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CATS-1: a model for predicting contaminant accumulation in a meadow ecosystem. The case of cadmium.

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Keywords: grassland, model, cadmium, simulation, bioaccumulation, food web

This investigation has been carried out by order and for account of the Directorate of Chemicals, Safety and Radiation Protection of the Dutch Ministry of Housing, Physical Planning and Environment, within the framework of the Project Ecological Sustainability of the Use of Chemicals (PEIS); Project no. 719103

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Abstract

A model has been developed for the ecological risk assessment of cadmium accumulation in meadow ecosystems, and is part of a model family called CATS. Ecosystem structure in CATS models is embedded in the classification of ecosystem units, so called ecotope system of the Centre for Environmental Science (CML).
The CATS model concept depends on the use of separate cycles for biomass and toxicants, which is the conceptual framework for risk assessment in all present and future versions. The model includes cycling of organic matter between litter, soil organic matter, plants and animals. The toxicant cycle consists of cadmium partitioning equilibria and leaching in soil and litter, as well as uptake by plants and animals and feedbacks to litter or soil. Biological availability of cadmium is simulated by modelling cadmium uptake from soil interstitial water.

Foodweb structure is based on functional groups, which implies that variability within the group exists with respect to both physiological and toxicokinetic parameters. A probabilistic treatment of model output, e.g. concentrations is used, to account for inherent biological variability and model uncertainty, and to assess ecotoxicological risks.
Cadmium accumulation was studied under different cadmium load scenarios, with reductions up to one eighth of the present load. Long term cadmium accumulation of all compartments follows the dynamics of accumulation in soil. It was shown that a reduction of about one half the present load is needed for this particular ecosystem, to stop the increase in cadmium concentration of all compartments. Further reductions of cadmium input take a long time to become effective, due to the high retention of cadmium in the top soil. Uncertainty analysis of the model showed that uncertainty in model outputs was within reasonable bounds, even though many parameters were highly uncertain. The use of a generic cadmium partitioning model with three adsorbing fractions, e.g. fresh organic material, processed (humified) organic material and inert soil, did not result in highly uncertain model predictions.

The probability distributions of concentrations in soil, plants, and functional groups were used to assess whether existing NOECs or environmental quality standards were exceeded. The Maximum Permissible Concentration (MPC) in soil, with regard to protecting 95% of the species, is exceeded at all cadmium load reduction scenarios in 2015 and 2050. Because of the high accumulation of earthworms, environmental standards for cadmium in food of moles and meadowbirds are exceeded at all loading scenarios. The probability that more than 5% of herbivorous species are unprotected against sublethal effects of cadmium, is predicted to be 45% in 2015 and 85% in 2050 at the present cadmium load. This example shows that with CATS models, a broad range of environmental quality standards can be compared in an integrated modelling effort.
With these NOECs or standards, we can pinpoint the most influential part of the ecosystem affecting risks for specific toxicants.

Samenvatting

In dit rapport wordt het eerste model uit de CATS modelfamilie gepresenteerd voor de ecotoxicologische risicoanalyse van accumulatie van cadmium in grasland. De ecosysteem structuur in CATS modellen is ingebed in een classificatie van ecosysteem-eenheden, het zogenaamde ecotopensysteem van het CML, Leiden.
De CATS modelstructuur gaat uit van afzonderlijke cycli voor biomassa en toxicanten. Dit vormt het conceptuele raamwerk voor risicoanalyse in de huidige en toekomstige modellen. Het model bevat de kringloop van organische stof tussen strooisel, organisch materiaal in de grond, planten en dieren. De cyclus van de toxische stof bestaat uit een milieuchemische partitioneringsmodule in bodem en strooisel, uitspoeling, opname door planten en dieren en feedbacks naar strooisel of grond. Biologische beschikbaarheid van cadmium is gesimuleerd door cadmium opname uit het interstitiële water mogelijk te maken.

De voedselwebstructuur van CATS modellen is gebaseerd op functionele groepen, hetgeen impliceert dat toxicokinetische en fysiologische parameters variabel zijn. Een probabilistische benadering van de modeluitkomsten, o.a. concentraties, wordt gebruikt om rekening te houden met inherente biologische variatie en overige modelonzekerheid, en voor een ecotoxicologische risicoanalyse.
Accumulatie van cadmium werd bestudeerd met verschillende reductiescenario's tot één achtste van de huidige cadmiumbelasting. De lange-termijn accumulatie van alle compartimenten volgt de dynamiek van accumulatie in de grond. Een reductie van de cadmium belasting tot ongeveer de helft van de huidige belasting is nodig om de toename van de cadmium concentratie in alle compartimenten te stabiliseren op het huidige niveau. Sterkere reducties van de belasting worden niet onmiddelijk effectief, vanwege de sterke retentie van cadmium in de bovenlaag van de grond. Uit een onzekerheidsanalyse van het model blijkt dat onzekerheid in modeluitkomsten binnen redelijke grenzen valt, ondanks grote onzekerheid in veel parameters. De formulering van het algemene partitioneringsmodel voor cadmium met drie adsorberende fracties, te weten vers organisch materiaal, ouder gehumificeerd organisch materiaal en inert materiaal, had niet tot gevolg dat modeluitkomsten heel erg onzeker zijn.

De kansverdelingen van concentraties in grond, planten en functionele groepen werden gebruikt om overschrijding van NOEC's, milieunormen en grenswaarde vast te kunnen stellen. De maximum toelaatbare concentratie in de grond, waarbij 95% van de soorten beschermd is, wordt overschreden voor alle belastingsscenario's in 2015 en 2050. Vanwege de sterke accumulatie van cadmium in regenwormen, worden maximum toelaatbare concentraties in het voedsel van mollen en weidevogels overschreden bij alle scenario's. De kans dat meer dan 5% van de herbivoren onbeschermd is tegen sublethale effecten van cadmium, is 45% in 2015 en 85% in 2050 bij het huidige belastingsscenario. Deze voorbeelden laten zien dat het mogelijk is met CATS modellen een groot aantal verschillende milieukwaliteitsnormen te vergelijken. Met deze stofspecifieke normen of NOEC's kan de schakel in het ecosysteem die het grootste risico loopt, worden aangewezen.

Preface

This report is part of the project Ecological Sustainability of the Use of Chemicals (PEIS) and is specifically dealing with the 'ecological benefit' of measures taken with regard to reducing emissions of chemicals. The investigation has been carried out by order of the the Directorate General for Environmental Protection (DGM), Directorate for Chemicals, Safety and Radiation Protection of the Netherlands' Ministry of Housing, Physical Planning and Environment (VROM). This study is being conducted coherently by three national research institutes: the National Institute of Public Health and Environmental Protection (RIVM), the Centre of Environmental Science, Leiden University (CML) and the Institute of Forestry and Nature Research (IBN-DLO). Together they work towards modelling the risks of contaminants and the succes of their removal, measured in ecosystem quality improvements ('ecological benefit'). The model has a geographical basis of about 40 ecodistricts, for which a Geographical Information System (GIS) is applicable.

The project therefore:
- classifies ecosystems (aquatic and terrestrial) and their geographical aspects (CML and IBN-DLO);
- ranks ecotoxicological effects of toxicants and recovery potential of ecosystems after being affected (IBN-DLO); and finally
- models the risks of toxicants and the rehabilitation potential in ecosystems (RIVM).

The model presented in this report regarding cadmium is the first of a family, called CATS, which is an acronym for Contaminants in Aquatic and Terrestrial ecoSystems. Cadmium accumulation modelling in meadows is exemplified for the case study area of the Lowland Peat Ecodistrict in the Netherlands. Knowledge about ecology, ecotoxicology and environmental chemistry has been integrated in the present model. The chosen approach looks promising and will set an example how to predict the risk of other chemicals in similar or other ecosystems in the next phase of the project. This report should stimulate the international discussion on how to implement general ecotoxicological data mainly from laboratory studies into the setting of 'real' ecosystems. This report is also to be considered as first of a series on CATS.

project manager PEIS
Dr. G.P. Hekstra

1. Introduction

Background and goal

The Netherlands' Ministry of Housing, Physical Planning and Environment has been funding a research programme on Ecological Sustainability of the Use of Chemicals, abbreviated PEIS (Hekstra 1990). This programme is directed towards developing environmental protection standards which minimize the ecological damage of pollutants. In this context, a policy instrument is required to assess the effects of measures aimed at reducing chronic pollution with persistent toxicants. This instrument for ecosystem-specific predictions should at least answer the following questions:

- where are certain kinds of ecosystems located,
- which effects do certain toxicants have on specific ecosystems,
- how do we value these effects.

The Directorate for Chemicals, Safety and Radiation Protection has commissioned several institutes to develop such an ecosystem-based prediction system. It should lead to environmental protection standards that take the difference in sensitivity to pollutant loadings between ecosystems into account. The Directorate has asked the RIVM to develop ecosystem models for this goal. These models are being developed for both terrestrial and aquatic ecosystems, and are identified by the use of the acronym CATS, short for Contaminants in Aquatic and Terrestrial ecoSystems.

CATS-1: a model for meadow ecosystems

The model presented here describes cadmium accumulation in a meadow on moist, nutrient-rich peat soil in the low-land peat district of the Netherlands. This region has been chosen for the case study in the development phase of the prediction system. In this phase, both aquatic and terrestrial models are being or have been developed. CATS-1 can be used in specific, well defined ecosystems

- to assess the effectiveness of a reduction of the pollutant load, in terms of reduced pollutant bioaccumulation.
- to derive standards for a maximum permissable pollutant input based on existing environmental standards or no-observed effect concentrations (NOECs) within the modelled ecosystem.

The model described in this report is CATS-1 version 2.28. Discussions on model structure with experts led to subsequent modifications. CATS-1 is based on the NMPCulty model of Knoop & Aldenberg (1989), which was used to calculate maximum permissable cadmium levels in Dutch agricultural soils (Langeweg et al. 1989). Because NMPCulty did not include any biota apart from the crop, more ecological realism has been brought into the model by incorporating a simplified food web for a meadow.

Report organization

This report serves two goals, firstly the description of the CATS model concept, and secondly the description and analysis of an example ecosystem model. The first four chapters are meant for those readers with a general interest in the CATS model concept. Chapters 5, 6 and 7 deal with the mathematical aspects of the model. The last chapter may be of general interest.

The structure and organisation of the prediction system is described in Chapter 2. After a brief introduction of the characteristics of the meadow ecosystem (Chapter 3), an overview of the model concept and model components (Chapter 4) is presented. The incorporated ecosystem processes are discussed in more detail in chapter 5. Model calibration and implementation procedures are explained in Chapter 6. The results of performed simulations are given in Chapter 7. Though some attention is paid to simulations with nominal values, i.e. model runs with single parameter values, much attention will be paid to results from model runs with incorporated uncertainty. An evaluation of predicted concentrations with respect to existing NOECs and environmental quality standards is presented in the last section of chapter 7. In Chapter 8, model predictions are discussed.

2. Scope of the Project

The CATS-1 model is an example of the models that will be used within the framework of the Project 'Ecological Benefit'. Every part of the project contributes to the realization of the prediction system. We will present a short overview of the component parts of the project and how they are to be linked together.

2.1 Elements of the project

The Project 'Ecological Benefit' consists of three parts:

1. The development of an ecosystem classification to differentiate between ecosystems with respect to biotic and abiotic parameters, by the Centre of Environmental Science, Leiden University (CML) and the Institute of Forestry and Nature Research (IBN-DLO)
2. The development of ecosystem models to predict dose-response or process-response relationships for thus distinguished ecosystem types, by the National Institute of Public Health and Environmental Protection (RIVM). This report is the description of such a model.
3. The description of ecosystem recovery from disturbance by pollutants, by the Institute for Forestry and Nature Research (IBN-DLO).

2.2 Ecosystem classification

Ecosystems in the Netherlands have been classified according to abiotic and biotic habitat factors for soil fauna (Sinnige et al. 1991). Essentially, it is an extension of the classification made on the basis of vegetation (Runhaar et al. 1987). Vegetation is thought to be less sensitive to pollutants than soil fauna. Since soil fauna is also important with respect to nutrient cycling and pollutant transfer to higher trophic levels, this classification serves as a basis for ecosystem modelling. It consists of basic ecosystem units called ecotopes, which are considered homogeneous with respect to both biotic and abiotic habitat factors determining the species composition of soil fauna (Sinnige et al. 1992). Several factors that appear to be decisive in explaining the species composition of soil fauna, have been distinguished: salinity, moisture condition, texture/parent material, acidity and nutrient availability. Every factor is divided into classes. A maximum of 136 ecologically sound combinations can be distinguished (Sinnige et al 1991). By studying the distribution of soil fauna, we can assign species of the soil fauna to different ecotope-types. Thus each ecotope-type is characterized by an ecological species group. To test the validity of the system, a limited number of taxa will be assigned to ecotope-types.

2.2.1 Importance for model development

When operational, this ecotope system determines important model characteristics:

- The abiotic habitat factors of the ecotope-type (at a higher hierarchical level, called ecoseries) govern the biological availability of the pollutant. The discriminative

factors for the presence of soil fauna, as used to classify the fauna, also determine the fate of the pollutant. For instance, high organic matter in the soil of productive systems causes low availability of pesticides. For many toxicants, pH influences sorption equilibria.

- Ecotoxicological effects of pollutants take place within the defined ecotope-types. Due to the nature of diffuse chronic pollution, we hypothesize that the toxicant does not change ecosystem structure. Clearly, very large toxicant discharges can cause drastic effects on the ecosystem structure, like in the neighbourhood of large smelters. The present model is not meant to predict changes in ecosystem structure, but can be used to predict changes in ecosystem function. So, the primary effects of the pollutant (dose-effect relations) take place within the trophic structure of the ecotope, determined by the ecological species group. The toxic compound is not a master factor that can cause a shift to another ecotope-type with a different group of species.
- The location of specific ecotope-types can be plotted using a Geographical Information System (GIS). Model predictions on maximum permissable concentrations or predicted concentrations in specific ecotope types can be plotted on a map using the GIS to locate the ecotope-types (fig. 1). This feature is not yet operational.

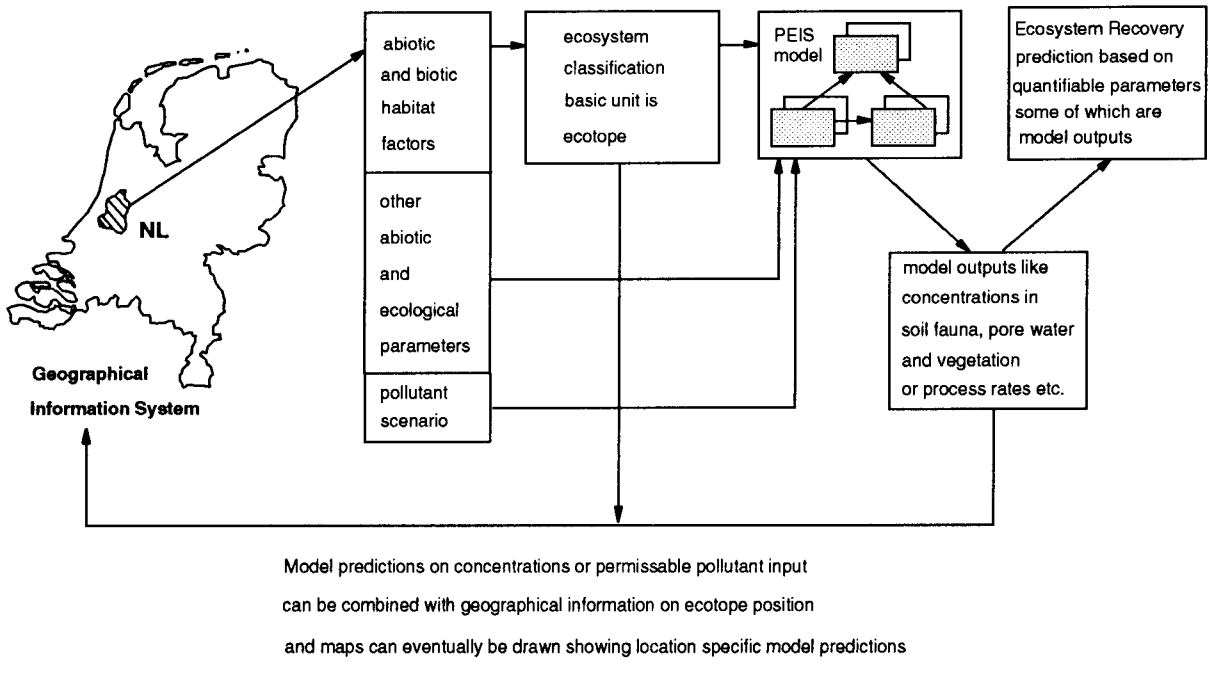

Fig. 1. Presentation of the relations between the elements of the Project Ecosystem Benefit

2.3 Ecosystem Modelling

The ecotope system distinguishes many ecotope types. It is not possible to develop integrated ecological models for all of them, so a very rigorous clustering is applied. The original vegetation system (Runhaar et al. 1987) distinguished five vegetation structures; pioneer vegetation, grassland, ruderal vegetation, shrubland and forest. We decided *a priori* to develop general ecosystem models for these vegetation structures.

