/ were converted into plant uptake coefficients (K_{BCF}, m^3/gC), by converting the volume into cubic metres and the biomass into gram carbon. The wet weights to carbon weight ratios used were 0.033 kg wet weight/gC for phytoplankton and 0.018 kg wet weight/gC for benthic plants /compiled in Kautsky, 1995/.

5.2.2 Radionuclide uptake in consumers

The total intake of radionuclides to consumers, X_{in} (Bq/yr), was calculated according to:

$$X_{in} = X_{in\,int} + X_{in\,ext} \tag{15}$$

where,

$X_{in\,int}$ was the intake of internally stored radionuclides of prey (Bq/yr),

$X_{in\,ext}$ was the intake of externally stored radionuclides on prey (Bq/yr).

The intake of radionuclides stored inside the prey ($X_{in\,int}$) was assumed to be proportional to the consumption (intake of carbon) and the radionuclide concentration in the prey according to:

$$X_{in\,int} = C_{in} \times \frac{X_{prey}}{C_{prey}} \tag{16}$$

where,

C_{in} was the carbon consumption (gC/yr),

X_{prey} was the amount of radionuclide in the food source (Bq), and

C_{prey} was the carbon content in the prey (gC).

The intake of radionuclides externally stored or adsorbed to the surfaces of the preys ($X_{in\,ext}$) was calculated according to:

$$X_{in\,ext} = \frac{C_{in}}{C_{prey}} \times X_{surf\,org} \tag{17}$$

where,

C_{in} was the consumption rate (gC/yr),

C_{prey} was the carbon content of prey (gC), and

$X_{surf\,org}$ was the radionuclides adsorbed to surface of prey (Bq) (see below).

5.2.3 Excretion of radionuclides by consumers

The radionuclide excretion by animals was modelled with an excretion coefficient, K_e (Bq gC^{-1}). This mechanism was designed to enable evaluation of the effect of excretion over a range from retention ($K_e < 1$) to active excretion of the radionuclide ($K_e > 1$). Radionuclides with similar retention properties as carbon would have a K_e close to 1. The excretion of radionuclides, X_{out} (Bq yr^{-1}), was calculated according to:

$$X_{out} = C_{out} \times K_e \tag{18}$$

where,

C_{out} was the excretion of carbon (gC/yr), i.e. respiration, and

K_e was the excretion coefficient (Bq/gC).

Excretion coefficients in the range 0 to 2 were analysed in this study. The maximum excretion coefficient was arbitrary chosen as a high excretion coefficient (excretion at the double rate compared to carbon respiration), whereas the lowest represent cases where all ingested radionuclides were retained within the organism.

5.2.4 Radionuclide adsorption to organic surfaces

The total radionuclide adsorption to organic surfaces, $X_{surfaces}$ (Bq), was calculated according to:

$$X_{surfaces} = \frac{\frac{X_{DIM}}{V} \times K_{dPOM}}{K_{SC\ for\ POM}} \times S_{total} \tag{19}$$

where,

X_{DIM} was the amount of radionuclide in the water (Bq),

V was the volume of the water (m^3),

K_{dPOM} was the distribution coefficient for POM (m^3/gC, see below),

$K_{SC\ for\ POM}$ was the surface to carbon content ratio for POM (m^2/gC, see below), and

S_{total} was the total area of POM and organisms in the area (m^2, see below).

The surface-associated radionuclides were distributed between organisms ($X_{surf\ org}$, Bq) and POM ($X_{surf\ POM}$, Bq) according to:

$$X_{surf\ org} = K_{ads} \times S_{org} \tag{20}$$

$$X_{surf\ POM} = K_{ads} \times S_{POM} \tag{21}$$

where,

K_{ads} was a surface specific association constant (Bq/m^2, see below),

S_{org} was the surface of the organisms (m^2, see below), and

S_{POM} was the surface of POM (m^2, see below).

Since the radionuclides associated to the surfaces of plants already is accounted for in the plant BCF values, no additional radionuclide adsorption to plant surfaces was included in the model calculations.

Calculation of K_{dPOM}

K_{dPOM} ($m^3\ gC^{-1}$) was a distribution coefficient that was adapted to our system from literature values of K_d (m^3 kg dry weight^{-1}) /IAEA, 1985/ by converting the mass into gram carbon. The dry weights to carbon content ratios for POM used were 0.006 kg dry weight gC^{-1}.

Calculation of K_{ads}

The partitioning of radionuclides in solution and attached to surfaces are often described with a distribution coefficient, K_d (m^3 kg dry weight^{-1}), which mostly is derived empirically according to:

$$K_d = \frac{\left(\frac{X_{POM}}{M_{POM}}\right)}{\left(\frac{X_{DIM}}{V}\right)} \qquad (22)$$

where,

X_{POM} was the amount of radionuclides in the particulate fraction (Bq),

M_{POM} was the mass of the particulate fraction (kg dry weight),

X_{DIM} was the amount of dissolved radionuclides in the water (Bq), and

V was the volume of the water (m^3).

Solving for the radionuclide concentration in the particulate fraction (X_{POM}) gives:

$$\frac{X_{POM}}{M_{POM}} = K_d \times \frac{X_{DIM}}{V}$$

A surface to volume ratio for particulate matter (K_{svPOM}) was calculated according to the following assumptions:

- the carbon content of particulate matter is 30 g wet weight/gC (7 g dry weight/gC),
- an average particle is spherical and has a radius of 25 μm,
- the density (δ) of POM is 1 g wet weight/cm^3 (0.23 g dry weight/cm^3, 0.03 gC/cm^3).

This gave the following estimations:

- area of an average particle: 7,850 μm^2,
- average volume of an average particle: 65,400 μm^3,
- amount of particles in the area: 1.3×10^{16},
- area and volume of all particles in the system: 104 km^2 and 867 m^3,
- surface to volume ratio for POM (K_{svPOM}): 1.2×10^5 m^2/m^3,
- surface to carbon content ratio for POM (K_{scPOM}): 3.6 m^2/gC.

These assumptions and calculations allowed us to derive radionuclide specific adsorption coefficients (K_{ads}, Bq/m^2) that were proportional to distribution coefficients for organic matter (K_{dPOM} m^3/gC) but related to the amount of surfaces possible to attach to, rather than the weights of the particles:

$$K_{ads} = \frac{K_{dPOM}}{K_{svPOM}} \times \frac{X_{DIM}}{V} \times \delta \quad (23)$$

Surface calculations

To enable estimations of the total surface area of the organisms, a weighed average for the surface area was calculated for each compartment. Sampling data expressing abundance and biomass was used /Jansson et al. 1982/. The average individual weight of each taxonomic entity was calculated by dividing the total biomass with the number of individuals. The organisms were assumed to have a density of 1g wet weight/cm^3 and to have a spherical or cylindrical form with a radius according to Table 5-4. In addition to the body surface for fish the gills has considerable surface area, which was calculated according to /Wootton, 1998/.

5.2.5 Radionuclide decay

The radionuclide decay, X_{decay} (Bq/yr), was calculated according to:

$$X_{decay} = X_{comp} \times \lambda \quad (24)$$

$$\lambda = \frac{\ln(2)}{T_{1/2}} \quad (25)$$

where,

λ was the decay constant (yr^{-1}),

$T_{1/2}$ was the half-life of the radionuclide (yr), and

X_{comp} was the radioactivity of the compartment (Bq).

5.3 Construction of the RN-model (a description of the Simulink model)

Since the RN-model is based on the CNP-model and thus has almost the same structure of the Simulink compartments, only the differences from the CNP model is described below.

5.3.1 Dissolved inorganic and Particulate organic matter (DIM and POM)

The reservoir compartments DIM and POM only differ from the corresponding compartments in the CNP-model in terms of three equations. Also, the import/export variable in the POM compartment in the CNP-model is lacking in the POM compartment in the RN-model.

Equations

Content of matter in DIM

mass = inflow – outflow – surface exchange – decay

Outflow from DIM

outflow = c × minimum of (requested[1], mass[1]) × (((mass[1]/water volume) × BCF) muxed with a constant (signal 1 becomes 1 in the vector))

- requested = requested demand of DIM by primary producers
- BCF = Bioconcentration factor

Outflow from POM

outflow = minimum of (inflow [1] + mass [1]) × c

Table 5-1. Input parameters.

Parameter	Value	Unit
BCF	see Table 5-3	kg wet weight^{-1}
Water volume	1.11×10^8	m^3

5.3.2 Phytoplankton

Equations

Demand of DIM by phytoplankton

Dedim of DIM = (light × kprod × biomass)[1] × ratioCNPX

- kprod = phytoplankton productivity coefficient
- ratioCNPX = ratio of carbon, nitrogen, phosphorus and radionuclides (X)

5.3.3 Consumer compartments (general for all consumers)

The compartments for consumers (i.e. zooplankton, grazers, fish, and benthos) in the generic radionuclide model differ from the consumer compartments in the CNP model in three aspects: there is no resex-block and the biomass- and excess equations are different.

Equations

Biomass

biomass = consumption – faeces – respiration – decay – (predation[1] × concentration) + import/export – excess

Excess

excess = ((consumption – faeces – respiration – decay – (predation[1] × concentration) + biomass)[1] – max biomass) × concentration

5.3.4 Exchangers

In the generic radionuclide model the equation for import/export of matter in the exchangers for POM, phytoplankton and zooplankton differs from corresponding equations used in the CNP-model.

Equations

Import/export = (external level – biomass) × water exchange

- biomass of the compartment

5.3.5 Radionuclide surface associatior

In the generic radionuclide model, four compartments (grazers, zooplankton, benthos and POM) have a module that adds particle reactive radionuclides to the surface of the organisms/matter in the compartment. The surface associated radionuclides are then assumed to be a part of the organism and will thus become transferred to the next trophic level when predated.

Variables

Sass: surface associated radionuclides (comes from SURFACER in surface subsystem).

Predation: predation of grazers/zooplankton/benthos or POM by fish or benthos.

Biomass: biomass of grazers/zooplankton/benthos or POM.

Predation of internal associated RNs: amount of radionuclides in predation that originates from internal radiation (= within prey/matter).

Predation of external associated RNs: amount of radionuclides in predation that originates from external radiation (= on prey/matter).

Equations

Predation of external associated RNs = (sass[2] × (predation [1]/biomass[1])), muxed" with C

- C = constant (= 0)

predation of internal associated RNs = predation + predation of external associated RNs

5.3.6 Surface subsystem

The surface subsystem or SURFACER is function that calculates the amount of surface-associated nuclides.

Variables

RNs in DIM: radionuclides in DIM (mass[2] of DIM).

RNs on surfaces: surfaces associated radionuclides (total).

Phase exchange: exchange of radionuclides between dissolved and particulate phases.

RNs on phytoplankton: surfaces associated radionuclides on phytoplankton.

RNs on benthic plants: surfaces associated radionuclides on benthic plants.

RNs on zooplankton: surfaces associated radionuclides on zooplankton.

RNs on grazers: surfaces associated radionuclides on grazers.

RNs on benthos: surfaces associated radionuclides on benthos.

RNs on POM: surfaces associated radionuclides on POM.

Total organism area: total organism area.

Equations

RNs on surfaces:

$$RNs\ on\ surfaces = \left(\frac{\frac{RNs\ in\ DIM}{total\ water\ wolume} \times Kd_{POM} \times \frac{dw}{C}}{POM\ area} \times total\ organism\ area\right) - RN\ phase\ exchange - (\text{predation of external associated RNs}[2])$$

RNs on phytoplankton:

RNs on phytoplankton = (area phytoplankton/total organism area) × RNs on surfaces

RNs on benthic plants:

RNs on benthic plants = (area benthic plants/total organism area) × RNs on surfaces

RNs on zooplankton:

RNs on zooplankton = (area zooplankton/total organism area) × RNs on surfaces

RNs on grazers:

RNs on grazers = (area grazers/total organism area) × RNs on surfaces

RNs on benthos:

RNs on benthos = (area benthos/total organism area) × RNs on surfaces

RNs on fish:

RNs on fish = (area fish/total organism area) × RNs on surfaces

RNs on POM:

RNs on POM = (area POM/total organism area) × RNs on surfaces

Total organism area:

total organism area = area phytoplankton + area benthic plants + area zooplankton + area grazers + area benthos + area fish + area POM

Table 5-2. Input parameters.

Parameter	Value	Unit
area phytoplankton	2.11×10^{8}	m^2
area benthic plants	1.01×10^{8}	m^2
area zooplankton	1.51×10^{6}	m^2
area grazers	9.03×10^{4}	m^2
area fish	4.34×10^{4}	m^2

Parameter	Value	Unit
area benthos	1.97×10^{5}	m^2
area POM	9.87×10^{7}	m^2
Kd_{POM}	see Table 5-3	–
$POM_{dw\ per\ C}$	7	dw/gC

5.3.7 Radionuclide point source

To the compartment for dissolved inorganic matter a point source compartment is connected. The point source compartment is a constant that provides the model with a release of radionuclides to the model system at each time step (per year). The point source term is vectorised into a signal with a constant (0) to complete the array without simulating an inflow of carbon to the system via the point source release.

5.3.8 Distribution coefficients (K_d) and bioconcentration factors (BCF) used in the simulations

The distribution coefficients (K_d) for coastal areas and bioconcentration factors for marine plants (BCF) used in for the model simulations originated from /IAEA, 1985/ (Table 5-3).

Table 5-3. Distribution coefficients (K_d) for coastal areas (Bq/kg dry weight)/(Bq/m³) and bioconcentration factors (BCF) for marine plants (Bq/kg wet weight)/(Bq/l) used in the model simulations /IAEA, 1985/.

	K_d (m^3/kg dry weight)	BCF (l/kg wet weight)		K_d (m^3/kg dry weight)	BCF (l/kg wet weight)
Ac	2.0×10^{3}	1.0×10^{3}	**Pb**	2.0×10^{2}	1.0×10^{3}
Ag	1.0×10^{0}	2.0×10^{3}	**Pd**	5.0×10^{1}	1.0×10^{3}
Am	2.0×10^{3}	8.0×10^{3}	**Pu**	1.0×10^{2}	2.0×10^{3}
Cl	3.0×10^{-5}	5.0×10^{-2}	**Ra**	5.0×10^{0}	1.0×10^{2}
Cm	2.0×10^{3}	8.0×10^{3}	**Se**	1.0×10^{2}	1.0×10^{3}
Co	2.0×10^{2}	1.0×10^{4}	**Sm**	2.0×10^{3}	3.0×10^{3}
Cs	3.0×10^{0}	5.0×10^{1}	**Sn**	1.0×10^{0}	2.0×10^{4}
H	1.0×10^{-3}	1.0×10^{0}	**Sr**	1.0×10^{0}	5.0×10^{0}
I	2.0×10^{-2}	1.0×10^{3}	**Tc**	1.0×10^{-1}	1.0×10^{3}
Nb	5.0×10^{2}	3.0×10^{3}	**Th**	2.0×10^{3}	2.0×10^{2}
Ni	1.0×10^{2}	2.0×10^{3}	**U**	1.0×10^{0}	1.0×10^{2}
Np	1.0×10^{0}	5.0×10^{1}	**Zr**	1.0×10^{3}	3.0×10^{3}
Pa	5.0×10^{3}	1.0×10^{2}			

5.3.9 Modelling tools and simulation parameters

The model was implemented and simulated in the software Matlab with Simulink (version 7.0/6.0; The Mathworks Inc.). The simulations time unit was year, and each simulation was run from zero to 100 years. This was sufficient to establish steady-state conditions. The radionuclide inflow in all simulations was 1 Bq/yr. The equation solver used in Simulink was ode23t with variable step size. Initial time step was 10^{-100} and step length together with tolerance parameters were all set to auto. Zero crossing detection was not used.

In the simulations, only the element specific properties of the radionuclides were included, thus not the decay of the radionuclides. This has, however, negligible effect on the modelling results since the half-life of most radionuclides of interest for safety assessments of radioactive waste is much longer than the 100 years the model simulations were run for.

5.3.10 Tools used for probabilistic simulations and sensitivity analyses

Probabilistic simulations were undertaken to investigate the effect of uncertainties in parameter estimations of ecosystem parameters. For these analyses the software @Risk was used (version 4.5; Palisade Corporation). In @Risk, it was possible to assign distributions to selected model parameters and obtain statistics from probabilistic simulations where the parameter estimations were randomly sampled from the assigned distributions. The probabilistic simulations presented in this paper were carried out using 10,000 realisations and Latin Hypercube sampling. Thirty input parameters were selected for the probabilistic simulations and their distributions with average and range of variation were assigned according to Table 5-4.

Selected input parameters were correlated to each other according to Table 5-5. Sensitivity analysis using rank correlations was calculated in @Risk. The results express the relative output correlations (–1 to 1) of the input parameters on the model result. Negative output correlations should be interpreted that the output parameter generally is high when the input parameter is low, and vice versa.

Table 5-4. Input parameters for probabilistic simulations and their distributions, average and standard deviations (SD), or minimum and maximum values. All normal distributions were truncated at a small positive value, 10^{-30}. LN = log-normal, N = normal, T = triangular, U = uniform. Averages presented in this table were used as input parameters in deterministic simulations.