It may seem that such a drastic reduction of variability ignores the variation of ecotope-types. However, the differences between ecotopes in abiotic site factors are used to parametrize a limited number of ecosystem models. In this way, the general models are made specific for an ecotope type by the parameter values generated by the ecotope type: moisture, pH, texture etc. and biotic parameters like biomass and presence of functional soil fauna groups. This output of the ecotope system is part of the input of the model (fig. 1). Because the ecotope system uses a restricted set of factors for the classification, not all model parameters are generated automatically by the ecotope system. So, additional input is needed. Model output is determined by the structure and processes of the model, which are described in the next chapters.

2.4 Ecosystem recovery

The goal of the project Ecosystem Recovery is the development of a tool for the indication of ecosystem recovery from pollutant effects. Consequently, measures for the sensitivity of ecosystems are needed enabling the assessment of recovery. Both structural and functional aspects of ecosystems are used for this purpose (Leon & van Dijk 1992). This led to the selection of a number of quantifiable parameters such as overall decomposition, microbial activity, net primary production, diversity, but also concentrations in both biota and abiotic compartments (Leon & van Dijk 1992). The most ideal situation would be the total compatibility of model outputs and ecosystem recovery parameters. Then, the model would predict how the recovery parameter (e.g. diversity) would change as a result of different pollutant scenario's. Many selected recovery parameters are not compatible with the present model concept. Enzyme activities as measures for microbial activity are not a model output. Because of the necessary reduction in complexity, the model uses the functional group concept for generalizing the food web. Consequently, there is no model output based on data for single species, such as a diversity index. A recovery parameter such as overall decomposition rate [y^{-1}] can be a model output if we not only model bioaccumulation of pollutants, but also the effect of the accumulated pollutant on nutrient cycling. The recovery of pollutant concentrations after load reductions towards background levels can also be predicted by the model.

3. Description of example ecosystem

In order to develop the CATS prediction system, an area for a first case study has been chosen. The study area is the lowland peat region, where over 90 percent of the area is covered with meadows for dairy farming. A substantial part of meadows in the Netherlands are situated on peaty soils in polders (fig. 2), defined as rich in fossile organic material (> 22.5%) and poor in clay. In the definition according to the ecotope system, cover layers of sand or clay on peat are not considered peat soils. Fen meadows often are situated in open, rural landscapes characterized by many ditches, reed vegetation and lake systems. Generally, these meadows are very nutrient rich due to fertilization and aerobic mineralization of fossile material due to lowered water tables (Grootjans 1985). Within this ecodistrict (H5 according to Klijn (1988)), we chose an abundant ecotope type: grassland on moist, nutrient rich peat soils with a pH between 4.5 and 6.5, coded G48-Mull (Sinnige et al. 1991). CATS-1 has been developed for this ecotope type. The first aquatic CATS model (Janse in prep.) is being made for shallow lakes within the same ecodistrict.
A thorough description of grassland ecosystems is given in IBP volumes 18 (1979) and 19 (1980), and more specific and extensive for fen meadows (Leon & van Dijk 1992); only a brief summary will follow here.

Over the last two decades, vegetation of these meadows has lost most of its former diversity due to lowered water tables and eutrophication. The most important nature values are meadow birds like lapwings (*Vanellus vanellus*) and black-tailed godwits (*Limosa limosa*). These meadow birds forage on soil and litter invertebrates, mostly earthworms and diptera larvae, from early spring to late summer. Above-ground invertebrates are an important food source for meadow bird chicks (Beintema et al. 1990). In the autumn, these birds migrate southwards. The most important herbivores are cattle, mostly cows but also sheep. A large part of the primary production is used by cattle that graze the field. Stocking density may be quite high, up to 3 cows per hectare. About 30 percent of the farms also have sheep. Depending on land use, a certain proportion of primary production is harvested for winter feeding. Smaller herbivores, are also present: wigeon (*Anas penelope*), coot (*Fulica atra*) and field vole (*Microtus spec.*). Wigeons are only present in significant numbers between October and April. During winter, they are the most common duck in this region, except for the mallard (*Anas platyrhynchos*). Coot and mallard are rather numerous the whole year round. All of these birds have other food sources; coots also eat macrophytes, geese may eat fresh reeds, wigeons also eat *Salicornia* on flood plains. The most common raptor in this area is the kestrel (*Falco tinnunculus*) which predates mostly on the continental field vole (*Microtus arvalis*).

Microorganisms are important in most decomposition processes, so we must consider their contribution in fen meadows. The most important invertebrate taxa are Enchytraeidae, Lumbricidae, Nematoda and Tipulidae. Microarthropods like Collembola and Acarina are less abundant (Leon & van Dijk 1992), probably due to the influence of high nitrogen fertilization (Siepel & van de Bund 1988). The most abundant detritivores/microbivores are potworms and earthworms, though biomass of potworms is negligible. Nematodes

show a wide variety of feeding habits, but herbivores are considered to be dominant in grasslands (Freckman 1982). Since microarthropods are not very abundant, low predation pressure on nematodes is expected. Larvae from Diptera, such as Tipulidae and Bibionidae ('rauwvliegen') live on grass roots. *Tipulida palidosa* is remarkably abundant in moist meadows.
An important predator of earthworms and to a lesser extent Diptera larvae is the mole, which can be present in densities of up to 20 per ha (Haeck 1969). Dung pats of cows are an important food source for a large variety of species, especially Nematoda, Diptera and Coleoptera (Sudhaus et al. 1988). Most nematodes in dung are considered to be microbivores, though some predate on other nematodes. Some species of Coleoptera and Diptera in dung pats are coprophagous, others are predators (Sudhaus et al. 1988). Adults often have a different feeding strategy than larvae. Their density shows strong seasonal variation. Above-ground insects, including those from dung pats are important as food for small insect eating birds such as swallows (*Hirundo rustica*).

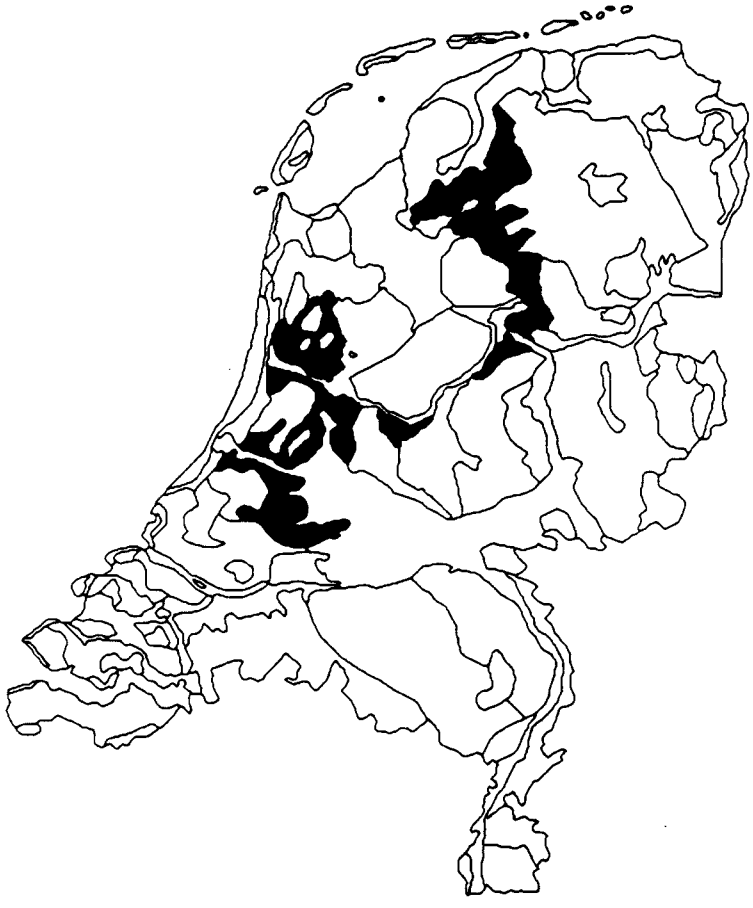

Fig. 2. Location of lowland peat ecodistricts (H5) in the Netherlands.

4. Model overview

4.1 Model concept

The choice for a certain kind of model is influenced by many factors, of which the most important are (Janssen & Heuberger 1992):
- the goal and application of the model
- the available knowledge about the processes or systems
- knowledge, experience and preference of the modeller(s).

Moreover, as in any ecological model, a number of assumptions with regard to ecosystem function and structure have to be made. Some of these assumptions are necessary because of adaptations between the different elements of the project, others are necessary to guarantee the robustness of the model. The CATS model concept has been strongly influenced by recent developments in eutrophication models (Janse & Aldenberg 1991, Janse et al. 1992).

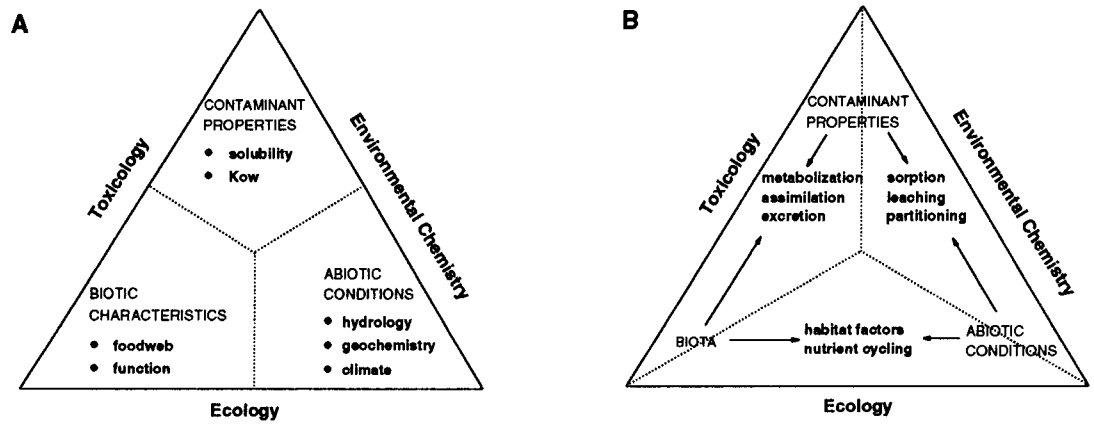

Fig. 3. Integrated ecotoxicological models use data from three disciplines (A). Processes can only be described adequately when integrating knowledge from these disciplines (B). Modified after Koeman 1984.

4.1.1 Integrated modelling

This project is specifically dealing with the 'ecological benefit' of measures taken with regard to reducing emissions of chemicals. The effects of these measures on ecosystem processes are studied. A thorough linking of abiotic and biotic processes within the model is needed because interactions of organisms with their environment are considered to be vital to ecosystem function (O'Neill et al. 1986) and thus to ecosystem modelling (Douben & Aldenberg 1991). The framework for integrated ecotoxicological modelling is illustrated in the triangle diagrams presented above (fig. 3). Ecotoxicology can be seen as an

integration of toxicology, environmental chemistry and ecology (Koeman 1984). Therefore, integrated ecotoxicological models integrate aspects of these disciplines. Fig. 3 shows that we need to consider abiotic conditions, contaminant properties and biotic characteristics to develop such models. Contaminant variables like solubility, K_{ow} and size determine their behaviour in different media. In many cases, these variables cannot fully explain exposure and uptake by organisms. We also need to consider the way of exposure, assimilation, elimination or metabolization. So, the physiology of an exposed organism needs to be taken into account. The fate of a toxicant is determined not only by its physico-chemical properties, but also by properties of the media (soil, water, air) in which it resides. Processes such as diffusion, leaching and sorption can be described by integrating knowledge about contaminant properties and abiotic conditions (fig. 3B). Many ecosystem variables of interest for ecotoxicological risk assessment, such as bioavailability of a compound, exposure of organisms, and effects on organisms, are influenced by all three sectors distinguished on the left (fig. 3A). These variables not only depend on the characteristics of the toxicant, but also on the behaviour of the animal and are influenced by abiotic site-specific factors. The relation between the parameters and variables from these disciplines can be studied in integrated ecotoxicological models.

4.1.2 Separate biomass and toxicant cycle

A major feature of the model is the conceptual division of the biomass cycle and the pollutant cycle (cf. Janse & Aldenberg 1990). It is not necessary to use biomass, any nutrient such as phosphorus or nitrogen will do. Simultaneous models of phosphorous, nitrogen and pollutant also fit in the same model concept. The two cycles we use here, are connected because pollutant mass is associated with biomass in both living and dead organic matter. If both cycles are considered simultaneously, we can explicitly model processes that only work on biomass or, conversely, on toxicant mass. In this kind of model, a change in biomass fluxes generally affects pollutant accumulation. The interaction between the cycles determines how a process in one cycle affects the other. This creates an important possibility. We can simulate the effect of pollutant accumulation on the functioning of the organisms.

If the concentration or body burden in some organism exceeds some no observed effect level (NOEC), an effect on the organism is expected. When a concentration-effect relationship with effects on biomass (growth reduction, mortality etc) is available, the resulting change of biomass will result in a rearrangement of biomass fluxes within the food web. This, in its turn, may cause a rearrangement of toxicant fluxes associated with biomass. Such a model is a so called type IV model (Douben & Aldenberg 1991). If we model bioaccumulation without effects on the nutrient cycle, the model is a type III model. At this stage of model development, CATS-1 is a type III model. However, any type III model structured like the present one, can be made into a type IV model given the availability of suitable dose-response, concentration-response or accumulated amount-response relationships.

4.1.3 Spatial resolution

The horizontal variation in ecosystems is described by the ecotope system. Ecotope types are considered homogeneous with respect to habitat factors. The same ecotope-type can be dispersed over the Netherlands, without necessarily forming a continuous area. Consequently, the model describes a horizontally homogeneous ecosystem which may be scattered over the Netherlands. A spatial differentiation of effects of pollutants on ecosystems requires different models for different types of ecosystems. Many different ecotope-types have been distinguished which precludes the development of models for every ecotope-type. The model is made specific for different ecotope-types by varying inputs, parameters and additional quantities.

Soils can exhibit strong vertical stratification. In many soils, a distinct litter layer is present in which the decomposers reside. Since litter can accumulate toxicants with a high affinity for organic matter, it is considered necessary to incorporate a litter layer in the model. In general, a very high percentage of all soil fauna can be found in the top 10 cm of the soil. For this reason we distinguish between a top soil layer and a deeper soil layer outside the system boundary. Since the model is horizontally homogeneous, the model is 1-dimensional in the vertical plane.

4.1.4 Functional groups

Species in an ecosystem can be subdivided into functional groups (Cummins 1974), regarding the fact that different species fulfil more or less the same role with respect to nutrient cycling (cf. Swift et al. 1979). Energy and nutrient fluxes have a characteristic pattern in different kinds of ecosystems. These fluxes lead to element cycles that are essential for a functioning ecosystem. In order to model effects on ecosystems, it is necessary to distinguish different exposure pathways yet end up with a manageable number of biotic compartments. The working hypothesis is, that we can model bioaccumulation and effects on ecosystem function at the level of functional groups, with enough resolution to distinguish between

- ecosystem types
- different exposure pathways.

Use has been made of the trophic group structure distinguished by Tamis (Sinnige et al. 1991). He proposed a clustering of invertebrates into 5 functional groups, and distinguished between detritivores and microbivores. We propose to fuse these two into one functional group (fig. 4), because many detritivores are also believed to consume microorganisms or can switch to a microbivore feeding habit and back again (Edwards & Lofty 1977).
The diagram depicted here is the minimum level of detail we would like to achieve in a CATS model. However, if we feel the data do not warrant that level of detail, we can aggregate functional groups. On the other hand, if we have detailed information on functional groups, we can also decide to split up groups.

For several reasons, policy makers often show an interest in specific vertebrates, like raptorial birds or species of Mustelidae. These animals are considered to represent the health of the ecosystems they live in. Furthermore, polyhalogenated pollutants have been shown to accumulate in several of these species and affect their reproduction. This warrants specific attention for vertebrates, resulting in several vertebrate compartments in the model. Feeding habits of most of the terrestrial vertebrates are quite well known, justifying a subdivision of trophic groups. Soil fauna feeding habits are much less known. Uncertainty analysis should tell us whether a certain level of aggregation is justified by the data.

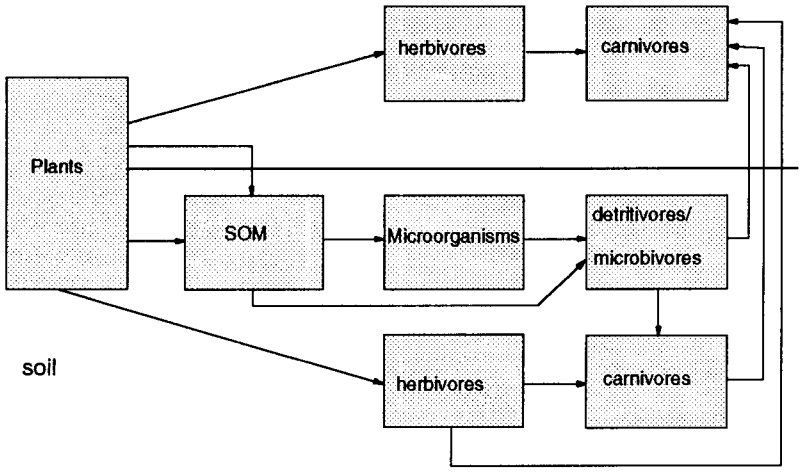

Fig. 4. Diagram of general functional groups in terrestrial CATS - models. Adaptations depend on local ecosystem.