Parameter	Distribution	Average	SD or min; max
Phytoplankton biomass (gC/m^3)	LN	1.1×10^{-1}	5.3×10^{-2}
Benthic plants biomass (gC/m^2)	LN	2.3×10^{1}	1.2×10^{1}
Zooplankton biomass (gC/m^3)	LN	1.1×10^{-2}	5.7×10^{-3}
Grazer biomass (gC/m^2)	LN	7.6×10^{-1}	3.8×10^{-1}
Fish biomass (gC/m^2)	LN	7.4×10^{-1}	3.7×10^{-1}
Benthos biomass (gC/m^2)	LN	2.1×10^{1}	1.0×10^{1}
Phytoplankton prod (gC/gC/yr)	LN	1.4×10^{1}	6.8×10^{0}
Benthic plants prod (gC/gC/yr)	LN	2.8×10^{0}	1.4×10^{0}
Zooplankton resp rate (gC/gC/yr)	LN	1.8×10^{1}	9.1×10^{0}
Grazers resp rate (gC/gC/yr)	LN	5.1×10^{0}	2.5×10^{0}
Fish resp rate (gC/gC/yr)	LN	2.2×10^{0}	1.1×10^{0}
Benthos resp rate (gC/gC/yr)	LN	2.2×10^{0}	1.1×10^{0}
Zooplankton cons rate (gC/gC/yr)	LN	3.0×10^{0}	1.5×10^{0}
Grazer cons rate (gC/gC/yr)	LN	3.0×10^{0}	1.5×10^{0}
Fish cons rate (gC/gC/yr)	LN	1.7×10^{0}	8.6×10^{-1}
Benthos cons. rate (gC/gC/yr)	LN	2.9×10^{0}	1.4×10^{0}
Radius phytoplankton (m)	N	5.0×10^{-6}	2.5×10^{-6}
Radius benthic plants (m)	N	1.0×10^{-3}	5.0×10^{-4}
Radius zooplankton (m)	N	5.0×10^{-5}	2.5×10^{-5}
Radius grazers (m)	N	3.5×10^{-3}	1.8×10^{-3}

Parameter	Distribution	Average	SD or min; max
Radius fish (m)	N	5.0×10^{-2}	2.5×10^{-2}
Radius benthos (m)	N	2.5×10^{-3}	1.3×10^{-3}
Radius POM (m)	N	2.5×10^{-5}	1.3×10^{-5}
Zooplankton AE (%)	T	8.0×10^{-1}	min = 1.0×10^{-1}; max = 1.0×10^{0}
Grazer AE (%)	T	8.0×10^{-1}	min = 1.0×10^{-1}; max = 1.0×10^{0}
Fish AE (%)	T	8.0×10^{-1}	min = 1.0×10^{-1}; max = 1.0×10^{0}
Benthos AE (%)	T	8.0×10^{-1}	min = 1.0×10^{-1}; max = 1.0×10^{0}
Fish cons of benthic plants – a	U	–	min = 5.0×10^{-2}; max = 2.0×10^{-1}
Fish cons of benthos – b	U	–	min = 5.0×10^{-2}; max = 2.0×10^{-1}
Fish cons of grazers – c	U	–	min = 5.0×10^{-2}; max = 1.5×10^{-1}
Fish cons of zooplankton	function	–	1 – a – b – c

Table 5-5. Rank correlations of input parameters used in the probabilistic simulations in @Risk. Parameter I was correlated to parameter II with the strength given in column three (1 to 1).

Parameter I	Parameter II	Strength of correlation
Correlation I		
Radius zooplankton	Zooplankton respiration rate	–0.85
Radius grazers	Grazers respiration rate	–0.85
Radius fish	Fish respiration rate	–0.85
Radius benthos	Benthos respiration rate	–0.85
Correlation II		
Zooplankton biomass	Phytoplankton productivity	0.35
Grazers biomass	Phytoplankton productivity	0.35
Fish biomass	Phytoplankton productivity	0.35
Benthos biomass	Phytoplankton productivity	0.35
Zooplankton biomass	Benthic plants productivity	0.35
Grazers biomass	Benthic plants productivity	0.35
Fish biomass	Benthic plants productivity	0.35
Benthos biomass	Benthic plants productivity	0.35

5.3.11 Statistical analyses

To identify input parameter combinations causing non-functioning ecosystems (i.e. biomass ≈ 0 for any organism group) and its underlying factors, statistical analyses including K-means clustering algorithms, SPSS Answer tree and Exhaustive CHAID analyses was used in the software SPSS Base (12.0, SPSS Inc.), and multiple logistic regression in the software Statistica (version 6.0, StatSoft inc.).

5.4 Results and Discussion

The performance, uncertainties and reliability of the model was tested in a series of analyses. These will be presented and discussed in due order. First, probabilistic and sensitivity analysis of caesium (Cs) was used to test the variability related to uncertainties in

ecological input parameters and to identify the strength of correlations between input and output parameters. Then, ecosystem-radionuclide interactions were examined in systematic analysis of the model mechanisms, which also included the overall radionuclide distribution in the ecosystem following a hypothetical point source discharge (exemplified with Cs, Sr and Th). Finally, to verify the model, bioconcentration factors (BCFs) calculated from modelling results from this study were compared to empirically derived BCFs /IAEA, 1985/.

5.4.1 Probabilistic simulations for caesium (Cs)

In the probabilistic simulations for caesium (Cs), approximately 77% of the randomly sampled combinations of ecological input parameters did not generate functioning ecosystems. That is, the biomass of one or several organisms approached zero shortly after the start of the simulation. In 42% of these cases, the fish biomass was not sustained given the combination of sampled input parameters. The consumption rate and the assimilation efficiency for fish were the main underlying factors for this result. To sustain the fish biomass in more than half of all simulations, these parameters were kept above 1.74 and 0.75 respectively (Table 5-4). Of the remaining 35% of the simulations it was the biomass of grazers (20%) and benthos (5%) that could not be sustained. The underlying factors for grazers were their consumption rate and assimilation efficiency. New lower limits to sustain their biomasses in more than 50% of the simulations were 1.47 and 0.35 respectively. For benthos it was the assimilation efficiency that caused the problem of sustaining the biomass (new lower limit 0.35). By changing these five ecological input parameters, the model gained stability and more than 65% of the simulations reached stable state, i.e. an improvement of 50%. Thus, the results from the model could be improved by constraining ecological input parameters within a range that is realistic in relation to measured values.

5.4.2 Sensitivity analysis

In the sensitivity analysis the calibrated ranges (c.f. above) for the model were used. Correlations numerically higher than 0.3 or less than –0.3 (range ± 1.0) between input and output parameters were interpreted as strong (Table 5-6).

The positive correlations between the ecological input parameters biomass, productivity and rates of respiration and consumption, and the three output parameters: biomass and total activity, demonstrate that the model performance was logic and follows common understanding of contamination dynamics. For instance, increased metabolic rates (e.g. productivity or respiration rate), increased the uptake and thereby the load of radionuclides.

Negative correlations were found between the radius of the organisms (or POM) and the radionuclide load in the respective compartment. These relationships indicated that a decreased radius increased the respiration rate, and consequently that smaller animals have higher weight specific respiration rate than larger /Dreyer and Puzio, 2001/, and in turn higher consumption rate and uptake of radionuclides.

The radius of POM was positively correlated with the radionuclide load of some organisms. This was due to the model assumptions that the surface specific association coefficient (K_{ads}) was scaled for the weight specific area of POM. Thus, K_{ads} was larger for low weight specific area to maintain the K_d value used.

This sensitivity analysis clearly showed that the total activities for each organism mainly were affected by the properties of the organism itself. However, the analysis did not include the effects of varying water exchange and uptake and elimination constants. This is discussed below.

Table 5-6. Summary of sensitivity analysis for Cs. The correlation (maximum ± 1.0) between the input parameters (rows) and the output parameters (columns). Only correlations stronger than ± 0.3 are presented. The biomass input parameters of different organisms refer to the initial biomass.

Biomass (gC)		Total activity (Bq)	
Phytoplankton			
0.80	phytoplankton biomass	0.49	phytoplankton biomass
		0.41	radius POM
		–0.39	radius phytoplankton
Benthic plants			
0.89	benthic plants biomass	0.82	benthic plants biomass
Zooplankton			
0.78	zooplankton biomass	0.43	zooplankton biomass
0.31	benthic plants productivity	0.40	radius POM
		–0.29	radius zooplankton
Grazers			
0.60	grazers biomass	0.60	grazer biomass
		0.38	benthic plants productivity
Fish			
0.43	fish biomass	0.38	fish biomass
0.30	fish consumption rate		
Benthos			
0.53	benthos biomass	0.52	benthos biomass
0.33	benthic plants productivity	0.47	benthic plants productivity
		0.39	benthic plants biomass
POM			
0.60	benthic plants biomass	0.61	benthic plants biomass
–0.39	benthos respiration rate	0.54	benthic plants productivity
0.38	benthic plants productivity		
0.32	radius benthos		
DIM			
		–0.41	benthic plants productivity
		–0.34	benthos biomass
		–0.32	benthic plants biomass

5.4.3 Comparison of probabilistic and deterministic simulations for caesium (Cs)

The deterministic and probabilistic simulations of Cs showed a good agreement regarding the output parameters: biomass and total activity (Table 5-7).

The differences between the deterministic and probabilistic simulations were a factor two or less for biomass and total activity for all the ecosystem components. For surface-associated activity the probabilistic estimations for grazers was a factor 6 higher, but well in between the 5 and 95% percentiles of variation.

The good conformity between the probabilistic and deterministic analyses suggested that the ecological input parameters used in the deterministic simulations gave estimates that were adequate. The remaining analyses were therefore performed only with deterministic

simulations. It is also worth to notice that the variability within the probabilistic simulations was low. The majority of the results varied less than one order of magnitude between the 5 and 95 percentiles in the probabilistic simulations. This suggests that even if some of the estimated ecological input parameters, such as the biomass or the metabolic rate of an organism group are uncertain, a well structured ecosystem model will produce reliable results.

Table 5-7. Biomass (gC), total activity (Bq) and activity on surface (Bq) for the ecosystem components from deterministic and probabilistic (average; 5 and 95% percentile) simulations of caesium (Cs). BCF, K_d and K_e were kept at 50, 3 and 1 respectively in both simulations.

Compartment	Deterministic	Probabilistic		
		average	5%	95%
Biomass (gC)				
Phytoplankton	1.1×10^{7}	1.1×10^{7}	4.5×10^{6}	2.1×10^{7}
Benthic plants	1.3×10^{8}	1.4×10^{8}	6.3×10^{7}	2.7×10^{8}
Zooplankton	1.3×10^{6}	1.2×10^{6}	5.0×10^{5}	2.4×10^{6}
Grazers	4.5×10^{6}	4.6×10^{6}	2.0×10^{6}	8.9×10^{6}
Fish	8.3×10^{6}	6.8×10^{6}	1.1×10^{6}	1.4×10^{7}
Benthos	1.2×10^{8}	1.1×10^{8}	4.9×10^{7}	2.1×10^{8}
POC	2.8×10^{7}	2.8×10^{7}	2.7×10^{7}	3.0×10^{7}
DIC	1.8×10^{9}	1.8×10^{9}	1.8×10^{9}	1.8×10^{9}
Total activity (Bq)				
Phytoplankton	7.7×10^{-8}	1.5×10^{-7}	1.8×10^{-8}	3.6×10^{-7}
Benthic plants	2.3×10^{-6}	2.4×10^{-6}	1.0×10^{-6}	4.5×10^{-6}
Zooplankton	1.2×10^{-9}	2.4×10^{-9}	2.2×10^{-10}	5.5×10^{-9}
Grazers	7.0×10^{-8}	7.0×10^{-8}	2.6×10^{-8}	1.4×10^{-7}
Fish	2.0×10^{-8}	3.1×10^{-8}	4.5×10^{-9}	7.6×10^{-8}
Benthos	2.2×10^{-7}	1.9×10^{-7}	6.4×10^{-8}	4.4×10^{-7}
POC	5.7×10^{-8}	6.1×10^{-8}	4.4×10^{-8}	9.5×10^{-8}
DIC	2.7×10^{-3}	2.7×10^{-3}	2.7×10^{-3}	2.7×10^{-3}
Activity on surface (Bq)				
Phytoplankton	6.8×10^{-8}	1.4×10^{-7}	1.2×10^{-8}	3.4×10^{-7}
Benthic plants	1.6×10^{-9}	4.1×10^{-9}	3.1×10^{-10}	8.2×10^{-9}
Zooplankton	4.9×10^{-10}	1.1×10^{-9}	8.1×10^{-11}	2.0×10^{-9}
Grazers	2.9×10^{-11}	2.0×10^{-10}	5.5×10^{-12}	1.3×10^{-10}
Fish	1.4×10^{-11}	1.5×10^{-11}	1.2×10^{-12}	3.6×10^{-11}
Benthos	6.4×10^{-10}	1.2×10^{-9}	1.2×10^{-10}	2.1×10^{-9}
POC	3.2×10^{-8}	3.4×10^{-8}	3.2×10^{-8}	3.5×10^{-8}

5.4.4 Model performance for radionuclide specific mechanisms

The model produced results in agreement with the mechanistic structure of the model and current knowledge of accumulation of contaminants in ecosystems. In all organism compartments, the exposure increased with increasing adsorption efficiency (K_d) and increasing bioaccumulation (BCF), and decreased with increasing elimination rate (K_e) (exemplified for concentration in fish in Figure 5-1). The response for K_d and BCF on the concentration was linear, whereas the concentrations decrease exponentially with increasing K_e.

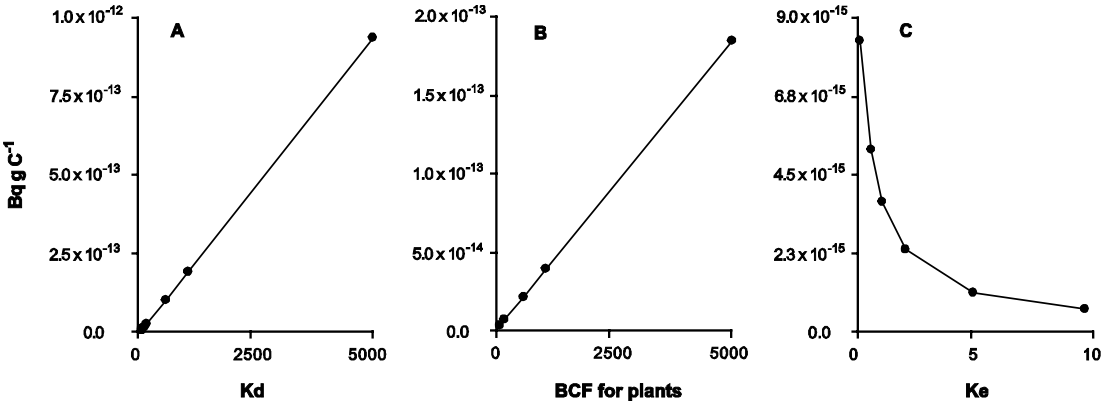

Figure 5-1. *Concentration (Bq/gC) in fish as a function of K_d, BCF and K_e. In A, BCF and K_e were kept constant at 50 and 1, in B, K_d and K_e at 10 and 1, and in C, K_d and BCF at 10 and 50, respectively.*

5.4.5 Influence of model mechanisms on the predicted endpoints

In a series of model analyses the importance of uptake efficiency of radionuclides in plants (BCF), the adsorption efficiency (partitioning coefficient, K_d), the radionuclide excretion rate (K_e), and the water retention time for the exposure of the ecosystem components were examined.

Plant uptake efficiency (BCF for plants)

The radionuclide concentration increased in all organism groups as the uptake efficiency, i.e. the bioconcentration factor for plants, increased, but the effect varied considerably between the organisms (Figure 5-2). A decreasing trend in radionuclide concentrations was found in the order: benthic plants ≥ grazers > fish > phytoplankton > benthos > zooplankton.

The observed pattern was likely a result of the three interacting mechanisms: trophic level, water exchange rate, and surface area. Organisms at the base of the food web were generally more affected by increases in BCFs than those at higher. Pelagic organisms, i.e. phyto- and zooplankton, were less influenced than benthic organisms. The water exchange continuously replaces the pelagic organisms and thus substitutes the contaminated organisms with uncontaminated from outside the system. Organisms having a large surface area exhibit a relatively higher external load of radionuclides than organisms with a smaller surface area. Since the amount of surface-associated radionuclides is independent of the consumption of contaminated food, organisms with a large surface were less influenced by increased plant uptake efficiency than organism with a small surface.

Surface adsorption (K_d)

The surface adsorption coefficients (K_d) are estimates of the partitioning of the radionuclides between the dissolved and particulate fraction. In the model they were used to regulate the amount of radionuclides associated to surfaces in the system, including organisms and POM. The influence of the surface adsorption on the radionuclide concentration in the organisms was explored in simulations with varying K_d values (Figure 5-3).

In grazers, a 10,000-fold increase of K_d had little effect on the radionuclide concentration compared to, e.g. zooplankton which occupy the same trophic level. This was presumably because, compared to phytoplankton and zooplankton, the grazers have a smaller weight specific surface area due to their low surface to volume ratio. The same mechanism applies indirectly for the uptake in the benthic animals, which mainly receive the radionuclides by their consumption of POM that has a high surface to volume ratio. The influence of K_d on the fish exposure was intermediate, due to the mixed diet, consisting of e.g. benthic plants and animals, zooplankton and grazers.

Excretion rate (K_e) – Biomagnification potential

Biomagnification is usually defined as the transfer of contaminants from food to an organism, resulting in a generally higher concentration within the organism than in the food source /Connell, 1989; Rand et al. 1995/. Once contaminants are within an organism, they may be metabolised and/or excreted so that the concentrations is a balance between the intake, by whatever means, and regulation /Gray, 2002/. Thus, when the intake rate is higher than the elimination rate, there is a potential for biomagnification to occur. To explore this mechanism with the present model, simulations for 25 different radionuclides with excretion rates (K_e) varying from full retention to active excretion were analysed (Table 5-8).