In the model description, names have been given to the functional groups according to the most dominant representative of that functional group, for reasons of easy identification of parameters and variables and association with animals valued by policy makers. So, small vertebrate herbivores are called mice, detritivores are worms, below ground predators are moles etc. A functional group in the model always exists of several species, next to the dominant one, but is identified with the dominant one.

4.1.5 Logistic growth

The food web of the model consists of functional groups, which represent densities of several species. Usually, we cannot describe all mechanisms acting on populations in their environment. Consequently, the dynamics of a more general population model do not have to be a true representation of the dynamics in the field. Because the goal of our model is not to predict true population field dynamics, but to study the impact of emission reduction, we choose to embed mass balance principles in the more phenomenological approach of logistic population growth. Since we model functional groups and not single populations, we feel that this justifies the use of this extended generic population model.

The much used logistic growth equation according to Verhulst (1838) can be written as

$$\frac{dx}{dt} = r \cdot x \cdot \left(1 - \frac{x}{K}\right) = r \cdot x - \frac{r}{K} \cdot x^2$$

with the intrinsic rate of increase r and the carrying capacity K for the growth of group X. This equation offers important dynamic advantages, and it also leads to general overall stability of the ecosystem model. We will consider K as the maximum observed density that occurs naturally. In a specific ecosystem (i.e. the ecotope type, cf. section 2.2) the observed density of a functional group can be much lower than K. Limitations on growth can be imposed by nutrients, pollutants, temperature etc. In such cases, the population will not reach K but stay somewhere below it. Following Hallam et al. (1983) and Smith (1982), we propose to combine limiting mechanisms with the logistic growth equation. Other limitations not explicitly modelled are represented by the environment as set by the carrying capacity K. The derivation of our extended logistic growth model from the original logistic growth equation is presented in Appendix C.

4.1.6 Probabilistic model treatment.

Within functional groups, species are clustered that can behave very different in nature with respect to processes such as growth, respiration, assimilation but also with respect to toxicants. Apart from this, other sources of model uncertainty exist (Janssen et al. 1990). This implies a probabilistic treatment, contrary to the usual deterministic treatment of these kinds of models. Consequently, predictions on the 'ecological benefit' of toxicant load reductions are given in terms of probabilities for certain events:

- the probability that a 'safe' concentration in food is exceeded (Romijn et al. 1991a,b).
- the probability that environmental standards for pollutant concentration in soil, drinking water or food are exceeded
- The percentage species that are protected in an ecosystem or functional group (Van Straalen & Denneman 1989, Aldenberg & Slob 1991).

This probabilistic approach fits well within the risk-philosophy of the Ministry (Tweede Kamer 1989).

4.2 Model structure

CATS-meadow version 2.28 is composed of 25 state variables, 10 of which represent the biotic part of the model and 10 their associated pollutant mass. Three state variables represent pollutant mass not associated with organic matter and two are used for mass balance checks. All state variables are expressed per square meter. One could visualize this by thinking of an aerial view at a square meter of soil, containing biomass of certain plants and animals in dry weight [gD/m^2], as well as dissolved pollutant mass, sorbed pollutant mass, indicated by *X* [gX/m^2]. Two soil layers are considered: litter and top soil. Deeper soil layers are outside the model boundary. The conceptual separation in biomass and pollutant mass is shown in figs. 5 and 6. Boxes represent state variables ([gD/m^2] or [gX/m^2]) and arrows depict fluxes going to or coming from compartments ([gD/m^2/y] or [gX/m^2/y]).

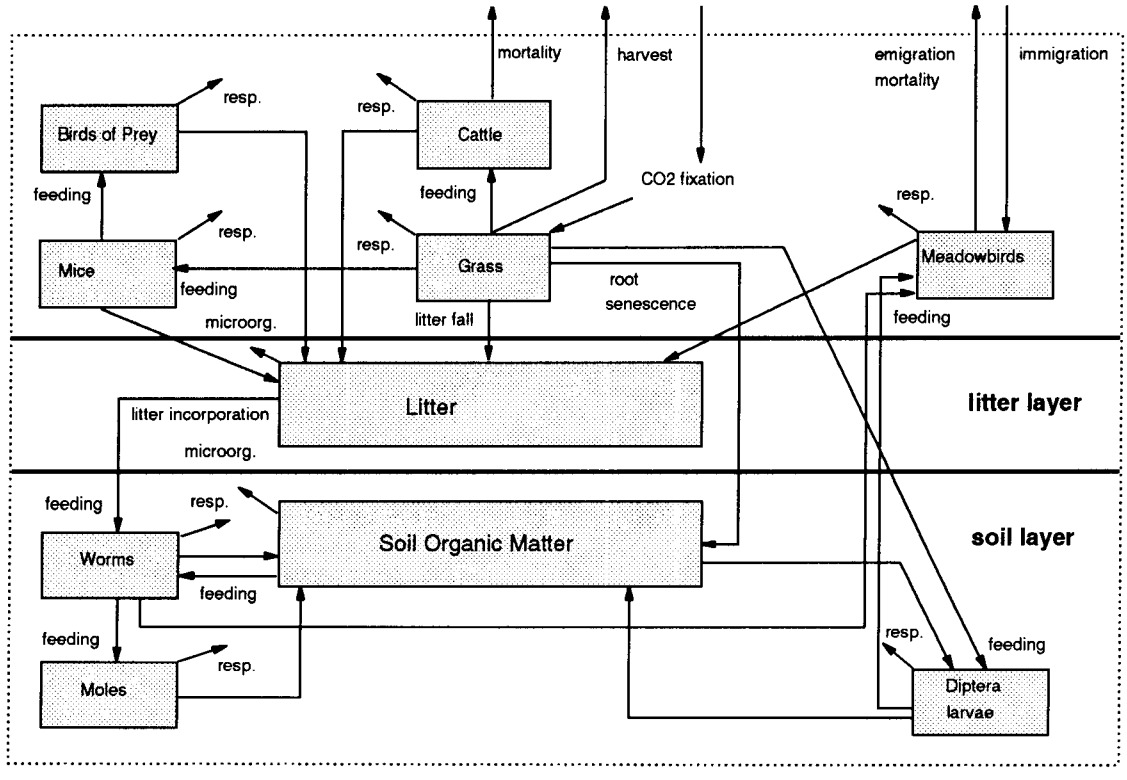

Fig. 5. Diagram of biomass (rectangles) and biomass fluxes (arrows) in the CATS model. Arrows for egestion and mortality fluxes bear no lable.

4.2.1 Biomass cycle

The biomass cycle consists of 8 functional groups and two organic pools in the soil. In meadows, a limited number of grasses are primary producers. This crop is harvested, but also grazed by small and large herbivores. Litter fall from the crop forms the litter layer, which is almost a virtual layer because it is very thin in a productive meadow. Below ground, soil organic matter is enriched by root senescence. Since inorganic carbon is not included in the model, primary production is an input of the model and all respiration terms are biomass losses. Microorganisms are not included as compartments. The modelling of microorganism biomass dynamics is outside the scope of this project. However, their respiratory activity in litter and SOM are included as processes. Detritivores and microbivores have been clustered into one group (detritivores/microbivores) represented by annelid worms. Studies on earthworms have shown that they eat both microorganisms and detritus (Edwards & Lofty 1977) and we can expect the same for many detritivores. Earthworms can eat organic matter from the litter layer and the top soil, depending on type of worm, palatability of the organic matter and the type of litter layer. Soil herbivores are represented by the dominant Tipula spec. larvae (Oudshoorn et al. 1984). They graze on both live and dead roots of grasses (pers. comm. De Goffau). The mole represents soil predators, and feeds mainly on earthworms. Above ground vertebrate predators are represented by two bird compartments, one for all meadow birds (eating soil invertebrates) and one for raptorial birds (eating small herbivorous vertebrates). The only allowed immigration is of meadow birds. During their migration and overwintering, they feed elsewhere but we do not incorporate this aspect in the present model. We can only calculate exposure due to foraging in the Netherlands. Cows and meadow birds are considered to die outside the system boundary, the harvest is taken from the system. Egestion of non-assimilated biomass is returned to either the soil layer or the litter layer, depending on whether the animal lives primarily above- or below ground. The same holds true for natural mortality (not due to predation).

4.2.2 Toxicant cycle

The pollutant cycle is depicted in fig. 6. The major feature of this diagram is the principal role of pollutant equilibria in determining the amount of Cd bound to the litter or soil organic matter (SOM) or Cd dissolved in interstitial water. A high binding constant means that the dissolved Cd concentration is relatively low and vice versa. It has been postulated that bioavailability of toxicants is primarily determined by the dissolved concentration (Boesten 1991). Both crop and earthworms are modelled to take up Cd from pore water, thus cadmium equilibria play a major role in determining bioavailability in the model. Some cadmium taken up by the crop is recycled into the system by litterfall and root senescence. As can be seen, pollutant associated with dead organic matter enters the biota through earthworm consumption of litter and SOM. These organic layers are continually enriched with pollutant because all egestion and excretion of pollutant by any functional group, or toxicant associated with decaying corpses, is added to either litter or soil organic matter. Pollutant enters the system by deposition, manure brought from outside the system and bird immigration.

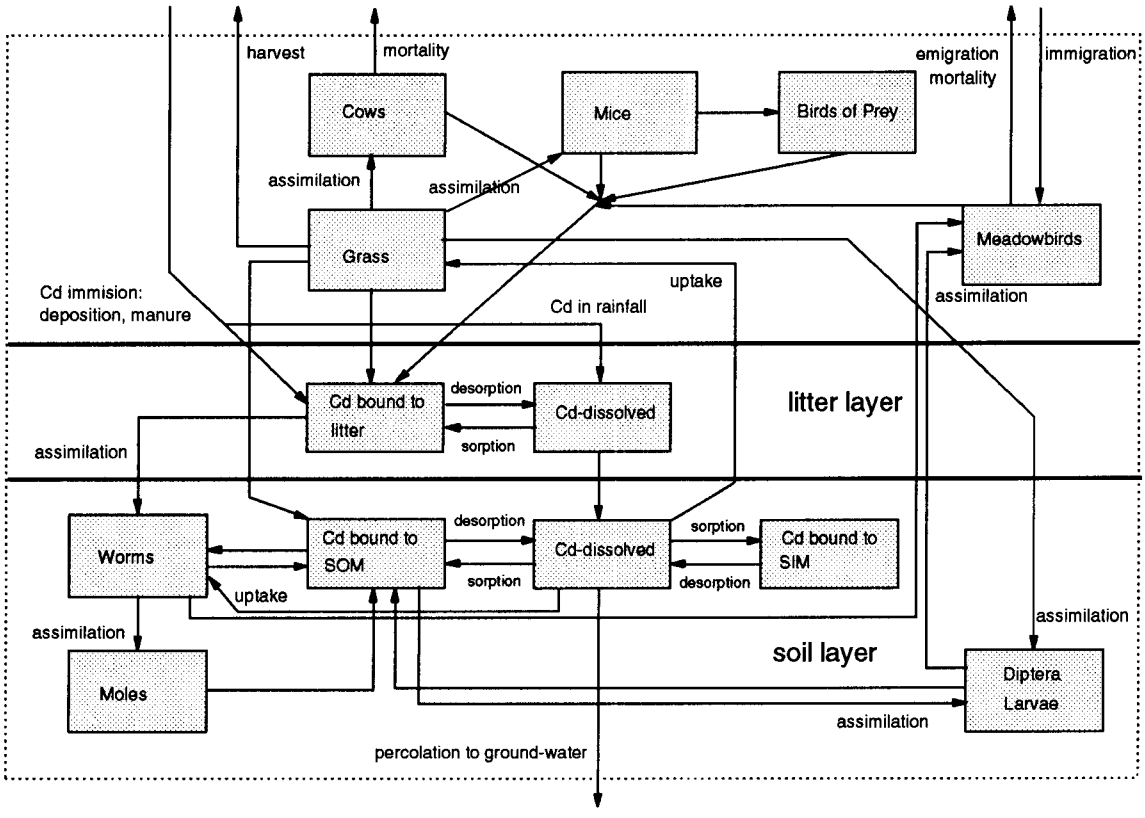

Fig. 6. Diagram of pollutant mass (rectangles) and fluxes (arrows). The dashed line is the system boundary. Arrows without subscripts indicate egestion, excretion, mortality.

Pollutant leaves the modelled ecosystem by a number of ways:
- percolation of the cadmium dissolved in rain water surplus to deeper soil layers
- with harvesting of crop
- with meadow bird emigration
- death of cows and meadow birds

If organic compounds are modelled, the model should also contain metabolization of organic compounds. A full description of all toxicant processes can be found in the next chapter.

4.2.3 Toxicokinetics

All functional groups are represented twice in the model because of the separate modelling of toxicant (X) and biomass (D). All masses are expressed in grammes per square meter. Mass flows going to and coming from a functional group are depicted in Fig. 7. Parallel processes are mortality and predation. These are proportional D and X processes, since the biomass that leaves the compartment in this way, has the same toxicant concentration as the compartment itself. Consequently, this does not change the ratio of X and D in the compartment. This ratio is important, since it is simply the concentration of toxicant:

gX/gD. Several toxicant processes have corresponding biomass processes that are not proportional. Assimilation, excretion and respiration can change the *X:D* ratio. Nutrients and toxicant can be assimilated by a functional group with different efficiencies: dry weight assimilation efficiency (*DAss*) and toxicant assimilation efficiency (*XAss*). The non-assimilated matter is egested (*DEges* and *XEges*). Uptake of pollutant (*XUp*) from the soil solution by vegetation or soft bodied insects is not matched at all by a corresponding nutrient uptake process. After pollutant assimilation, the toxicant is excreted from the compartment at a certain rate *XExcr* [y^{-1}]. The matching biomass process is respiration *DResp*, but this process is considered independent from *XExcr*. All these processes, acting on both cycles or on one separately, influence the concentration in a compartment.

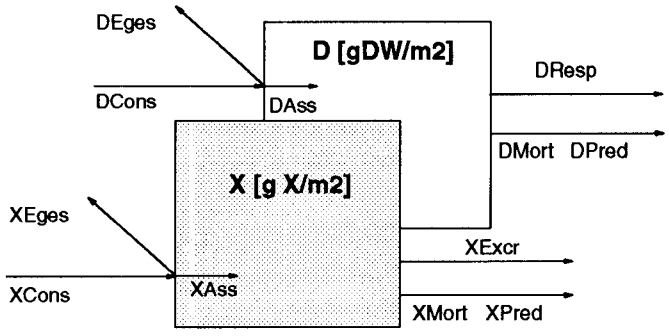

Fig. 7. Diagram of biotic (*D*) and pollutant (*X*) fluxes going to and coming from a functional group. See text for explanation.

5. Description of processes

A detailed description of processes included in this model is presented in this chapter. The precise mathematical process formulations are included in Appendix B.

5.1 Abiotic processes

5.1.1. External cadmium loading

Cadmium loading of the system is the sum of wet deposition, dry deposition and manure application. Wet deposition of pollutant results from cadmium dissolved in rain water. It can be calculated if total rainfall and pollutant concentration in rainwater is known. Dry deposition is the result of cadmium contaminated particulate fall out. Dry deposition depends on the location of the ecotope type. Cadmium input by manure comes from different sources, each one with a specific cadmium concentration:

- artificial fertilizer
- animal manure slurry from several sources applied to the field
- cattle manure produced when cattle is feeding in the field

The first two sources depend on agricultural land use and have been calculated for the NMPCulty model (Langeweg 1989). The last source depends on the number of cattle per ha. and the concentration of cadmium in the grass, and is calculated in the model. Since the cadmium input of manure from feeding cattle occurs within system boundaries, it is not a real input but part of the modelled pollutant cycle. Usually, cadmium input by manure (all sources) is higher than by wet and dry deposition.

5.1.2 Percolation of precipitation surplus

In general, more precipitation comes down than is evaporated or evapotranspirated, causing a net downward seepage of water. The usual amount of rainfall is a general figure for the western part of the Netherlands, and the precipitation surplus estimated at 40% of total rainfall (Knoop & Aldenberg 1989). In the litter layer, a certain fraction of the original amount is transferred to the soil layer. Soil pore water is taken up by crops and animals, and a part of it evaporates (fig. 8). A fixed moisture content of the litter and soil layer is assumed. The remaining seepage to deeper layers is the net precipitation surplus.