In the simulations where the ingested radionuclides were fully retained ($K_e = 0$), the concentration was only slightly higher (up to a factor 1.8 in fish) when compared to simulations where the excretion rate was kept equivalent to the carbon respiration ($K_e = 1$).

For zooplankton, grazers and benthos, the differences between full retention ($K_e = 0$) and active excretion ($K_e = 2$), were negligible for all radionuclides but for Cl, which increased up to a factor 3.4 in the benthos. As a consequence of changes in the excretion rate between the two extremes in fish, only up to a four fold increase of the radionuclide concentrations was observed. This implies that the biomagnification for fish is only a factor 4 or less. Similar results has been observed in experimental studies with Cs /Rowan et al. 1998; Zhao et al. 2001/. This was also concluded in a review study of biomagnification of metals in marine organisms /Gray, 2002/. With the exception of mercury, there was little evidence of biomagnification of metals.

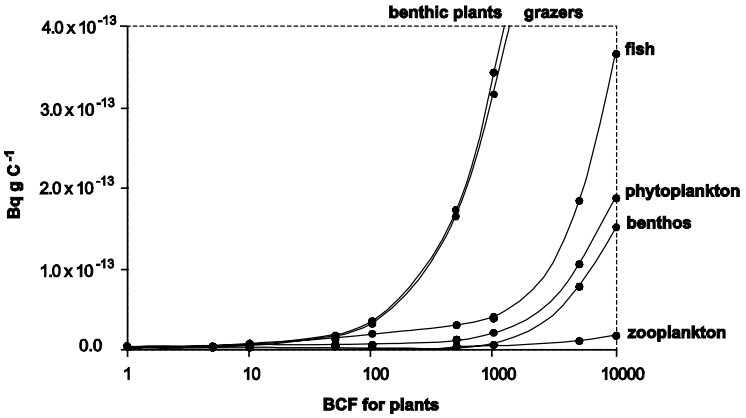

Figure 5-2. *Influence of plant BCF for plants (dm^3/kg wet weight) on the steady-state concentration (Bq/gC) in phytoplankton, benthic plants, zooplankton, grazers, benthos and fish. K_d and K_e were kept constant at 10 and 1.*

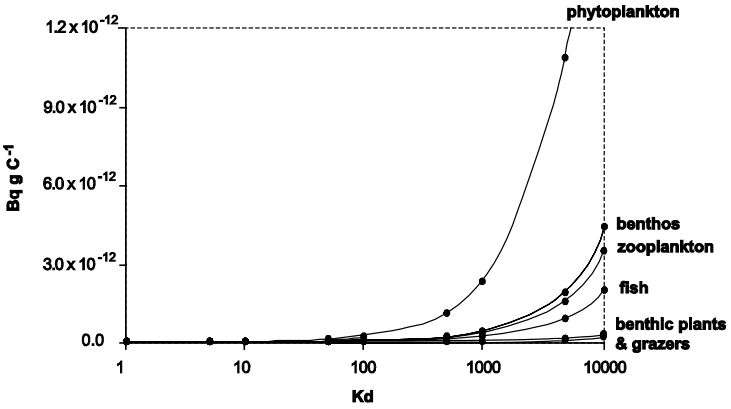

Figure 5-3. *Influence of K_d on the steady-state concentration (B/gC) in phytoplankton, benthic plants, zooplankton, grazers, benthos and fish. Plant BCF and K_e were kept constant at 50 and 1.*

Table 5-8. Potential for biomagnification for 25 radionuclides in zooplankton, grazers, benthos and fish. The biomagnification values were calculated as the ratio of maximum to minimum concentration, obtained in simulations with BCFs and K_d according to IAEA recommended values /IAEA, 1985/ and K_e at 0 (full retention; minimum) or 2 (active excretion; maximum).

	Zooplankton	Benthos	Grazers	Fish		Zooplankton	Benthos	Grazers	Fish
Ac	1.0	1.0	2.2	3.3	**Pb**	1.0	1.0	2.2	3.6
Ag	1.1	1.1	2.2	4.0	**Pd**	1.0	1.0	2.2	3.8
Am	1.0	1.0	2.2	3.5	**Pu**	1.0	1.0	2.2	3.8
Cl	1.1	3.4	2.2	4.3	**Ra**	1.0	1.0	2.2	3.8
Cm	1.0	1.0	2.2	3.5	**Se**	1.1	1.0	2.2	4.0
Co	1.0	1.0	2.2	3.9	**Sm**	1.0	1.0	2.2	3.4
Cs	1.0	1.0	2.2	3.8	**Sn**	1.1	1.1	2.2	4.0
H	1.1	1.3	2.2	4.0	**Sr**	1.0	1.0	2.2	3.6
I	1.1	1.1	2.2	4.0	**Tc**	1.1	1.1	2.2	4.0
Nb	1.0	1.0	2.2	3.6	**Th**	1.0	1.0	2.1	3.2
Ni	1.0	1.0	2.2	3.8	**U**	1.1	1.0	2.2	3.9
Np	1.0	1.0	2.2	3.9	**Zr**	1.0	1.0	2.2	3.5
Pa	1.0	1.0	1.8	3.2					

Water exchange rate

The water exchange rate in the area is high. The annual retention time is about a day /Engqvist and Andrejev, 1999/. Changes in water exchange rate have been found to have significant effects on the fate of ^{14}C in this ecosystem, including the concentrations in biota /Kumblad et al. 2003/. The implications of changes in the water exchange for the radionuclide dynamics were also tested in this study with Cs as an example. This was done in simulations with constant BCF, K_d and K_e, and varying water exchange rates between the normal water exchange rate of 365 exchanges per year and a reduction by a factor 10 and 100 (i.e. 36.5 and 3.65 exchanges per year respectively) (Table 5-9).

This test showed clearly that the larger the water exchange in the area was, the quicker the radionuclides were removed from the area, and the lower the concentrations in the organisms became. The response in benthic plants, grazers and DIC was equal to the change in water exchange rate, whereas in the other organisms, the response was larger

than the reduced water exchange rate. Zooplankton was the most affected organism. This was a consequence of that increased water exchange not only increase the dilution in the zooplankton compartment itself by replacing contaminated zooplankton with non-contaminated organisms, but also its food source (phytoplankton) and DIM (source for phytoplankton). This was also shown for zooplankton and ^{14}C in /Kumblad et al. 2003/. That study also demonstrated that the water turnover sets high constrains on the ecosystem itself in terms of e.g. nutrient recycling, which have implications for primary production rates etc. in the system and thus indirectly on radionuclide dynamics.

Table 5-9. Concentration (Bq/gC) in phytoplankton, benthic plants, zooplankton, grazers, fish, benthos, POM and DIM in simulations with constant BCF (50), K_d (3) and K_e (1), but varying water exchange rates (WE): 3.65, 36.5 and 365 exchanges per year.

	WE = 3.65	WE = 36.5	WE = 365
Phytoplankton	1.6×10^{-11}	5.2×10^{-13}	7.3×10^{-15}
Benthic plants	1.7×10^{-12}	1.7×10^{-13}	1.7×10^{-14}
Zooplankton	1.5×10^{-11}	2.7×10^{-13}	9.9×10^{-16}
Grazers	1.6×10^{-12}	1.6×10^{-13}	1.6×10^{-14}
Fish	8.9×10^{-12}	1.8×10^{-13}	2.4×10^{-15}
Benthos	6.3×10^{-12}	1.7×10^{-13}	1.8×10^{-15}
POM	7.1×10^{-12}	1.9×10^{-13}	2.1×10^{-15}
DIM	1.6×10^{-10}	1.5×10^{-11}	1.5×10^{-12}

5.4.6 Influence of radionuclide uptake pathway (plant uptake and adsorption)

The total load of contaminants organisms are exposed to is a result of intake via ingestion, diffusion and/or adsorption. The accumulated surface activity is the sum of the contribution of surface adsorption, independently if it is contained in the food at higher trophic levels, or associated to the surface. The adsorption process in relation to the plant uptake was analysed in simulations with only plant uptake of radionuclides, only adsorption to organic surfaces, and both mechanisms (Figure 5-4).

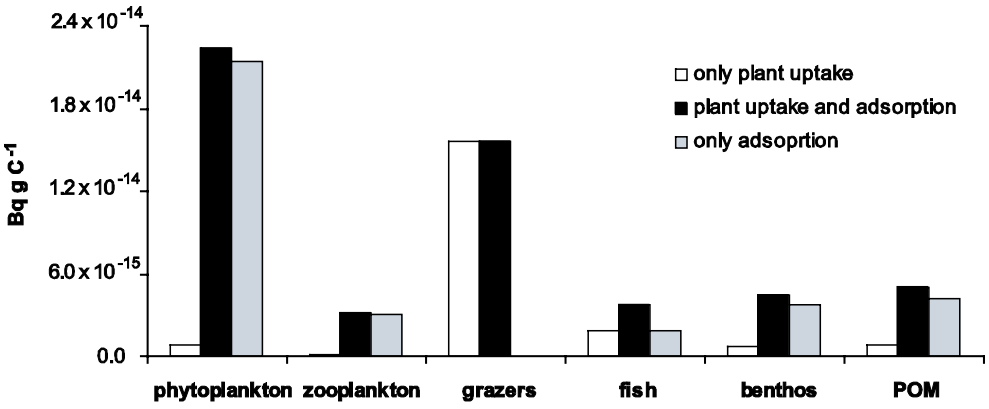

Figure 5-4. *Concentration (Bq/gC) in phytoplankton, zooplankton, grazers, fish, benthos and POM in three simulations: only plant uptake (plant BCF 50; K_d 0), plant uptake and adsorption (plant BCF 50; K_d 10), and only adsorption (plant BCF 0; K_d 10).*

The plant uptake mechanism only contributed with 2% and 4% of the total concentration for the phyto- and zooplankton, and about 17% for the benthos and POM. This was again primarily due to the large surface to volume ratio of phytoplankton, zooplankton and POM, compared to the other organisms in the model. The concentration in grazers, that have a small surface to volume ratio, increased less than 1% in simulations with both mechanisms compared to the plant uptake mechanism alone. Fish was found to be in between of these two extremes. They obtained the same concentration from the plant uptake mechanism (49%) compared to the surface adsorption mechanism (51%). This was a result of the location of fish in the food web. Their concentration was an integration of surface-associated radionuclides of most other compartments as they were defined as top-level consumer in this system.

5.4.7 Internal and external load of radionuclides

The distribution between external (adsorbed) and internal (ingested food) stored radionuclides in each organism was compared in Figure 5-5.

The externally stored radionuclides contributed little to the total activity compared to the ingested for all ecosystem components except phytoplankton, zooplankton and POM. For these components, the external radioactivity contributed to approximately 96%, 59% and 77% respectively of the total radioactivity in simulations having both surface adsorption and plant uptake mechanisms. Again, this was due to their large surface to volume ratio.

These results emphasise the importance of the radionuclide uptake via consumption. Thus, to obtain representative modelling results in exposure assessments of radionuclides, ingestion is a very important process to consider even for radionuclides having low bioconcentration factors. As the exposure situation seems to be strongly dependent on the food intake, one may also conclude that the conceptual description of uptake directly from water, i.e. bioconcentration factors, which often is used for instance for fish, is very misleading.

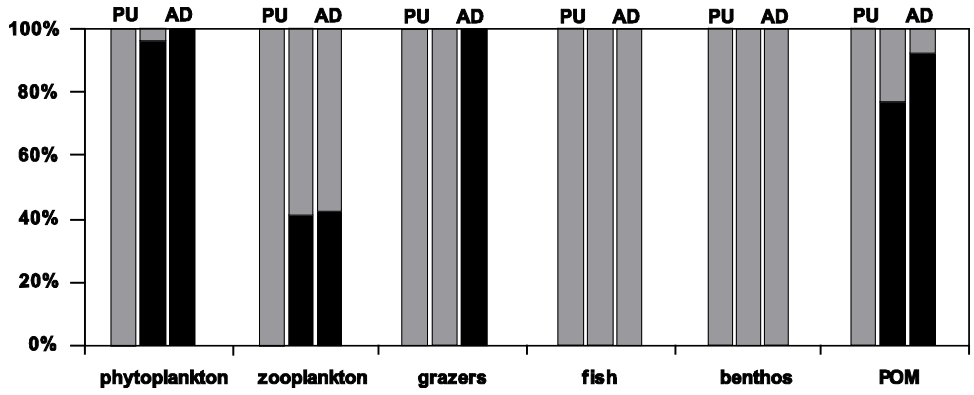

Figure 5-5. *Internal (grey) and external (black) radioactivity in phytoplankton, zooplankton, grazers, fish, benthos and POM for three simulations: PU – only plant uptake (plant BCF 50; K_d 0), plant uptake and adsorption (plant BCF 50; K_d 10), and AD – only adsorption (plant BCF 0; K_d 10).*

5.4.8 Fate of radionuclide discharges in the ecosystem

Since this model was based on mass balances of matter (including radionuclides) in the system, it was possible to trace the fate of simulated radionuclide releases and compare the distribution of radionuclides in the various compartments of the ecosystem. This was done for all 25 radionuclides, and is illustrated in Figure 5-6 for caesium (Cs), strontium (Sr) and thorium (Th), as they have different BCF and K_d values.

The major portion of the discharged radionuclides ended up in the dissolved fraction, i.e. in DIM (87.1–99.9%). The remaining part was mainly distributed between the benthic plants and benthos, e.g. for Cs and Sr, which primarily was a consequence of the biomass distribution in the ecosystem. The pattern of the distribution was similar for most radionuclides, although there were some discrepancies due to their adsorption and bioaccumulation ability. Protactinium (Pa) and thorium (Th) for instance, which have fairly low BCF and high K_d values, were distributed somewhat different than the other radionuclides. The radionuclides Pa and Th were mainly distributed between phytoplankton and benthos. This was primarily a result of surface adsorption to phytoplankton and POM and these compartments high surface to volume ratio.

There are few field studies that have analysed the relative distribution of radionuclide contamination in whole ecosystems. However, soon after the first Hanford reactors began to operate in the 1950's, such a study was performed. The major fraction of most radioactive contaminants accumulated by aquatic life was found to be held by the plankton and benthic algae due to their relatively large biomass /Davis and Foster, 1958/. This was in accordance with the findings of this study.

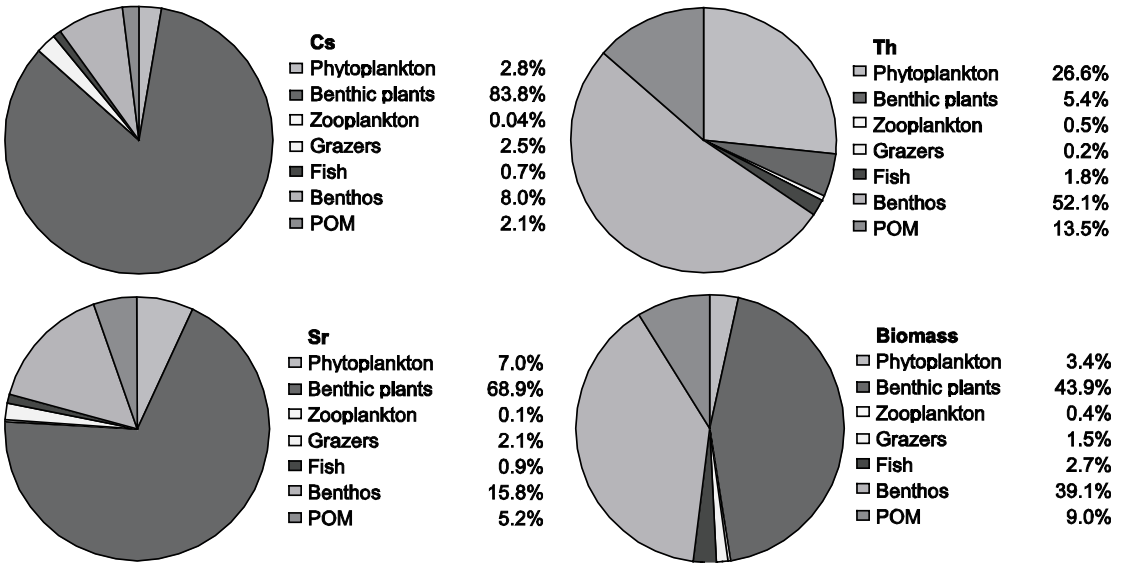

Figure 5-6. *Distribution (%) of particulate and accumulated caesium (Cs), strontium (Sr), and thorium (Th) (Bq) and biomass (gC) among the ecosystem components. The major fraction of the released radionuclides ended up in the DIM compartment (87.1–99.9%), but was not included in the distribution graphs (DIM makes up 85.3% of the total amount of carbon in the system).*

5.4.9 Comparison with IAEA recommended values

Bioconcentration factors (BCFs) for 25 different radionuclides were calculated for phytoplankton, zooplankton, grazers, fish and benthos from present modelling results and compared with empirically derived BCF values published by /IAEA, 1985/ (Table 5-10). The parameter settings used in the simulations for the initial BCFs for plants and K_d values for the respective radionuclides were the IAEA recommended values (Table 5-3). The excretion coefficient was kept at one, i.e. no retention or active excretion.

In general, the BCFs calculated in this study were in the same order of magnitude as the IAEA BCFs for most organism groups and radionuclides. This suggests that the model produce comparable results to empirical radionuclide data, even though the only radionuclide specific input parameters used were the adsorption efficiency (K_d) and the bioconcentration factor (BCF) for plants. That is, with only two values per radionuclide it was possible to estimate the concentrations (and BCFs) in all components of the modelled ecosystem. However, the comparison also identified some discrepancies. For instance, the BCFs for Ac, Am, Cm, I, Nb, Pa and Zr for fish were about a magnitude higher in this study than the IAEA BCFs. Even larger differences were found for Tc in benthic plants (compared with macro algae) and for I in grazers (compared with crustaceans). For phytoplankton and zooplankton, the opposite pattern was found. The IAEA BCFs for those organisms were often one or two magnitudes higher than in this study.