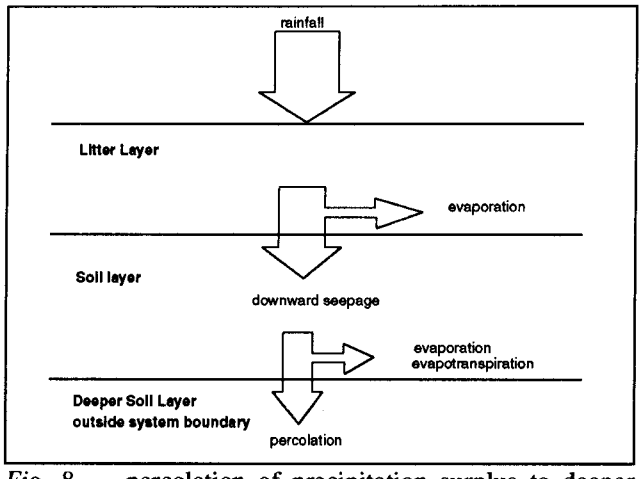

Fig. 8. percolation of precipitation surplus to deeper soil layers outside the system boundary.

5.2 Litter & Soil processes

In many models, soil is seen as a homogeneous mixture of organic and inorganic constituents. Organic matter is utilized by soil fauna as an energy source and as such a crucial aspect of soil fauna models. Therefore, organic matter is a state variable in the model. To incorporate organic matter turnover of soils in our model, we need to consider two aspects

- turnover of litter (100% organic) deposited *on* the top soil by vegetation, dead animals etc.
- turnover of organic matter *incorporated in* the top soil

5.2.1 Turnover of litter

Litter biomass results from plant littering but also from food egestion and natural mortality of animals (fig. 5). Litter is consumed by earthworms and respired by microorganisms. Microorganisms are not incorporated as a separate compartment, but their respiratory activity is. Earthworms contribute to a mixing of the litter and the soil through fragmentation and burrowing activity (Scheu & Wolters 1991). A net downward movement of processed litter exists to the top soil. Depending on the amount of litter input and soil fauna activity, the litter layer can grow thicker or decrease in height. Toxic effects on soil fauna probably inhibit their litter processing abilities (Denneman et al. 1986). The dynamics of the litter layer is modelled because of its importance in nutrient cycling and contaminant retention. Litter layer thickness is a model output, assuming a constant density [kg/m^3].

5.2.2 Turnover of Soil Organic Matter

Root senescence, egestion and natural mortality contribute to the formation of soil organic matter (SOM). SOM is consumed by earthworms and diptera larvae, and respired by microorganisms. Biomass of microorganisms is not a model variable, but their respiratory activity is modelled as a first order decay of organic matter. The composition of the soil layer is not constant, since activity of soil fauna can increase or decrease the organic matter content of the soil. A highly organic soil has a lower density than a very sandy soil. Since the density influences soil equilibria, the density must be calculated dynamically. For this reason, soil organic matter (*SOM*) is a state variable of the model. The rest of the non-palatable soil consists of persistent humic substances, and the inorganic soil matrix: sand or clay etc. In peat soils, a large fraction of the soil matrix is non-palatable organic matter. This non-palatable component of soil is called soil inert matter (*SIM*). SIM is not a dynamic variable.

A schematic view of a standard soil volume (1 m^2 · depth) is depicted in fig. 9. This volume is filled with particulate matter (organic and inorganic), filled with water (*Liquid*) and filled with air (*Air*). The model keeps track of the SOM mass. Since we have a fixed soil depth, only a part of the soil volume is filled with organic matter (fig. 9) and the remaining volume will be filled with soil inert matter. The more organic matter is mixed into the soil, the less inorganic matter remains in the top layer of the soil up to the limit where SOM fills the whole volume, and maximum SOM density is reached. If the organic content of soils changes, we can expect the porosity of the soil to change also. The change of porosity is small so we consider it constant.

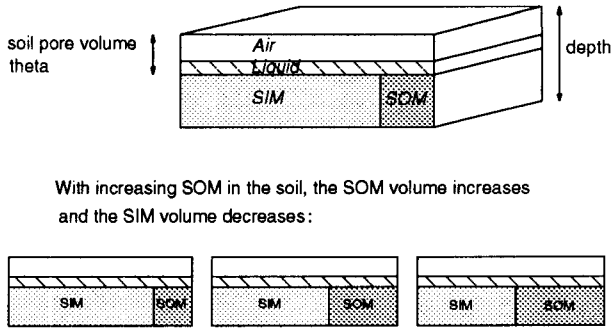

Fig 9. Representation of a standard soil volume. Due to increasing SOM, density will change. See text for explanation.

5.2.3 Litter and soil cadmium equilibria

An important feature of the CATS model is the turnover of litter by soil animals. Cadmium sorbed to litter is brought into the top soil by egestion and mortality of detritivores. Because SOM is a processed organic fraction, i.e. more humified, we can expect SOM to have a higher cadmium sorption capacity than the litter it originated from. Soil organic matter (SOM) is then available as food for other, soil dwelling invertebrates. These animals are exposed to the pollutant by their food, i.e. SOM. Therefore, it is necessary to know what the cadmium concentration is of the organic component of the soil. Usually, cadmium partitioning in soil is between Cd-dissolved and Cd-sorbed. The soil fraction to which the cadmium binds, is a mixture of all inorganic and organic soil fractions (Chardon 1984). Since we want to know the Cd concentration of the SOM, we must distinguish Cd binding to organic and inert (non palatable) soil components. So, cadmium equilibrium is between one dissolved fraction and two bound fractions, SIM and SOM (fig. 10). In the litter layer we distinguish only one sorbing, organic fraction.

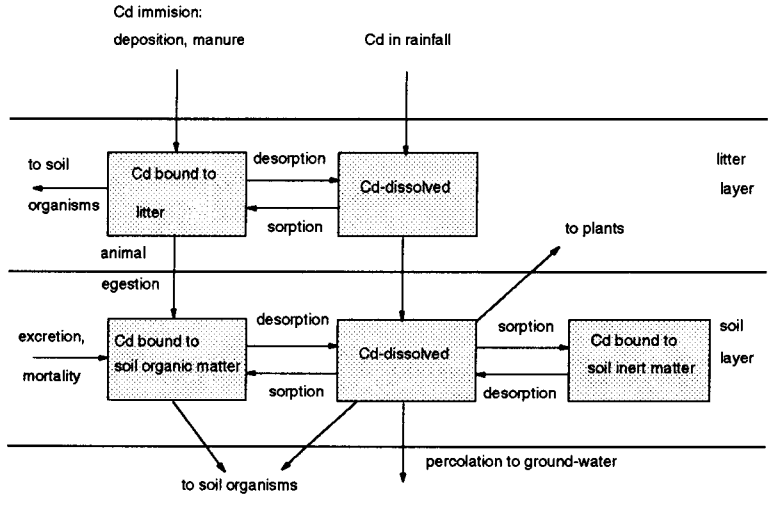

Fig. 10. diagram of cadmium equilibria in litter and in soil showing the fluxes that connect compartments.

Cadmium equilibria usually are described with the nonlinear Freundlich adsorption isotherm:

$$q = k \cdot c^{n}$$

with k = constant [l/kg]
q = sorbed cadmium [mg/kg]
c = steady state dissolved cadmium concentration [mg/l]
n = constant [-]

The soil factors pH and organic matter largely determine *k* (Boekhold et al. 1990), while *n* is rather constant. It should also be noted that the cadmium sorption isotherms are almost linear at low concentrations of cadmium in the soil solution (Chardon 1984). For this reason, we assume *n* to be unity at low cadmium field concentrations. Initial sorbed and dissolved amounts are estimated from the total cadmium content of dried litter or soil.

Soil organic matter content is a dynamic variable. Consequently, the overall binding constant of the soil, which is derived from both *SIM* and *SOM*, is a dynamic variable. The overall binding constant is a model output, and is tuned to binding constants as determined from soil samples (Chardon 1984). For this peaty soil, a high binding constant of about 1500 should be reasonable. Peat consists of organic, inert soil material (*SIM*) that is not consumed by soil animals. For this specific soil, we assumed binding constants of *SOM* and *SIM* to be not very different. Binding capacity of litter has been determined by Somers (1978).

The equilibria are implemented using Clasen's (1976) mechanism. He discerned slow and fast reactions. Slow reactions are fluxes due to leaching, mortality, egestion etc. Fast fluxes are equilibrating fluxes, assuming instantaneous equilibrium. For simple equilibria, it is possible to find an analytical solution yielding the fast fluxes (Appendix E). For more complex equilibria, a numeric solution is necessary (Wortelboer & Aldenberg 1991).

5.3 Vegetation processes

5.3.1 Biomass cycle

Primary production determines the magnitude of most biomass fluxes in an ecosystem. Primary production is set to a predefined level, which means that it can be seen as a forcing function. This is done for two reasons:

- vegetation usually is not very sensitive to toxic effects, except herbicides so we are not very interested in physiological mechanisms of crop growth
- the ecotope system for vegetation (Runhaar et al. 1987) is used for model input , and distinguishes only three classes of production (low, medium, high). No more level of detail is required for general purpose modelling.

In accordance with other biotic compartments, we will use the logistic growth equation also for vegetation modelling. The crop will grow to its carrying capacity *K* when no

limitations are operating except general environmental limitation. Since we expect the farmer to do anything in his power to raise production, we do not model nutrient limitations but use the carrying capacity to calibrate on known production levels. For crop growth, we consider the fluxes as shown in fig. 11:

- grass cut for silage (winter feeding)
- losses during cutting and grazing together with losses due to senescence of leaves and roots.

To complete the general crop processes, respiration and harvest are considered first order processes.

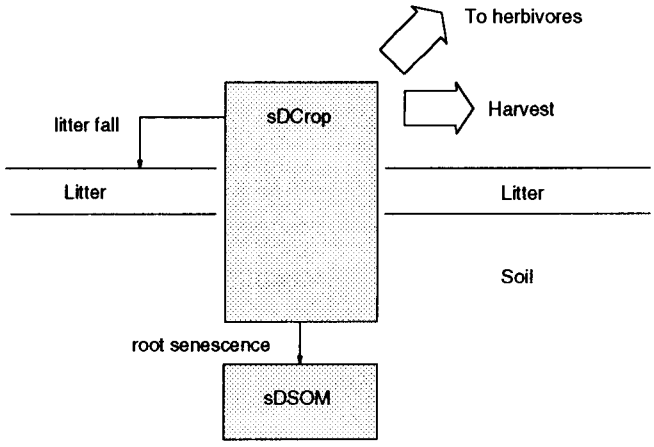

Fig. 11. Diagram of crop fluxes

In peaty meadows, average production ranges from 10.5 to 13.7 tons per hectare per year, depending on fertilization and water table (Boxem & Leusink 1978). The grass biomass, stubble and roots, can be estimated to be between 6 and 8 tons/ha. Since in spring, these grasslands usually produce more than cattle can eat, grass is mown for winter feeding. We take an average situation, where approx. 4.5 tons are mown, and the rest of the production is available for grazing (pers. comm. Van de Ven, CABO). It is estimated that about 20% of total production is lost to litter during grazing and mowing (Boxem & Leusink 1978). How much biomass is lost due to root senescence is not known, so we assume an equal distribution of detritus fluxes above and below ground.

5.3.2 Cadmium cycle

Cadmium uptake by the crop is supposed to have a nearly linear dependence on soil solution at low Cd concentrations, at higher concentrations this is not always true (Gerritse et al. 1983). Uptake from the soil solution is modelled with saturating Monod kinetics. From measurements on crop concentrations in similar soil, we can determine the Bioaccumulation Factor (BAF) of the crop which can be between 0.2 and 0.4 (van Baalen & Leendertse 1986, Langeweg 1989) for this kind of soil:

$$BAF = \frac{Cd\ conc.\ plant}{Cd\ conc.\ soil}$$

The uptake parameters are calibrated on the BAF, such that it remains constant at low Cd concentrations. At higher concentrations, the BAF becomes smaller. Cadmium taken up by the crop is transferred to the litter and back to the soil by litter fall and root senescence. Major cadmium fluxes from the crop are by grazing and harvesting. These fluxes are determined by the size of the biomass fluxes and the cadmium content of the crop.

5.4 Animal functional groups

Animal functional groups resemble one another strongly, sharing the same sort of processes: consumption, assimilation and egestion (fig. 12). In this section, we delineate the processes that are shared by all animal groups and those that differ between groups.

5.4.1 Biomass fluxes

All animal functional groups consume food (*DCons*) either from one or from several sources (fig. 12). Food is assimilated (*DAss*) with a certain efficiency (*fDAss*), and non-assimilated food is egested (*DEges*). Assimilated food is partitioned to growth, reproduction and respiration (*DResp*). All functional groups grow according to logistic growth (Appendix C). The logistic growth equation employed does not distinguish between growth and reproduction. Some natural mortality (*DMort*) is expected for any population, proportional to population density, and we have to estimate the mortality rate. Natural mortality and respiration are modelled as first order processes. Respiration rates have been estimated with an allometric body-size relationship (Peters 1983). Given average body weight, the rate constants can be estimated (Appendix B). Populations can be predated on by other functional groups. This represents a loss term. We can now form a generic mass balance equation for a functional group:

$$\frac{dD}{dt} = DAss - DResp - DMort - DPred$$

with
dD/dt = rate of biomass change [gD·m^{-2} ·y^{-1}]
DAss = assimilation [gD·m^{-2} ·y^{-1}]
DResp = respiration [gD·m^{-2} ·y^{-1}]
DMort = natural mortality [gD·m^{-2} ·y^{-1}]
DPred = predation [gD·m^{-2} ·y^{-1}].

5.4.2 Toxicant fluxes

Animals take up cadmium with their food, or from the soil solution (fig. 12). Cadmium consumption by a functional group (*XCons*) equals the dry weight consumption times the Cd concentration of the food. The actual amount of cadmium that enters the population (*XAss*) depends on the cadmium assimilation efficiency (*fXAss*), which is the fraction retained, of total cadmium ingested by the population. The non-assimilated fraction of cadmium in the food is egested with non-assimilated biomass (*XEges*), and is returned to litter or soil organic matter, depending on the habitat of the animal. Cd assimilation efficiency for mammals typically ranges between 1-10% (Ros & Slooff 1987). Another route of exposure to contaminants is by uptake directly from the soil solution. This phenomenon is believed to play an important role in the uptake of soft-bodied invertebrates, like earthworms (Van Gestel & Ma 1988, 1990). The modelled mechanism of

uptake is analogous to that of toxicant uptake by plants. The use of Monod saturation kinetics ensures a lower BAF at higher dissolved toxicant concentrations, as often observed (Ma 1982, Ma et al. 1983).

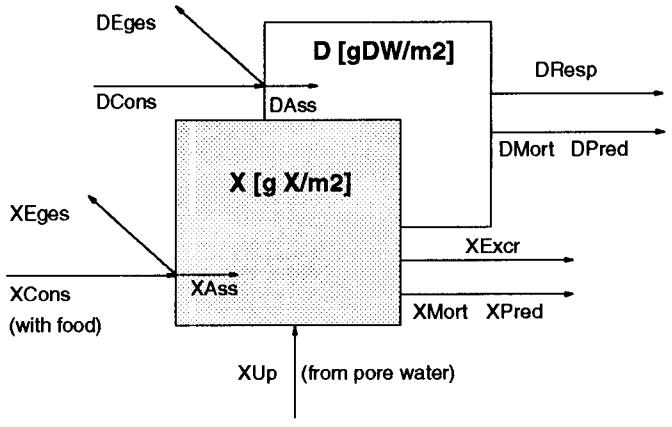

Fig. 12. Diagram of biotic (*D*) and pollutant (*X*) fluxes going to and coming from a functional group. See text for explanation.

The group looses cadmium by mortality (*XMort*), excretion (*XExcr*) and predation (*XPred*). Cadmium excretion is modelled as a first order process. Excretion constants are difficult to find in literature, but it is assumed that the larger the animal, the smaller the excretion constant (Jørgensen & Johnsen 1989). If we assume the compartment to be homogeneous, excretion constants (kXExcr) show a relationship with the half-time(*T1/2*) of the chemical, which is the time to excrete half of the initial body burden:

$$T(1/2) = \frac{ln2}{kXExcr}$$

Now we can also construct a general toxicant mass balance:

$$\frac{dX}{dt} = XAss\ (+\ XUp)\ -\ XExcr\ -\ XMort\ -\ XPred$$

with
dX/dt = rate of toxicant mass change [gX·m^{-2} ·y^{-1}]
XAss = Cd assimilation [gX·m^{-2} ·y^{-1}]
XExcr = Cd excretion [gX·m^{-2} ·y^{-1}]
XMort = Cd loss by natural mortality [gX·m^{-2} ·y^{-1}]
XPred = Cd loss by predation [gX·m^{-2} ·y^{-1}]

Functional groups in close contact with pore water require an additional Cd input:
XUp = Cd uptake from soil pore water [gX·m^{-2} ·y^{-1}]

5.4.3 Food limitation and growth

Population growth rate is set to a maximum growth rate, the actual growth rate depends on food supply. The maximum growth rate is multiplied by a reduction function, again we use a Monod saturation function. Meadow birds, Diptera larvae and worms have two food sources. Meadow birds eat worms and Diptera larvae, Diptera larvae eat roots and soil organic matter and worms eat litter and soil organic matter. For these groups, food saturation functions are used to allow for several food sources. Food saturation for more

than one food source can be modelled as Michaelis-Menten kinetics, as used by Smith (1982) for microorganisms having several energy sources. No food preference factors are used, though they can be easily incorporated when judged necessary. Maximal consumption rates have been estimated with allometric body-size relationships (Peters 1983).