Differences between the two data sets could be due to mechanisms that were not accounted for in the model, or differences in environmental conditions between the modelled ecosystem and the sites/or conditions where the IAEA BCFs were attained. The functional groups used in this study, did not always represent the groups IAEA presented BCFs for, e.g. benthos was compared with molluscs, which probably also contributed to the observed differences.

BCFs calculated in this study that were higher than the IAEA BCFs, could be due to (i) active excretion (i.e. $K_e > 1$) which was not included in the model simulations, (ii) inadequate estimations of input parameters for K_d and BCF values used in the simulations, or (iii) environmental factors that influenced the radionuclide transport in food web that were not accounted for in the simulations or in the derivations of the IAEA BCFs, or (iv) isotope dilution with stable isotopes (e.g. I, Cl). Similarly, BCF values lower than the IAEA BCFs could be a consequence of (i) retention of ingested radionuclides (< factor 4, see above) or (ii) diffusive uptake in the organisms which was not included in the simulations, or (iii) differences in environmental conditions.

The observed differences for phytoplankton and zooplankton were probably to a large extent due to the effect of water turnover on the exposure situation for plankton organisms. In this case, it would mean a factor of 365, since the water retention time in the modelled ecosystem is about a day /Engqvist and Andrejev, 1999/. This corresponds quite well to the observed differences in BCF values.

The comparison between this study and the IAEA database may be refined and improved by reconstructing the size and metabolic rates for the organism used in for derivation of the IAEA BCFs.

Table 5-10. Comparisons of bioconcentration factors (BCF) (dm^3/kg wet weight) derived in this study for phytoplankton, zooplankton, grazers, fish and benthos with recommended BCF values for exposure assessments /IAEA, 1985/.

	Phytoplankton		Zooplankton		Crustaceans/Grazers		Fish		Molluscs/Benthos	
	IAEA	this study	IAEA	this study	iaea	this study	iaea	this study	iaea	this study
Ac	1.0×10^{4}	5.3×10^{3}	1.0×10^{4}	1.2×10^{3}	1.0×10^{3}	2.0×10^{3}	5.0×10^{1}	2.0×10^{3}	1.0×10^{3}	2.3×10^{3}
Ag	1.0×10^{4}	5.6×10^{1}	5.0×10^{3}	8.0×10^{0}	5.0×10^{3}	1.4×10^{3}	5.0×10^{2}	3.9×10^{2}	1.0×10^{4}	1.2×10^{2}
Am	2.0×10^{5}	5.3×10^{3}	2.0×10^{3}	1.3×10^{3}	5.0×10^{2}	4.1×10^{3}	5.0×10^{1}	2.6×10^{3}	2.0×10^{4}	2.5×10^{3}
Cl	1.0×10^{0}	3.8×10^{-3}	1.0×10^{0}	5.3×10^{-4}	5.0×10^{-2}	1.0×10^{-1}	5.0×10^{-2}	2.7×10^{-2}	5.0×10^{-2}	1.1×10^{-2}
Cm	3.0×10^{5}	5.3×10^{3}	2.0×10^{3}	1.3×10^{3}	5.0×10^{2}	4.1×10^{3}	5.0×10^{1}	2.6×10^{3}	3.0×10^{4}	2.5×10^{3}
Co	5.0×10^{3}	9.3×10^{2}	2.0×10^{3}	1.8×10^{2}	5.0×10^{3}	1.1×10^{4}	1.0×10^{3}	3.1×10^{3}	5.0×10^{3}	1.1×10^{3}
Cs	2.0×10^{1}	9.0×10^{0}	3.0×10^{1}	2.0×10^{0}	3.0×10^{1}	3.2×10^{1}	1.0×10^{2}	1.1×10^{1}	3.0×10^{1}	5.9×10^{0}
H	–	7.7×10^{-2}	1.0×10^{0}	1.1×10^{-2}	1.0×10^{0}	2.0×10^{0}	1.0×10^{0}	5.4×10^{-1}	1.0×10^{0}	1.7×10^{-1}
I	1.0×10^{3}	4.4×10^{1}	3.0×10^{3}	6.0×10^{0}	1.0×10^{0}	1.2×10^{3}	1.0×10^{1}	3.1×10^{2}	1.0×10^{1}	9.4×10^{1}
Nb	1.0×10^{3}	1.4×10^{3}	2.0×10^{4}	3.2×10^{2}	2.0×10^{2}	1.5×10^{3}	3.0×10^{1}	7.8×10^{2}	1.0×10^{3}	6.7×10^{2}
Ni	3.0×10^{3}	3.1×10^{2}	1.0×10^{3}	7.0×10^{1}	1.0×10^{3}	1.4×10^{3}	1.0×10^{3}	4.6×10^{2}	2.0×10^{3}	2.2×10^{2}
Pa	1.0×10^{3}	1.3×10^{4}	1.0×10^{3}	3.0×10^{3}	1.0×10^{1}	2.1×10^{2}	5.0×10^{1}	3.7×10^{3}	5.0×10^{2}	5.4×10^{3}
Pb	7.0×10^{3}	6.0×10^{2}	1.0×10^{3}	1.3×10^{2}	1.0×10^{3}	2.0×10^{3}	2.0×10^{2}	6.9×10^{2}	1.0×10^{3}	3.8×10^{2}
Pd	1.0×10^{3}	2.1×10^{2}	1.0×10^{3}	4.1×10^{1}	3.0×10^{2}	2.0×10^{3}	3.0×10^{2}	5.7×10^{2}	3.0×10^{2}	2.1×10^{2}
Pu	1.0×10^{5}	3.1×10^{2}	1.0×10^{3}	6.9×10^{1}	3.0×10^{2}	1.4×10^{3}	4.0×10^{1}	4.4×10^{2}	3.0×10^{3}	2.2×10^{2}
Ra	2.0×10^{3}	2.1×10^{1}	1.0×10^{2}	4.1×10^{0}	1.0×10^{2}	2.0×10^{2}	5.0×10^{2}	5.8×10^{1}	1.0×10^{3}	2.1×10^{1}
Se	8.0×10^{3}	5.7×10^{1}	1.0×10^{4}	9.1×10^{0}	5.0×10^{3}	1.2×10^{3}	6.0×10^{3}	3.2×10^{2}	6.0×10^{3}	9.9×10^{1}
Sm	1.0×10^{4}	5.4×10^{3}	1.0×10^{3}	1.3×10^{3}	1.0×10^{3}	5.9×10^{3}	5.0×10^{2}	3.1×10^{3}	5.0×10^{3}	2.6×10^{3}
Sn	5.0×10^{4}	5.0×10^{2}	5.0×10^{4}	7.0×10^{1}	5.0×10^{4}	1.3×10^{4}	5.0×10^{4}	3.6×10^{3}	5.0×10^{4}	1.1×10^{3}
Sr	3.0×10^{0}	3.0×10^{0}	1.0×10^{0}	6.7×10^{-1}	2.0×10^{0}	1.0×10^{1}	2.0×10^{0}	3.5×10^{0}	1.0×10^{0}	1.9×10^{0}
Tc	5.0×10^{0}	6.7×10^{2}	1.0×10^{2}	9.3×10^{1}	1.0×10^{3}	1.8×10^{4}	3.0×10^{1}	4.8×10^{3}	1.0×10^{3}	1.4×10^{3}
Th	2.0×10^{4}	5.2×10^{3}	1.0×10^{4}	1.2×10^{3}	1.0×10^{3}	1.5×10^{2}	6.0×10^{2}	1.5×10^{3}	1.0×10^{3}	2.2×10^{3}
U	2.0×10^{1}	5.0×10^{0}	5.0×10^{0}	9.5×10^{-1}	1.0×10^{1}	6.3×10^{1}	1.0×10^{0}	1.8×10^{1}	3.0×10^{1}	6.1×10^{0}
Zr	6.0×10^{4}	2.7×10^{3}	2.0×10^{4}	6.3×10^{2}	2.0×10^{2}	1.5×10^{3}	2.0×10^{1}	1.2×10^{3}	5.0×10^{3}	1.2×10^{3}
Np	1.0×10^{2}	3.7×10^{0}	1.0×10^{2}	7.7×10^{-1}	1.0×10^{2}	2.8×10^{1}	1.0×10^{1}	8.3×10^{0}	4.0×10^{2}	3.3×10^{0}
Zr	6.0×10^{4}	2.7×10^{3}	2.0×10^{4}	6.3×10^{2}	2.0×10^{2}	1.5×10^{3}	2.0×10^{1}	1.2×10^{3}	5.0×10^{3}	1.2×10^{3}

5.5 Discussion

No model has the ability to fully describe a real ecosystem or the ultimate fate of contaminants. Nevertheless, models are inevitable and useful tools in many disciplines, for instance in safety assessments. The model presented and discussed in this report, based on site-specific carbon dynamics and two radionuclide specific input parameters, can be used to estimate the radionuclide concentration in all components of the modelled system. It can also describe the overall distribution of radionuclides in the ecosystem.

The accuracy of any model results depends on the model conceptualisation, and its parameter estimations and mathematical algorithms. Uncertainties related to modelling results may thus be divided into the three categories: conceptual, the input data and the representational uncertainties. The conceptualisation of this model is robust as it was designed according to well-known ecological principles and was based on the structure of the ecosystem at the actual site. The quality of the ecological input parameters was high, as the majority of the data originated from field measurements in the area. The probabilistic analysis also show that a realistic variability of these parameters would have little effect on modelling results, probably due to the robust conceptualisation and ecosystem constraints. Uncertainties related to the radionuclide specific input parameters, i.e. BCF for plants and K_d, was shown to vary in importance for the different organism groups. This was examined in the analyses of the radionuclide specific model mechanisms. Generally, the surface adsorption mechanism was of higher importance than the plant uptake mechanism. However, to the total exposure, the ingestion of surface-associated radionuclides contributed substantially more than the surface adsorption itself.

Sensitivity analysis of the present model showed that the magnitude of the radionuclide exposure to an organism mainly depended on the properties of the organism itself, such as size, biomass and metabolic rate. A model validation was performed by comparing BCFs calculated in this study with BFCs from IAEA's database. The comparison showed that concentration factors calculated from results from this model were in fair agreement with BCFs based on empirical measurements.

5.6 Conclusions

With a model based on site-specific carbon dynamics and three radionuclide specific mechanisms, it was possible to estimate the radionuclide concentrations in all components of the modelled ecosystem with only two radionuclide-specific input parameters (bioconcentration factors (BCF) for plants and adsorption coefficients (K_d)). Comparisons of BCFs derived in this study with BFCs recommended by IAEA, suggest that this model produces analogous results to empirically derived data for more than 20 different radionuclides. Analyses of the importance of three radionuclide specific mechanisms: radionuclide uptake by plants, excretion of radionuclides by animals, and adsorption of radionuclides to organic surfaces, suggest that:

- The water exchange rate in the area has a major effect on the radionuclide exposure to organisms, both by dilution of the water and by replacing the plankton with uncontaminated organisms.
- The biomagnification of radionuclides in fish, or any other organism group is small, not larger than a factor 4.

- For most organisms the surface adsorption mechanism is more important than the plant uptake mechanism. However, for fish, both were equally important.
- The overall distribution of most radionuclides in the receiving ecosystem declined from water solution > benthic plants > benthos > phytoplankton to particulate organic matter.
- The ingestion is a very important mechanism to consider even for radionuclides having low BCF values as most of the internal body contents of radionuclides originated from the ingestion of surface-associated radio-nuclides. The bioconcentration factor concept is therefore misleading.

This study show that ecologically sound models can successfully be used either directly in assessment modelling or to produce site-specific transfer factors. This is especially valuable when future changes of the environment need to be taken into account.

6 Concluding discussion

SKB has adopted an ecosystem modelling approach for the exposure modelling of radionuclides as a complement to traditional exposure model chains in their safety assessment of underground repositories for nuclear waste. The reasons for employing this concept were many. Of most importance was perhaps that ecosystem models clearly distinguish radionuclide specific properties, such as half-life, surface adsorption and uptake efficiencies, from non-nuclide specific conditions, such as insolation, water balance, composition of ecosystem, food web structure. This makes the models scalable for changes of the environment, which is of particular importance for the assessments of radionuclides since many have very long half-lives and posing a potential threat during a long period of time, during which the environment likely will change considerably. Another important reason is that ecosystem models can provide realistic estimates also for radionuclides for which data on e.g. uptake rates are lacking. As high level waste includes a multitude of different radioactive isotopes having different chemical and physical properties and there are many different ecosystem types with a variety of species of interest, this feature is extremely valuable. A realistic description of the biosphere is also needed for the understanding of the receiving environment, which is essential for the interpretation of the modelling results, and to get credibility from authorities and the rest of society.

Although ecosystem exposure models both for both terrestrial and aquatic environments are under development and will be used in coming safety assessments of the deep repository, the focus has to date been on the aquatic models due to lack of data on the terrestrial environment. The aquatic models has been fully applied for the brackish water area above the underground waste repository SFR, and is presently being adapted and applied for other marine areas and limnic ecosystems, both in the Forsmark and Oskarshamn area.

In this report three models were described: (i) the CNP-model (describing the distribution and fluxes of carbon and nutrients for the coastal ecosystem off Forsmark), (ii) the C-14 model (describing the transport and distribution of hypothetically released C-14 from the underground repository SFR-1 to the ecosystem above), and (iii) the RN-model (describing the transport and distribution of radionuclides other than C-14 hypothetically discharged to the ecosystem).

In the CNP model it was shown that the carbon dynamics in the area was constrained by the amount of nitrogen and phosphorous available for primary production. Moreover the CNP model showed that the phytobenthic community dominate both the biomass and primary production in the area whereas the major part of the consumption was taken place in the soft bottom community and pelagic community. The most significant carbon flows in the system was found to be the export of excess carbon produced in the phytobenthic community to the other communities or away from the area trough water movements.

The distribution and flows of hypothetically discharged C-14 was analysed with the C-14 flow model. The analyses clearly illustrate that the route of C-14 entry into the food web and the water exchange rates significantly influence the modelled radionuclide exposure of the organisms. The highest concentrations were observed in benthic organisms exposed to C-14 released in the photic zone at a low water exchange rate. However, even in the most pessimistic simulations, the concentrations were far below the background levels. The extent, to which the water exchange influenced different organisms, mirrored their location in the food web and how their food sources were affected by the water exchange.

During normal water exchange conditions and C-14 discharge to the aphotic zone, more than 99% of the discharge was flushed out from the system immediately and only 0.2% was assimilated into plants.

The concentrations of more than 20 hypothetically released radionuclides were estimated for all the organisms groups in the generic radionuclide model, which was based on the CNP model and three additional radionuclide specific mechanisms. Comparisons of bio-concentration factors (BCFs) derived by the model with BCFs recommended by IAEA suggests that the generic radionuclide model produces analogous results to empirically derived data. Other model analyses show that (i) the water exchange rate had a large effect on the radionuclide exposure, (ii) the biomagnification potential for any radionuclide or organism was less than a factor 4, (iii) the surface adsorption mechanism is equal or more important than the plant uptake mechanism, and (iv) that ingestion is a very important mechanism to consider even for radionuclides having low BCF values.

In contrast to bioconcentration factor based exposure models, a major advantage with the use of models based on an ecosystem approach is that as long as the basic CNP-flow model is adequate, unrealistic results cannot be produced. This is because the radionuclide uptake is constrained by the metabolic uptake rates of the respective organism group, i.e. primary production or consumption, and the radionuclides available for uptake in the respective compartment from where the food source come, i.e. in the water or in the prey. As a consequence, in this type of models, biota can never accumulate more radionuclides than the total amount released into the system, or to a larger extent than the total amount of matter ingested (food). This may be self-evident, but is not always the case for BCF-based transfer models, as these are neither mass balanced nor consider recirculation processes in the system or changes in radionuclide availability. This problem with BCF-based models was also identified in a validation project of radioecological transfer models /IAEA, 1996/, where the modelling results varied by up to five orders of magnitude for the same type of simulations.

Although the advantages with the use ecosystem models are many, there are also drawbacks that need to be mentioned. For instance, the development of ecosystem models are quite complex and requires a good understanding about the site. A comprehensive ecological knowledge is also needed for the interpretation of the modelling results. In contrast to BCF-based models, ecologically sound models not only require ecological knowledge, but also site-specific ecosystem data, which may be difficult and costly to attain. Although the ecological parameters are generic for all radionuclides, this may of practical and economical reasons be the major drawback for the possibilities of using this approach. However, safety assessments of nuclear facilities such as waste repositories will eventually always be site-specific, and a well-documented description of the ecosystem is likely to be required before building permits can be given. Many parameters required for ecosystem modelling can also be estimated and extrapolated from abundance data on species present or other monitoring data. A BCF-based model on the other hand requires a vast amount of radionuclide specific information (one BCF for each organism-radionuclide-ecosystem type of interest), of which many are absent or rather uncertain. In ecosystem models of the type presented in this report, only BCFs for plants are needed to get estimates of the radionuclide concentrations in all organisms included in the food web model, and thus not only those that are parts of the human food chain.

The models described in this report demonstrate that the ecosystem modelling approach is a possible, flexible and realistic methodology to use in transfer modelling of radionuclides in aquatic ecosystems. The methodology has also shown to have the ability to handle many of the identified modelling problems related to BCF-models.

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