Consumption of earthworms received special attention, since these animals eat their way through soil or litter, filtering organic particles from the matrix. We modelled the consumption of earthworms in a way comparable to the filtering of aquatic organisms (Janse & Aldenberg 1990). In soil with a high (palatable) organic matter content, the worms ingest a small amount of soil to obtain their food. In soils with low organic matter content, the filtering rate will be increased (the worms will eat more soil) up to a fixed maximum filtering rate. Food availability governs where the earthworms will forage. If litter is abundant, worms will primarily filter the litter layer. If there is hardly any litter, worms will filter the top soil.

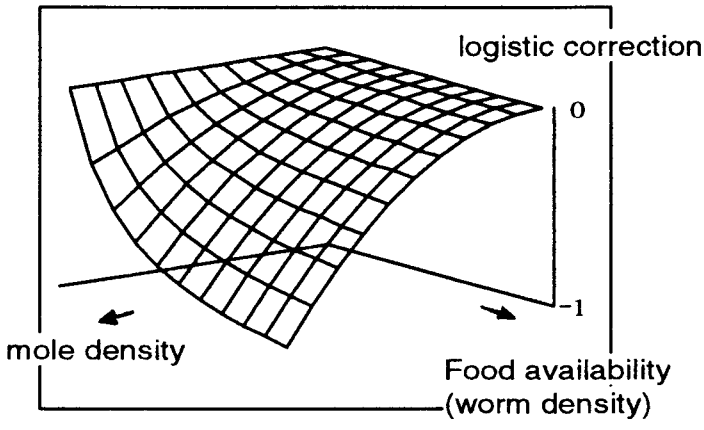

Fig. 13. Logistic correction on mole assimilation depends on model density and food availability (worm density).

All animal functional groups grow according to logistic growth, if they are not predated upon or limited by an explicitly modelled factor, such as pH, temperature, toxicants etc. Biomass assimilation is not a first order processes like respiration, but is influenced by a correction from the logistic growth equation (cf. appendix C). The logistic correction on mole assimilation is shown in fig. 13. The positive x axis points towards the reader, and the y axis is plotted from left to right. The logistic correction is the z axis (vertical). At low mole densities (back of the plane), food availability does not influence the correction and the population can attain almost exponential growth. At mole densities close to the carrying capacity (front of the plane), high food availability brings about the highest negative feedback, slowing down population growth.

5.4.4. Mortality

In the original definition of logistic growth, mortality rises with increasing population density due to competition and aggression (as reproduced in Wilson & Bossert 1971). In our derivation of logistic growth, this 'environmental correction' on mortality depends also on food availability (Appendix C). The correction function on mole mortality is depicted in fig 14. The positive x-axis points towards the reader, and the y axis is plotted from left to right. The logistic correction is the z axis (vertical). This surface plot shows, that with rising mole density, the intraspecific competition causes mortality to rise. At high food availability, this effect is much less pronounced than at low food availability, meaning that at low food density crowding and competition cause more deaths than at higher food density.

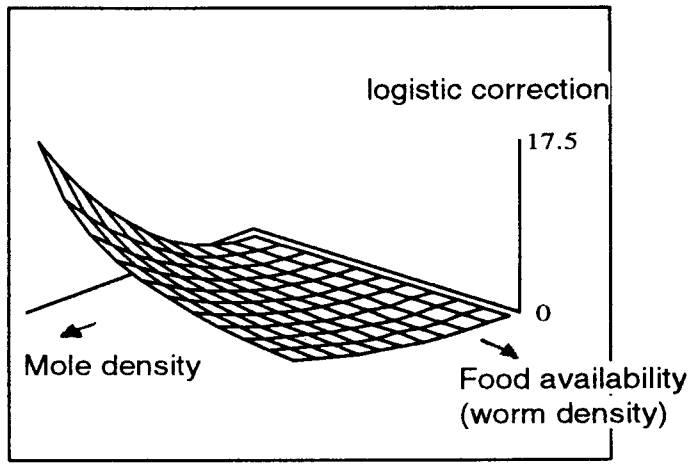

Fig 14. Logistic correction on mortality of moles depends on mole density and food availability (worm density).

6 Parameter estimation, calibration and model analysis

6.1 Data requirements

The CATS models are integrated ecotoxicological models, and therefore require parameters from different categories (table 1). A full description of model parameters and references can be found in Appendix B. General soil characteristics (table 1, cat. 1) such as density, moisture content, and porosity influence leaching and partition of toxicant over dissolved and sorbed phase. In general, these characteristics are relatively easy to collect. Primary production (cat. 2) is defined in three classes in the ecotope system (see section 2.1), so no great level of detail is required. Parameters are calibrated on known production data (see next section).

Table 1. Number of parameters per model category. nGroups = number of functional groups in the CATS model.

category	description	number
1. soilcharacteristics	density, moisture, porosity etc.	13
2. primary production	growth, harvest, litterfall	7
3. biomass cycle	growth, respiration, mortality etc.	nGroups * 7
4. toxicant sorption	sorption constants	3
5. toxicant uptake & excretion	uptake, assimilation, excretion	nGroups * 3 or nGroups * 5

The biomass cycle (cat. 3) requires rate parameters for growth, respiration, mortality, half saturation constants, carrying capacity and initial biomass. Most parameters can be estimated with the aid of body-size relationships (appendix B) or can be collected, but little is known about natural mortality rates. Sorption requires three sorption constants (cat. 4). For organic micropollutants, sorption to inorganic matter (SIM) is not very important (Boesten 1991), in contrast to heavy metals. The separate sorption constants must be calibrated on a known overall sorption constant. This overall sorption constant is a model output to facilitate comparison with data. Parameters for toxicant uptake and excretion (cat. 5) are collected for every functional group. Plants or animals that take up toxicant from the pore water require two additional parameters, uptake rate and a half saturation constant. In general, assimilation efficiencies are better known than excretion rates. Uptake rates from pore water are not available, but are determined by calibration on Bioaccumulation Factors (BAF).

The model can be applied to a different toxicant by changing those parameters that determine behaviour in soil and organisms: sorption constants, assimilation efficiencies, excretion and or degradation rates and initial concentrations. Parameters concerning the food web, constituting over half of all parameters, remain the same. A grassland on different soil with the same type of food web requires the change of a few soil and sorption characteristics.

6.2 Model output

The model is designed to calculate toxicant concentrations in all relevant compartments. So, model output consists of concentrations in soil, litter, pore water, crop and all animal functional groups. Since we are also interested in the process of food-chain transfer of toxicants, bioaccumulation factors (BAFs) are also model output. The biomass cycle is the backbone of the model, and therefore biomass of litter, soil organic matter, grass and all animal functional groups are model output too.

6.3 Calibration and Range-Check procedures

Submodels of CATS-1 have been calibrated manually on known averages such as biomass, Cd concentrations and BAFs. The interaction of submodels in the total model can be difficult to understand, especially since biomass and toxicant cycle interact in CATS models. Therefore, runs have been performed with simultaneous sampling of most parameters to calibrate the model on known data. A calibration procedure has been employed using a calibration procedure described by Janse et al. (1992). This procedure consists of the next steps:

- Parameters are sampled from uniform parameters distributions, a prerequisite for Bayesian analysis. Use has been made of the software package UNCSAM to generate the samples (Janssen et al. 1992).
- Model runs are performed with successive parameter samples, using an interface between UNCSAM and the simulation software ACSL, called TREATSAM (Traas et al. in prep.).
- Model output such as concentrations and BAFs is compared with ranges of acceptable output (Appendix B). If the output is acceptable, the run is completed. If the output is not acceptable (i.e. outside the range), the run is stopped.
- Successful model runs are subjected to a procedure to determine the best fit to available data (appendix B). This procedure is based on Bayesian statistics (Box & Tiao 1973), and is implemented in the program BACT, an acronym for Bayesian Calibration Technique (Aldenberg & Kramer in prep).

The run with the best fit to available data according to BACT, has been used to study the general model behaviour, as shown in section 7.1.

6.4 Model analysis

6.4.1 A probabilistic model treatment and uncertainty analysis.

Models contain several sources of uncertainty. Some of this uncertainty is due to the model structure itself, because we do not know whether the model is correct. Often, we do not know the exact initial conditions of a modelled situation, or the influence of the environment on the system (Janssen et al. 1990). The parameters of the model itself are often not known exactly. In the CATS model, many parameters are inherently variable because we use the concept of functional groups, and because of spatial and temporal

variation. This means that respiration rates, consumption etc. are variables with a certain probability distribution. So, in CATS we have different sources of uncertainty:
- unintentional uncertainty
- intentional uncertainty,

due to the concept of functional groups and biological variability. Inherent natural variability is seen as one of the reasons for an uncertainty analysis (Kros et al. 1990). In this regard, there is no difference between our wish to express model output as probability distributions, and the results of an uncertainty analysis, which are also distributions. With uncertainty analysis, we can quantify uncertainty associated with different cadmium-loading scenario's.

Uncertainty analysis was performed in a similar way as described for the calibration procedure. Parameter distributions as used in the analysis are specified in the parameter listing of appendix B. Only the initial soil concentration is specified as a normal distribution. A correlation is specified between the sorption constant for soil organic matter and initial soil concentration. A few parameters have not been taken into account in this analysis, most notably soil depth, carrying capacities and average annual rainfall. Uncertainty in Cd input has also not been taken into account, since cadmium loading is the subject of the scenario studies.
The Range Check procedure was used, and rejected runs excluded from the uncertainty analysis. With UNCSAM we generated 2200 parameter sets from specified distributions, and, depending on the loading scenario, between 739 and 765 runs were accepted (with output within specified ranges). These runs were used for uncertainty analysis.

6.4.2 Uncertainty measures

The uncertainty in model output such as bioaccumulation factors and toxicant concentrations is analyzed by
- the geometric average, standard deviation and coefficient of variation, in 2015 and 2050, for all Cd scenario's.
- the histograms of the probability distributions in 2015 at three loading scenario's.
- uncertainty measures.

Properties of different uncertainty measures and how to choose a suitable one have been treated in full elsewhere (Janssen et al. 1990, 1992). The most important aspects with regard to the choice of a measure are mentioned below:
- the Coefficient of Determination (COD) or R^2 of a linear regression model is used to determine whether the linear model is suitable. If COD is larger than 0.7, the use can be justified. If COD is below 0.7, data transformation should be used to achieve a better fit, for instance rank correlation. The linear regression model without data transformation was always used.
- to use the linear regression model, independent variables may not show significant correlations. A measure for collinearity is the Variance Inflation Factor (VIF), as calculated by UNCSAM. Collinearity is within bounds if the VIF is not larger than 5 to 10. In all the presented cases, VIFs were smaller than 6 so we accepted the linear model.

When these conditions are satisfied, the uncertainty measure RTU (Root of Partial Uncertainty Contribution (PUC)) is a suitable measure (Kros et al. 1990). The disadvantage of the RTU is that weak sources score high if they are correlated with strong sources. It is advised to compare the RTU with the SRC. If a weak source according to the SRC scores high with the RTU, a possible correlation with a strong source can be identified (Janssen et al. 1990). In the tables with uncertainty measures, we present both the RTU and the SRC.

6.5 Evaluation of environmental standards

The reference model run can be used to assess whether predicted concentrations in soil, litter pose any threat to soil organisms. Since food chain transfer of the toxicant is integrated in the model, we can do the same for larger terrestrial vertebrates. However, since uncertainty is associated with every model output, we need the distribution of this output to assess the *probability* that an NOEC, or any applicable environmental standard is exceeded. Several NOEC's and suitable environmental standards have been collected, and applied to the matching output. To determine this probability, we calculate the right-tail probability that the standard or NOEC is exceeded, as shown by the shaded area in fig. 15. Exceedance probabilities are expressed as percentages and calculated in 2015 and 2015, for all loading scenario's. The error of this estimate, due to the limited number of samples, was not determined.

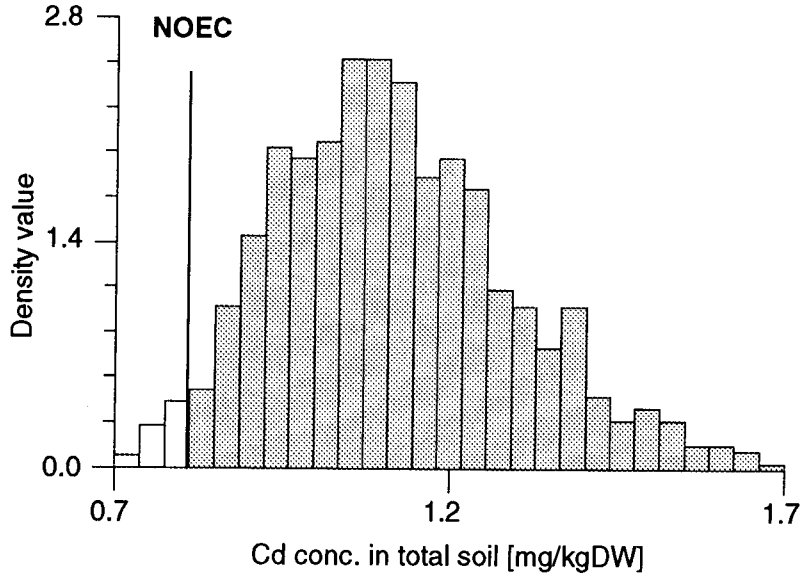

Fig. 15. Histogram of probability distribution of total cadmium in top soil. The right tail probability that the NOEC is exceeded, is calculated from the hatched area.

7. Results

In this chapter, results are presented for a reference run and from an uncertainty analysis of the model. Firstly, general model behaviour is shown. Secondly, the results of the uncertainty analysis using Monte Carlo simulations are shown and model uncertainty can be analyzed. Thirdly, with the results of the uncertainty analysis we can assess whether load reductions lead to an improvement in ecosystem quality, as judged by NOECs, environmental quality standards etc.

7.1 General model behaviour.

7.1.1 Biomass cycle

The reference simulation has been carried out for the period 1990 - 2015. Simulations shown are for the present Cd load, since the cadmium load does not influence the biomass cycle. The results clearly show, that a steady state is reached within a period of three years (Fig 16a,b,c). This is true not only for the functional groups shown here, but also for litter biomass, soil organic matter, mice and moles.

The characteristic response time of the system with respect to the biomass cycle, independent of parameter variation, appears to be very small indeed. For this reason, calculated biomass is compared with acceptable ranges of biomass (the Range Check procedure) 5 years after the start of the simulation. Because the reference run has been allowed to equilibrate, all steady states are very close to the starting point (the y axes show very little variation).

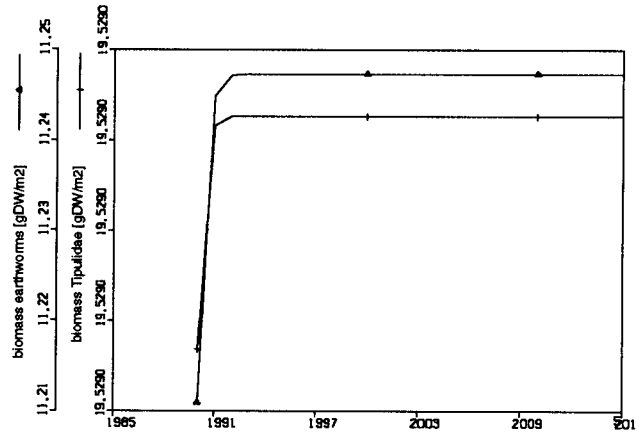

Fig. 16a. Biomass of soilfauna in reference run from 1990 to 2015. Two different y axes are used.

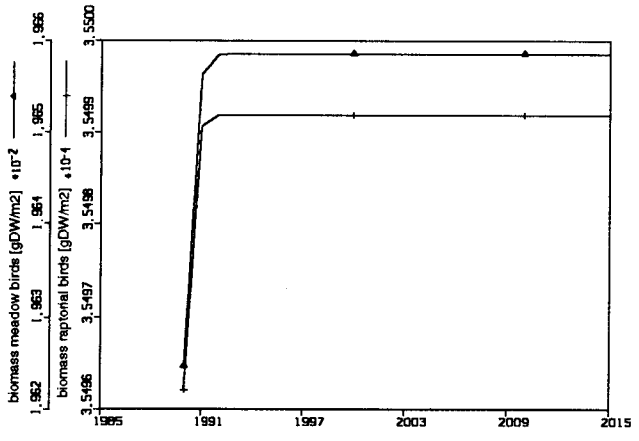

Fig. 16b. Biomass of birds in reference run from 1990 to 2015. Two different y axes are used.

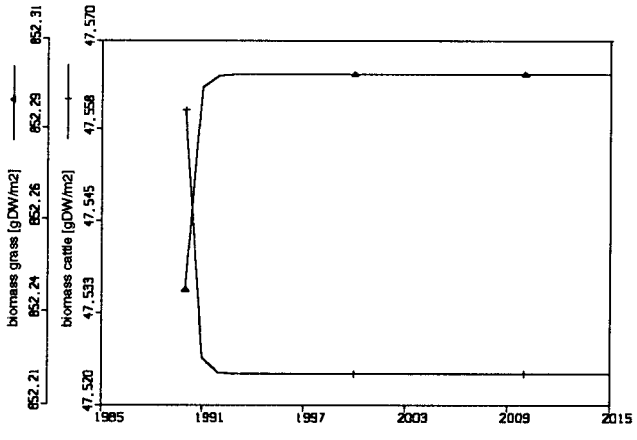

Fig. 16c. Biomass of grass and cattle in the reference run from 1990 to 2015. Two different y axes are used.

7.1.2 Concentrations

Concentrations are model output, and can be calculated any time during the simulation. Concentrations in all model compartments react to the cadmium loading and are calculated for the period 1990 to 2050 (fig. 17a-f). The initial cadmium concentration in the top soil (Fig. 17a) starts at about 0.7 mg/kgDW, a high value because of the location of these lowland peat meadows in a densely populated and industrialised region. In these soils, cadmium values of 0.2 to 1.0 mg/kg are measured (CCRX 1985).

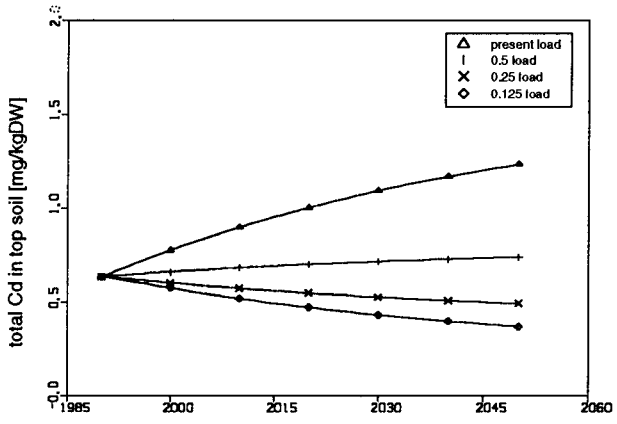

Fig. 17a. Cd concentration in top soil at all loading scenario's, of reference run.

It can be seen that at the present level (uppermost line), Cd content continues to rise, even after 2050. A steady state is reached somewhere around 2300, with Cd concentrations of approx. 1.6 mg-/kgDW (results not shown). Half the present Cd load almost stops the increase in cadmium concentration, and steady state is achieved at approx. 0.8 mg/kgDW (results not shown).
If we lower the Cd input to one-eighth, we reach values of relatively clean grass-lands (Ma et al. 1991) in 2050, and steady state is reached at approx. 0.2 mg/kgDW.

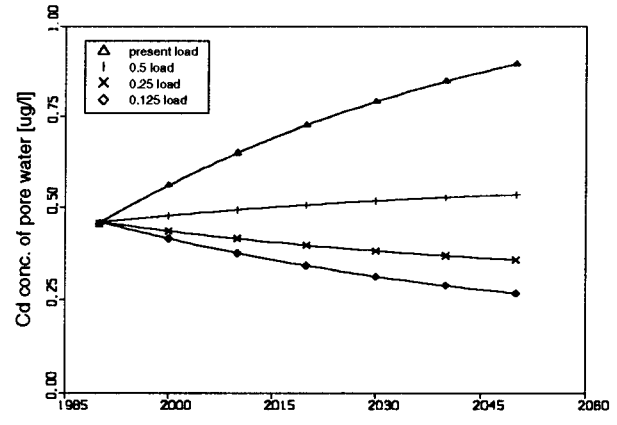

Fig. 17b. Cd concentration in pore water, at all loading scenario's, reference run.

Since dissolved cadmium is supposed to be in equilibrium with sorbed cadmium (Boesten 1991), and modelled as such, it follows the same pattern and dynamics as total cadmium (Fig. 17b).
Crop concentrations also show the same reaction to cadmium loading scenario's, since we modelled cadmium uptake of the crop from the pore water (fig. 17c). Earthworms and all other functional groups (fig. 17d-f) show the same accumulation pattern. Kidney concentrations of moles and mice were calculated using BAFs, and they also show the same accumulation pattern and dynamics.

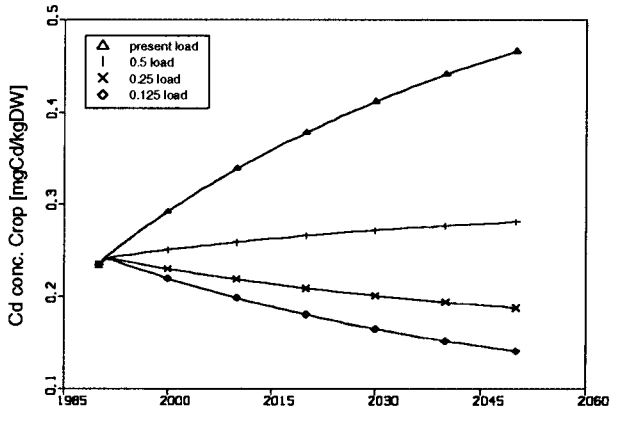

Fig. 17c. Cd concentration of grass at all loading scenario's, reference run.

We can conclude that cadmium accumulation in all compartments show the same dependency on top soil concentrations, and that steady state concentrations for all compartments are reached somewhere around the year 2300. For this type of model, with no feedback between accumulation level and the biomass cycle, an almost linear relation seems to exist between soil concentrations and concentrations in all functional groups. This suggests that bioaccumulation factors can be derived from the model to predict the pseudo steady state concentration in functional groups.

The calculated concentrations could be used to evaluate whether certain environmental standards are exceeded, if we would assume that this reference run is representing the true state of the grassland ecosystem. Since inherent natural variability is not incorporated in this run, this single run can never represent the natural variability of the system. We must make use of Monte-Carlo simulations to calculate the probability that environmental standards are exceeded. This matter will be dealt with in the next section.

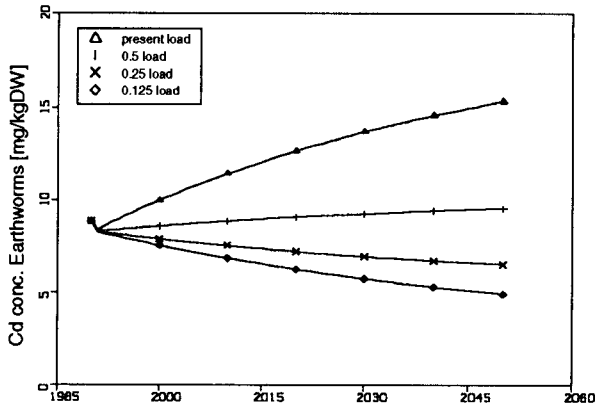

Fig. 17d. Cd concentration in earthworms, at all loading scenario's, reference run.

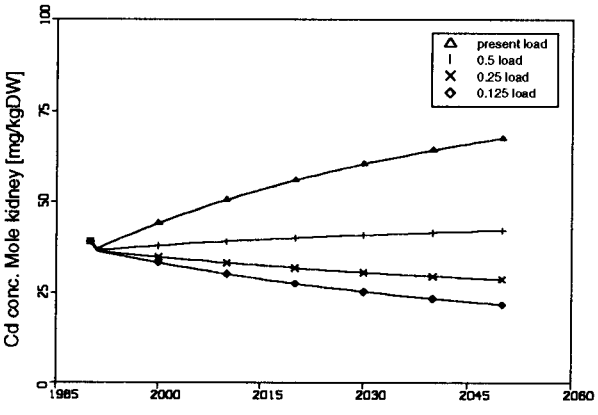

Fig. 17e. Predicted cadmium concentration in kidney of moles for all loading scenario's, reference run.

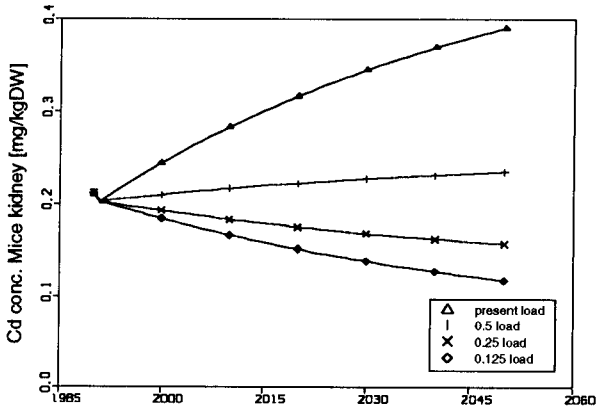

Fig. 17f. Predicted cadmium concentration in the kidney of mice, for all loading scenario's, reference run.

7.2 Uncertainty analysis

7.2.1 Biomass

The realized biomass distributions after the uncertainty analysis runs are depicted in figs 18a-h, for the year 2015. Different cadmium loads do not influence the biomass cycle, so the same biomass distributions are calculated for every scenario. These distributions result from uncertainty in the parameters for food intake, growth, mortality and respiration as incorporated in the modified logistic growth equations. They are influenced by the range check procedure, in which the calculated biomass is compared with acceptable ranges as soon as a steady state is reached. As a result of this procedure, uncertainty of the biomass estimates is reduced, thereby reducing uncertainty of the toxicant part of the model because the concentration is calculated from both cycles. The acceptable ranges of biomass are often much wider than the actual realized biomass distributions. This is the case for grass, Tipulidae and earthworms. It is expected that a low biomass of soil fauna groups, would prevent the predators (moles and birds) to reach a high density (biomass). Therefore, if the predators are experiencing food limitation in the model, biomass distributions would be expected to be skewed to the right. The results show that most biomass estimates, except for cattle and grass, are skewed to the left.

7.2.2 Bioaccumulation factors

Mathematical model analysis

On the basis of mathematical analysis, we can gain insight into the bioaccumulation process. In Appendix D, a formula is derived from the model equations for the maximum Bioaccumulation Factor (BAF), but only for animals exposed through their food only.
The BAF calculated with this formula, can be used to predict the equilibrium concentration in a functional group by multiplying the Cd concentration of the food with the BAF. The BAF depends not only on toxicokinetic parameters, but also on parameters of the biomass cycle such as respiration and mortality rate:

$$BAF = fXDass \cdot \frac{kDResp + kDMort}{kXExcr + kDMort}$$

with
fXDAss ratio of the ass. efficiency of cadmium and ass. efficiency of biomass [-]
kDResp respiration rate constant of functional group [1/y]
kDMort mortality rate constant [1/y]
kXExcr excretion constant for cadmium [1/y]

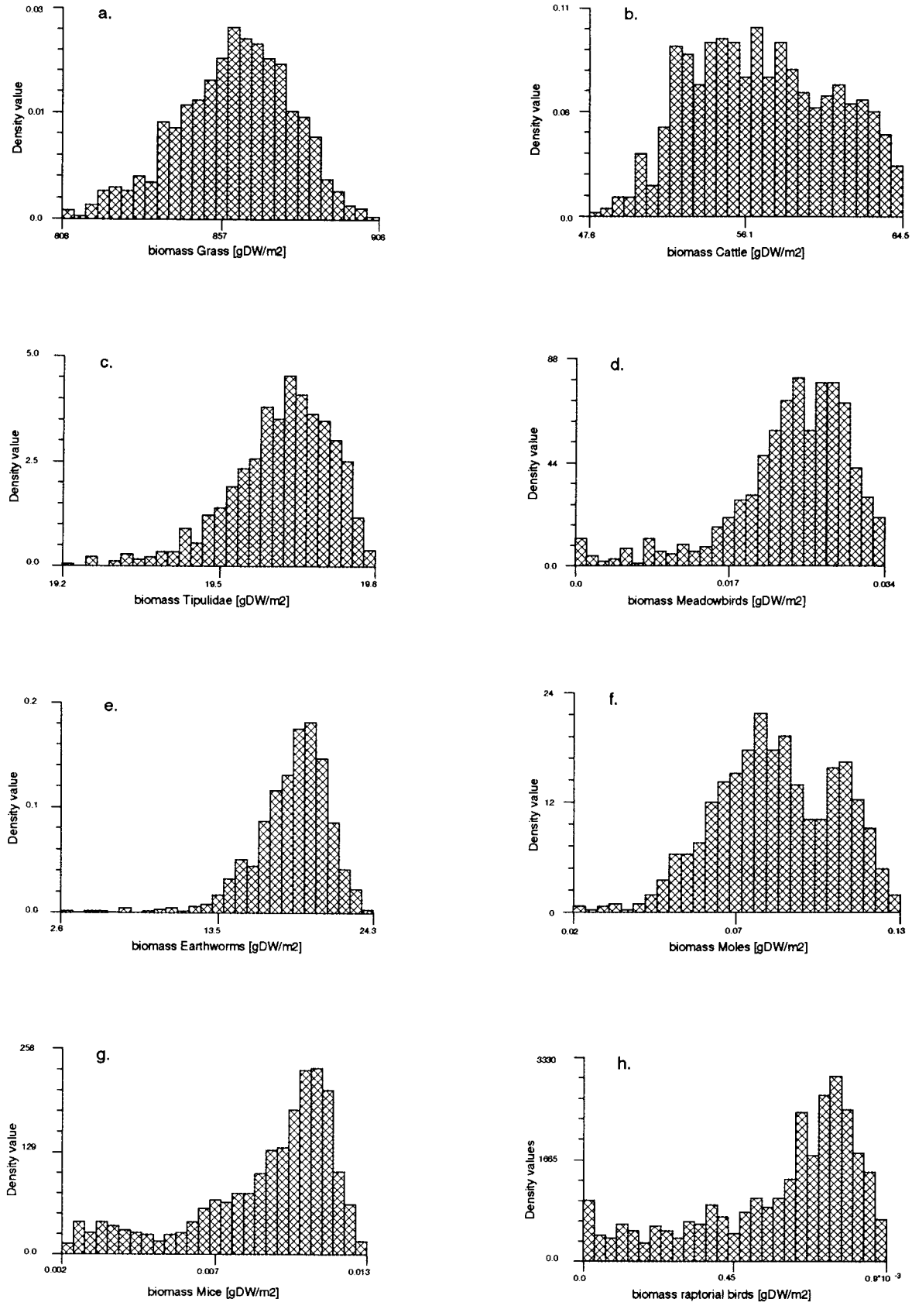

Fig. 18. Probability distributions of the biomass of all functional groups in the year 2015.

In general, the assimilation efficiencies, and respiration rate are relatively well known. Mortality and Excretion rates are less well known. We varied the excretion constant over a range of realistic values (Ros et al. 1986), between half times of 85 to 500 days. A low excretion constant corresponds with a long half time, a high excretion constant with a short half time. For this group, uncertainty in excretion rate influences the BAF considerably (fig. 19).

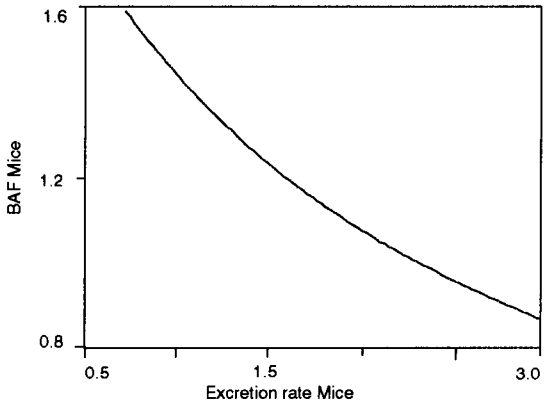

Fig. 19. The influence of the half time of cadmium on the bioaccumulation factor for Mice.

This formula can be used to predict the uncertainty in the bioaccumulation factor, if the uncertainty of the parameters can be determined. It can also be of use to calibrate parameters whose values are less well known on measured concentrations. The excretion rate (kXExcr) is such a parameter. The uncertainty analysis based on regression will show if the parameters of the formula for the maximum BAF are indeed important sources of uncertainty. If this proves to be the case, we have an easy to use analytical tool to predict the worst case scenario for food chain transfer of a toxicant.

7.2.3 Uncertainty analysis based on regression

Apart from mathematical model analysis, numerical methods have been devised based on regression models. The next section presents the result of this type of analysis, not only for bioaccumulation factors but also for predicted concentrations in different model compartments. Uncertainty measures are only calculated for 2015, and three loading scenarios. The influence of a parameter, input or initial value on the uncertainty of the model output is studied with uncertainty measures, calculated from the regression model. Parameters are listed in order of importance, according to the RTU of the present load scenario (first two columns). The values are followed by the ranking. The rank of a parameter may differ, depending on the uncertainty measure used and the Cd loading scenario.

7.2.3.1 Bioaccumulation factor grass

The bioaccumulation factor (BAF) for the grass is the quotient of the concentration in grass and the concentration in total soil. The distribution of the bioaccumulation factor is shown in fig. 20. It is truncated because of the Range Check procedure, the total allowed range is between 0.20 and 0.46 (appendix B). The BAF of the crop appears to be a normal distribution. Distributions for the BAF are not exactly the same, since the number of successful runs differs between the scenario's used, but differ too little to be plotted in one figure. Therefore, only one distribution is shown in fig. 20.

The average of the bioaccumulation factor is about 0.31, and hardly differs between different scenario's (table 3). In 2050, a slight increase can be seen when the cadmium loading is reduced. This is expected, since the uptake of cadmium from the soil solution is modelled with Monod saturation kinetics. If the cadmium concentration falls, the uptake saturation becomes less and the BAF can increase. The absolute uncertainty (standard deviation) and relative uncertainty (average divided by the standard deviation) do not change over the simulation period. Relative uncertainty is not very large, and is determined largely by the applied Range Check procedure, based on available data.

Uncertainty measures have been calculated with the program UNCSAM, and a ranking of sources (parameters) based on the RTU in the first scenario is presented in table. 2. The calculated uncertainty measure is printed first, followed by the ranking. A high ranking source contributes much to uncertainty. The first 5 parameters contribute most to uncertainty, and this does not change for any scenario. The ranking according to the RTU hardly differs from that according to the SRC, and their values do not differ much. If the RTU and the SRC are equal, no correlations exist between parameters (Kros et al. 1990). The rate parameter (kXUpCr) and half saturation constant (hXUpCr) for uptake of cadmium from the soil are strong sources, just as the sorption constant for soil inert matter. The biomass cycle of the model clearly is important, because the fraction of crop production that goes to litter (fDEnvCr), the rate constant for harvest (kDHarvest) and the assimilation efficiency of cattle (kDAssC) also influence the BAF. This is an example of how interaction between the two cycles can influence the concentration in a compartment of the model.

Table 2. Ranking of uncertainty sources for the BAF grass at different loading scenario's, in 2015.

Scenario	Present load		0.5 load		0.125 load	
parameter	RTU	SRC	RTU	SRC	RTU	SRC
kXUpCr	0.62 (1)	0.67 (1)	0.58 (1)	0.67 (1)	0.51 (1)	0.56 (1)
cXAdsSimIn	0.54 (2)	-0.56 (2)	0.51 (2)	-0.54 (2)	0.46 (2)	-0.48 (2)
hXUpCr	0.45 (3)	-0.48 (3)	0.42 (3)	-0.46 (3)	0.36 (3)	-0.39 (3)
fDEnvCr	0.20 (4)	0.23 (4)	0.20 (5)	0.23 (4)	0.19 (4)	0.22 (4)
kDHarvest	0.19 (5)	-0.16 (6)	0.20 (4)	-0.18 (5)	0.19 (5)	-0.17 (5)
fDAssC	0.18 (6)	0.18 (5)	0.15 (6)	0.15 (6)	0.15 (6)	0.14 (6)
kDRespC	0.10 (7)	0.11 (7)	0.09 (7)	-0.09 (7)	0.07 (8)	-0.07 (8)
kDGrCr	0.07 (8)	-0.07 (9)	0.07 (8)	-0.07 (9)	0.09 (7)	-0.09 (7)
kDAssC	0.06 (9)	-0.07 (8)	0.06(12)	-0.07(10)	0.07(11)	-0.08 (9)
cDTip0	0.06(10)	0.00(89)	0.07 (9)	-0.02(89)	<0.06	<|0.06|
R^2	0.99		0.91		0.74	

Table 3. Basic statistics for the bioaccumulation factor of the grass for all loading scenario's, in 2015 and 2050.

	2015				2050			
	1/1	1/2	1/4	1/8	1/1	1/2	1/4	1/8
average	0.314	0.315	0.316	0.316	0.313	0.315	0.316	0.317
standard deviation	0.061	0.062	0.062	0.062	0.061	0.062	0.062	0.062
coeff. of variation	0.196	0.196	0.196	0.196	0.196	0.196	0.196	0.196

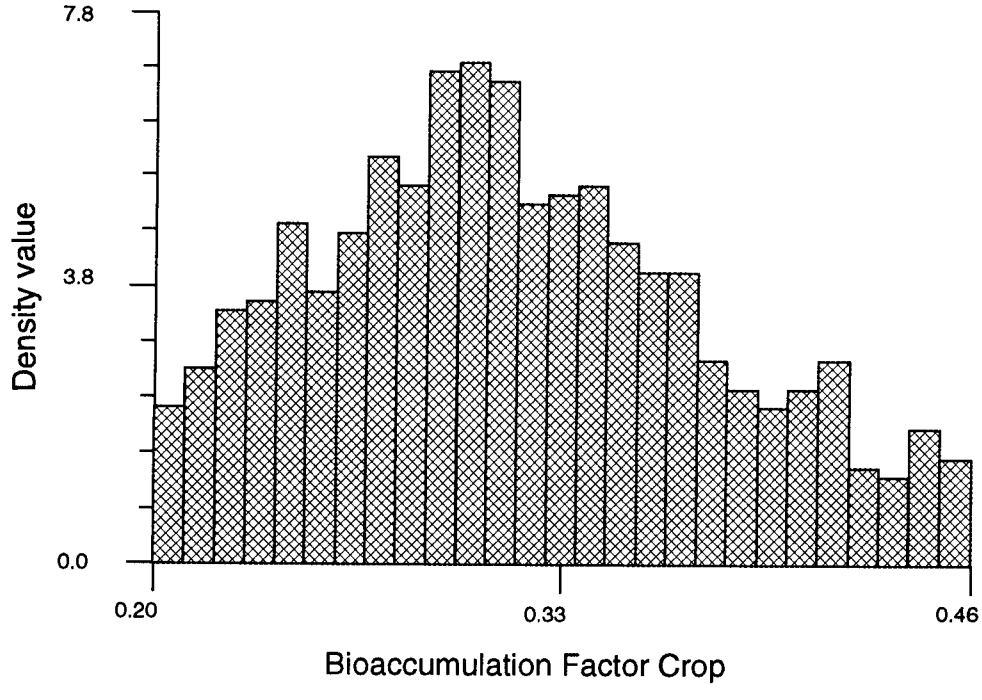

Fig 20. Distribution of the bioaccumulation factor of the grass in 2015 at present Cd loading.

7.2.3.2 Bioaccumulation factor Mice.

The bioaccumulation factor for mice is the quotient of the concentration in mice and the concentration in grass. The distribution is influenced by the applied range check, BAFs outside the range 0.2 - 1.0 are rejected.
The BAF for the present loading is shown and appears to be skewed to the right (fig. 21). The average, standard deviation and coefficient of variation do not change (table 5), therefore the BAF appears to be independent of the cadmium load reductions that were studied.

Uncertainty in the BAF mice is determined largely by the assimilation efficiency of cadmium (fXAssMi), which varies over the range of 1 to 10 percent (table 4). Other parameters that influence uncertainty in BAF are respiration rate (kDRespMi), excretion rate (kXExcrMi), mortality rate (kDMortMi) and the assimilation efficiency of biomass (kDAssMi). These parameters all appear in the BAF formula presented in section 7.2.2. Parameters of the biomass cycle of raptorial birds such as maximum production rate (kDAssMi) and the half saturation for assimilation (hDPrMiR) determine uncertainty to a lesser degree.

The R^2 of the regression in table 4 shows that the fit of the regression model is quite acceptable at the present load, but gets worse with each reduction in loading scenario's. Apparently, model behaviour is becoming increasingly non-linear when loads are reduced. It would be interesting to see whether the fit would improve again, if a steady state is reached after load reduction.

Table 4. Ranking of uncertainty sources for BAF mice at different loading scenario's in 2015.

Scenario	Present load		0.5 load		0.125 load	
parameter	RTU	SRC	RTU	SRC	RTU	SRC
fXAssMi	0.81 (1)	0.86 (1)	0.78 (1)	0.83 (1)	0.72 (1)	0.77 (1)
kDRespMi	0.28 (2)	0.34 (2)	0.26 (2)	0.32 (2)	0.25 (2)	0.31 (2)
kXExcrMi	0.24 (3)	-0.27 (3)	0.42 (3)	-0.46 (3)	0.23 (3)	-0.26 (3)
kDMortMi	0.18 (4)	-0.21 (4)	0.16 (5)	-0.19 (5)	0.15 (5)	-0.18 (5)
fDAssMi	0.16 (5)	-0.21 (5)	0.17 (4)	-0.21 (4)	0.17 (4)	-0.21 (4)
kDAssR	0.16 (6)	-0.19 (6)	0.14 (6)	-0.17 (6)	0.13 (6)	-0.17 (6)
kDAssMi	0.16 (7)	-0.12 (8)	0.09 (9)	-0.10 (9)	0.09 (7)	-0.10 (9)
hDPrMiR	0.11 (8)	0.13 (7)	0.10 (8)	0.06 (9)	0.09 (9)	0.12 (7)
hDConsCrMi	0.10 (9)	-0.07(10)	0.10 (7)	-0.06(11)	0.09 (8)	-0.06(14)
fDAssR	0.07(10)	0.10 (9)	0.08(10)	0.11 (8)	0.09(10)	0.11 (8)
R^2	0.89		0.84		0.73	

Table 5. Basic statistics for the bioaccumulation factor of Mice for all loading scenario's in 2015 and 2050.

	2015				2050			
	1/1	1/2	1/4	1/8	1/1	1/2	1/4	1/8
average	0.454	0.453	0.453	0.454	0.454	0.453	0.453	0.454
standard deviation	0.176	0.176	0.175	0.176	0.176	0.176	0.175	0.176
coeff. of variation	0.388	0.388	0.387	0.388	0.388	0.388	0.387	0.387

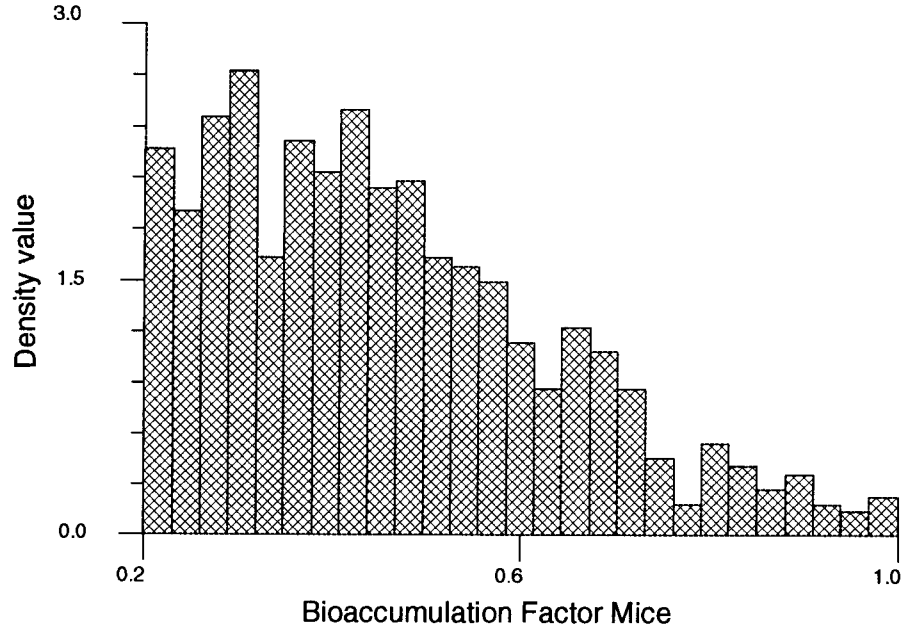

Fig. 21. distribution of the bioaccumulation factor of Mice in 2015, at present Cd loading.

7.2.3.3. Bioaccumulation factor Earthworms

The bioaccumulation factor for earthworms is the quotient of the concentration in worms and the concentration in *total* soil. Uptake of contaminants is from interstitial water and soil properties such as pH, CEC and organic matter content obviously influence the dissolved concentrations. A BAF based on dissolved concentrations shows far less variation than the one used here, for total soil (Boesten 1991). The BAF of earthworms has been shown to be very dependent on soil properties mentioned above (Ma 1982). BAFs based on total soil should therefore be calibrated on BAFs from similar soils. In our model, soil properties are used to determine the value of the sorption constant for the soil inert matter (cXAdsSIMIn). The uptake of cadmium from the soil solution was calibrated on the BAF based on total soil, determined in similar peaty soils. Even so, other factors also influence the BAF so we applied a range check to ensure that the BAF for earthworms would be within an appropriate range for this type of soil.

The distribution of the BAF shows that it is skewed to the right, with a low probability for high BAFs and a high probability for lower BAFs (fig. 22). The average BAF of earthworms and the standard deviation increase with a decrease in loading scenario's (table 7). Relative uncertainty (coeff. of variation) increases with the first load reduction, to remain constant afterwards.

Ranking of uncertainty sources hardly differs between the RTU and the SRC, and between the loading scenario's, apparently correlations between sources are not important (table 6). A surprisingly strong source is the half saturation constant for cadmium uptake from the soil solution (hXUpW), while the uptake rate (kXupW) is ranked 4 or 5. The sorption constant cXadsSIMIn and the excretion rate kXExcrW are also very strong sources. Again, parameters from the biomass cycle also influence the BAF, like kDMortW and kDAssW. It is not surprising that uncertainty is determined most by uptake from the soil, since Cd uptake from food is only a fraction of the uptake from the soil solution.

Table 6. Ranking of uncertainty sources for the BAF Earthworms at different loading scenario's in 2015.

Scenario	Present load		0.5 load		0.125 load	
parameter	RTU	SRC	RTU	SRC	RTU	SRC
hXUpW	0.55 (1)	-0.57 (1)	0.53 (1)	-0.55 (1)	0.47 (1)	0.50 (1)
cXAdsSimIn	0.44 (2)	-0.44 (3)	0.45 (2)	-0.44 (3)	0.36 (2)	-0.38 (3)
kXExcrW	0.44 (3)	-0.46 (2)	0.42 (3)	-0.44 (2)	0.36 (3)	-0.35 (2)
kDMortW	0.35 (4)	-0.36 (4)	0.34 (5)	-0.35 (5)	0.32 (4)	-0.34 (4)
kXUpW	0.28 (5)	0.30 (5)	0.27 (4)	0.29 (4)	0.23 (5)	-0.24 (5)
hDEatW	0.20 (6)	-0.26 (6)	0.21 (6)	-0.26 (6)	0.16 (7)	-0.16 (6)
kDAssW	0.15 (7)	-0.16 (7)	0.15 (9)	-0.17 (7)	0.15 (6)	-0.20 (7)
kDRespW	0.09 (8)	0.09 (8)	0.09 (8)	0.19 (8)	0.08 (8)	0.09 (9)
fDEnvCR	0.05 (9)	-0.03(12)	0.05 (7)	-0.03(11)	0.06(13)	-0.05(12)
fXAssW	0.05(10)	0.04(11)	0.04(14)	0.02(14)	<0.06	<|0.05|
R^2	0.96		0.92		0.72	

Table 7. Basic statistics for the bioaccumulation factor of earthworms for all loading scenario's in 2015 and 2050.

	2015				2050			
	1/1	1/2	1/4	1/8	1/1	1/2	1/4	1/8
average	11.90	12.10	12.22	12.28	11.71	12.11	12.34	12.46
standard deviation	2.88	2.98	3.02	3.04	2.82	2.99	3.07	3.11
coeff. of variation	0.20	0.25	0.25	0.25	0.24	0.25	0.25	0.25

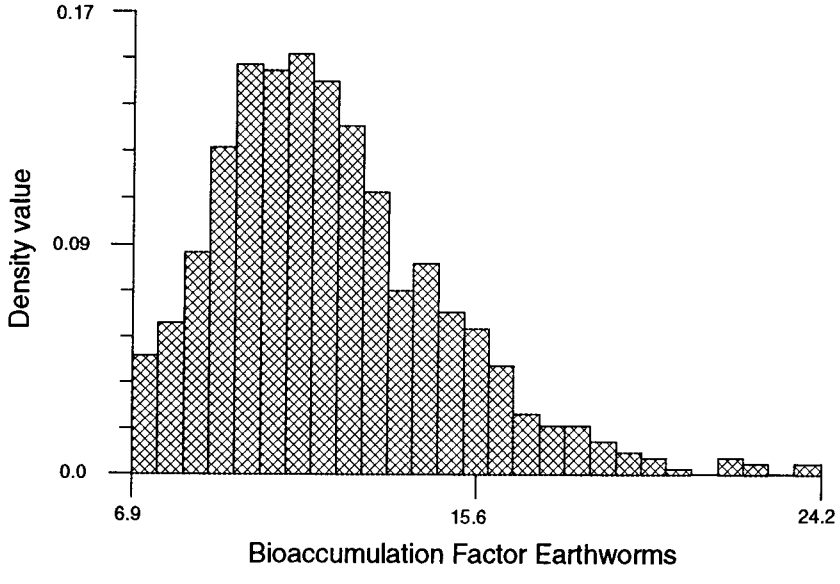

Fig. 22. Distribution of the bioaccumulation factor of Earthworms in 2015, at present Cd loading.

7.2.3.4 Cd concentration of total soil

Total soil concentration is an important soil output, since the exposure of many organisms is via the soil or the soil solution. Protection levels for soil fauna (Van Straalen & Denneman 1989) and mammals and birds have been derived (Romijn et al. 1991b). With these extrapolation methods, a maximum permissible concentration is calculated for a standardized soil. The predicted soil concentration is also used to predict concentrations in higher trophic levels with the use of BAFs.

Histograms of probability distributions for the soil concentration at different cadmium loads are depicted in fig. 23. The y axis is the density value, which should be multiplied with a corresponding value on the x axis to get the probability that a certain concentration occurs. As the load is reduced, the distributions become more peaked, and less wide, i.e., the standard deviation decreases (Table 9). The coefficient of variation (CV) is a measure for the relative uncertainty in the soil concentration. The CV increases when Cd load is reduced, indicating that the average concentration is decreasing at a slower rate than the standard deviation. This indicates that uncertainty increases with Cd load reductions, but in 2050 relative uncertainty has become smaller than in 2015.

The RTU value and ranking is very different from the SRC for the cadmium sorption constant for soil organic matter *cXAdsSOMIn* (table 8).. The SRC ranks this parameter as 45, i.e. 44 sources have a greater influence on uncertainty. According to the RTU, cXAdsSOMIn is one of the most important sources. This is a typical case of correlation of a weak source with a strong source: cXAdsSOMIn was correlated on purpose with high initial soil concentrations. This makes sense, since low initial soil concentrations would generally be found in soils with a low cXAdsSOMIn. In this case, the prediction of the SRC should be used, and the RTU overestimates the importance of this source. The same probably holds true for the initial concentration of Mice (cXDMiceIn), which the SRC ranks as 89 (very weak source) and the RTU as 8.

The density of the soil (RhoSIM) is a very strong source of uncertainty, together with initial soil concentration which becomes first if Cd load decreases. Ranking of most other parameters does not change much when loads are reduced. It is no surprise that the sorption constant for soil inert matter is important, since it influences cadmium equilibrium directly. Parameters determining cadmium uptake of the crop are weaker sources of uncertainty. Because of its high biomass, the grass takes up much cadmium from the soil, thereby influencing cadmium concentration in the soil.

Table 8. Ranking of uncertainty sources for Cd conc. in total soil at different loading scenario's in 2015.

Scenario	Present load		0.5 load		0.125 load	
parameter	RTU	SRC	RTU	SRC	RTU	SRC
RhoSIM	0.70 (1)	-0.70 (1)	0.57 (2)	-0.58 (2)	0.45 (2)	-0.45 (2)
cXTotSoilIn	0.66 (2)	0.67 (2)	0.74 (1)	0.75 (1)	0.72 (1)	0.71 (1)
cXAdsSOMIn	0.40 (3)	0.00(45)	0.44 (3)	-0.02(18)	0.44 (3)	0.01(76)
cXAdsSIMIn	0.18 (4)	0.20 (3)	0.17 (4)	0.19 (3)	0.13 (4)	0.14 (3)
hXUpCr	0.13 (5)	0.10 (5)	0.12 (6)	0.10 (5)	0.07 (9)	0.05 (7)
kXUpCr	0.12 (6)	-0.13 (4)	0.12 (5)	-0.13 (4)	0.11 (5)	-0.11 (4)
kXUpW	0.07 (7)	0.00(44)	<0.06	<|0.03|	<0.07	<|0.04|
cXDMiceIn	0.07 (8)	0.00(89)	0.07 (7)	0.00(75)	0.08 (6)	0.01(73)
fPreSoilDeep	0.06 (9)	-0.06 (6)	0.06 (8)	-0.06 (7)	<0.07	<|0.04|
hDPrB	0.06(10)	-0.01(25)	0.06(10)	-0.01(59)	0.05(19)	0.02(42)
R^2	0.99		0.94		0.79	

Table 9. Basic statistics for Cd conc. in total soil for all loading scenario's in 2015 and 2050.

	2015				2050			
	1/1	1/2	1/4	1/8	1/1	1/2	1/4	1/8
average	1.13	0.886	0.765	0.706	1.35	0.877	0.642	0.525
standard deviation	0.171	0.150	0.141	0.137	0.154	0.114	0.098	0.091
coeff. of variation	0.152	0.169	0.185	0.194	0.114	0.130	0.152	0.173

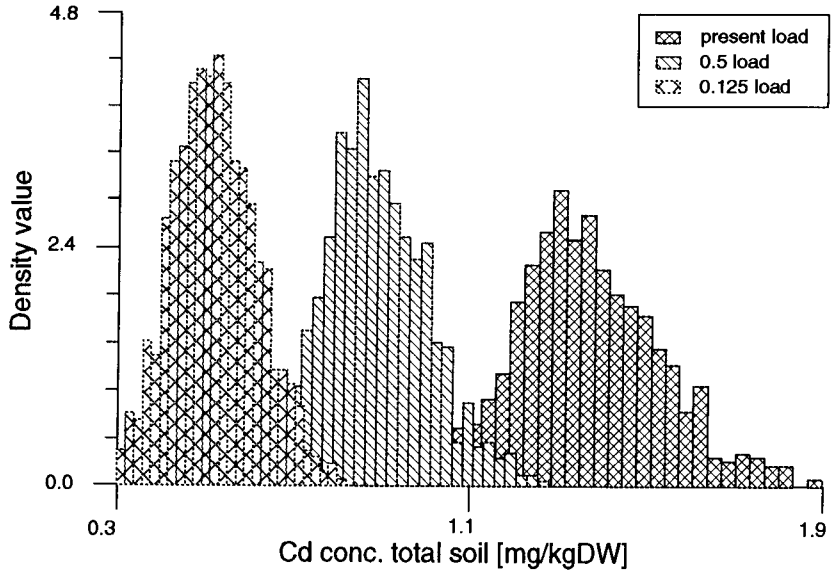

Fig. 23. Distribution of the Cd concentration in total soil in 2015, at different Cd loading scenario's.

7.2.3.5 Cd concentration in pore water

Dissolved cadmium is taken up by crops and earthworms. It can be expected that uncertainty in dissolved cadmium is reflected in the concentration of connected compartments, which prompts us to analyze uncertainty of this output. Another reason for analysis is the use of dissolved cadmium concentrations to evaluate the environmental standard for ground water quality (next section).

Cd concentrations in soil interstitial water are in the range of 0.2 to 1.3 microgrammes per litre (fig. 24). The average concentration will continue to rise at present Cd input, but halving the input starts a slow decline of the concentration (table 11). The coefficient of variation shows that the relative uncertainty increases, but is still rather small, and that uncertainty is reduced as time progresses.

The values for the uncertainty measures RTU and SRC are quite similar, which indicates that strong correlations between parameters (sources) are absent (table 10). The only discrepancy between RTU and SRC is shown once again for the sorption constant for soil organic matter (cXAdsSOMIn), but this is a weak source. The initial soil concentration becomes the strongest source when Cd load is reduced. Surprisingly, the density of the soil (RhoSIM) is a very strong source. RhoSIM was only varied between 0.3 and 0.5. Clearly, RhoSIM is very important in the initial calculation of the dissolved concentration (assuming steady state between the two fractions). As expected, the sorption constant for soil inert matter (cXAdsSIMIn) is a strong source.
Cadmium uptake by the crop from the soil solution also influences uncertainty (kXUpCr, hXUpCr), but these are weaker sources.

Table 10. Ranking of uncertainty sources for Cd conc. in pore water at different loading scenario's in 2015.

Scenario	Present load		0.5 load		0.125 load	
parameter	RTU	SRC	RTU	SRC	RTU	SRC
RhoSIM	0.62 (1)	-0.61 (1)	0.53 (2)	-0.52 (2)	0.41 (2)	-0.40 (2)
cXTotSoilIn	0.58 (2)	0.59 (2)	0.67 (1)	0.68 (1)	0.67 (1)	0.67 (1)
cXAdsSIMIn	0.49 (3)	-0.47 (3)	0.42 (3)	-0.41 (3)	0.33 (4)	-0.32 (3)
cXAdsSOMIn	0.35 (4)	-0.01(20)	0.39 (4)	-0.03(10)	0.40 (3)	-0.02(44)
kXUpCr	0.13 (5)	-0.12 (4)	0.14 (5)	-0.13 (4)	0.13 (5)	-0.12 (4)
hXUpCr	0.12 (6)	0.08 (5)	0.11 (6)	0.08 (5)	0.08 (7)	0.06 (6)
kDHarvest	0.07 (7)	-0.05 (8)	0.07 (8)	-0.04 (8)	<0.05	<|0.03|
cXDMiceIn	0.07 (8)	-0.01(18)	0.07 (7)	-0.01(45)	0.08 (6)	-0.01(74)
kXUpW	0.06 (9)	0.00(63)	0.05(14)	0.00(63)	<0.05	<|0.03|
fPreSoilDeep	0.05(10)	-0.05 (6)	0.06(10)	-0.05 (7)	<0.05	<|0.03|
R^2	0.99		0.93		0.75	

Table 11. Basic statistics for Cd conc. in pore water for all loading scenario's in 2015 and 2050.

	2015				2050			
	1/1	1/2	1/4	1/8	1/1	1/2	1/4	1/8
average	0.751	0.591	0.510	0.471	0.897	0.583	0.427	0.348
standard deviation	0.130	0.111	0.102	0.098	0.109	0.076	0.063	0.058
coeff. of variation	0.173	0.188	0.209	0.209	0.122	0.131	0.147	0.165

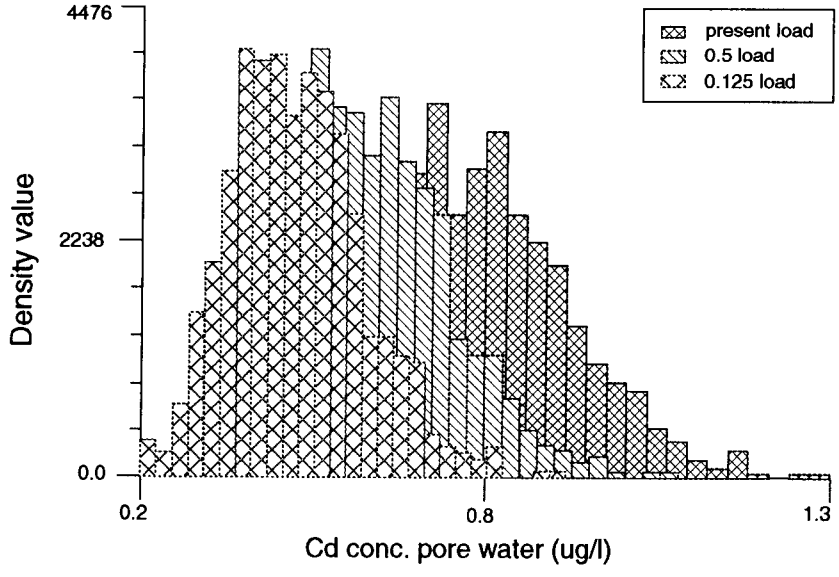

Fig. 24. Distribution of the Cd concentration in pore water in 2015, at different Cd loading scenario's.

7.2.3.6 Cadmium concentration Grass

The cadmium concentration of the grass is determined by the allowed range of the bioaccumulation factor of the grass. The resulting probability distribution is shown in fig. 25. The average concentration already shows a decline from 2015 to 2050 if the Cd loading is halved (Table 13). The absolute uncertainty is reduced, if the Cd loading is reduced but relative uncertainty (coeff. of variation) increases. As time progresses, uncertainty becomes smaller.

Since the concentration of the grass is the product of the bioaccumulation factor and the soil concentration, we can expect both to be important sources of uncertainty. Indeed, the soil density RhoSIM and uptake rate of Cd from the soil solution are strong sources. The initial soil concentration becomes more important when load is reduced (table 12). The partitioning of biomass over harvest (kDHarvest) and litter (fDEnvCr) also influences grass concentration. A difference between RTU and SRC can be seen once more for cXAdsSOMIn, which is a weak source according to the SRC. Parameters of the cattle grazing the crop (fDAssC, kDRespC) are weaker sources that influence uncertainty.

Table 12. Ranking of uncertainty sources for Cd conc. in grass at different loading scenario's in 2015.

Scenario	Present load		0.5 load		0.125 load	
parameter	RTU	SRC	RTU	SRC	RTU	SRC
RhoSIM	0.48 (1)	-0.47 (2)	0.41 (2)	-0.53 (1)	0.33 (2)	-0.33 (3)
kXUpCr	0.47 (2)	0.51 (1)	0.41 (3)	0.40 (3)	0.33 (3)	0.37 (2)
cXTotSoilIn	0.45 (3)	0.45 (3)	0.53 (1)	0.44 (2)	0.55 (1)	0.56 (1)
cXAdsSIMIn	0.35 (4)	-0.36 (5)	0.31 (5)	-0.32 (4)	0.26 (5)	-0.27 (5)
hXUpCr	0.32 (5)	-0.36 (4)	0.28 (6)	-0.32 (5)	0.23 (6)	-0.27 (4)
cXAdsSOMIn	0.28 (6)	0.00(47)	0.32 (4)	-0.01(75)	0.32 (4)	-0.02(28)
kDHarvest	0.21 (7)	-0.19 (6)	0.21 (7)	-0.19 (6)	0.17 (7)	-0.16 (6)
fDEnvCr	0.17 (8)	0.18 (7)	0.15 (8)	0.17 (7)	0.13 (8)	0.14 (7)
fDAssC	0.16 (9)	0.13 (8)	0.13 (9)	0.10 (8)	0.09 (9)	0.07(10)
kDRespC	0.08(10)	-0.08 (9)	0.07(10)	-0.06(10)	<0.08	<|0.06|
R^2	0.99		0.90		0.73	

Table 13. Basic statistics for Cd conc. in grass for all loading scenario's in 2015 and 2050.

	2015				2050			
	1/1	1/2	1/4	1/8	1/1	1/2	1/4	1/8
average	0.351	0.277	0.240	0.222	0.418	0.273	0.200	0.164
standard deviation	0.078	0.065	0.058	0.055	0.071	0.047	0.036	0.031
coeff. of variation	0.222	0.233	0.242	0.248	0.169	0.171	0.180	0.190

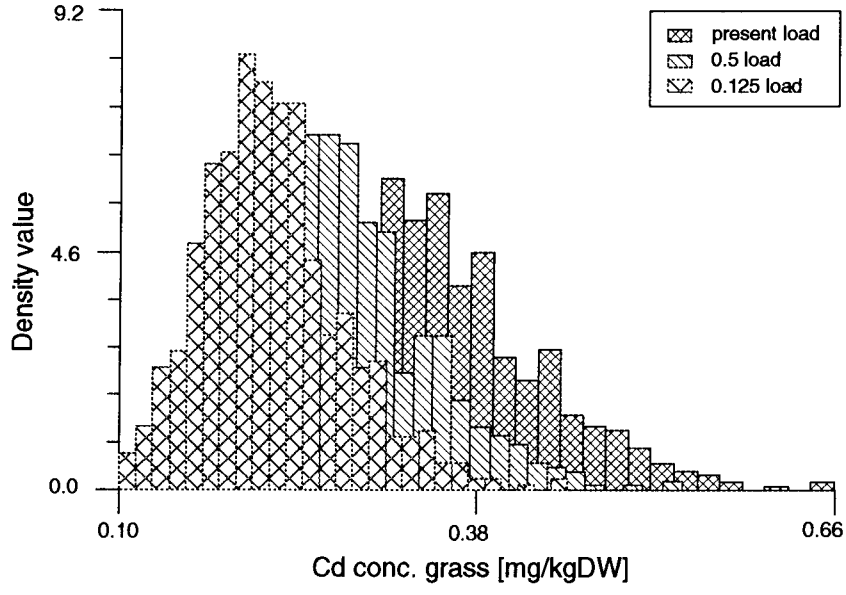

Fig. 25. Distribution of the Cd concentration in grass in 2015, at different loading scenario's.

7.2.3.7 Cd concentration earthworms.

The uncertainty in the prediction of the Cd concentration of worms is studied because worms are an important source of cadmium for meadow birds and especially moles. The probability distributions for cadmium concentrations in earthworms are also skewed to the right (fig. 26). Load reductions show the same dynamics as in compartments. Halving the present load causes a slight decrease of the average concentration in 2050, compared to 2015 (table 15). The reference run still shows a slight increase in 2050 at half the present load, indicating that overall behaviour is a little bit different from the reference run. The standard deviation of all runs decreases and relative uncertainty (coeff. of variation) decreases with a decrease in loading.

RTU and SRC usually have the same ranking of parameters, except for cXAdsSOMIn, which is a weak source according to the SRC, but correlated with the strong source cXTotSoilIn. The half saturation constant for cadmium uptake (hXUpW) from pore water is a very strong source, indicating that the shape of the Monod saturation function is important with respect to uncertainty table 14). The density if the bulk of the top soil, RhoSIM, is important in the calculation of the dissolved concentration, which shows in the ranking of sources. When cd loading decreases, initial soil concentration (cXTotSoilIn) becomes more important and the soil density becomes less important. The uncertainty in the sorption constant of the soil, even though quite a wide range has been used, is a weaker source than the density of the soil (RhoSIM). this reflects that important sources for uncertainty in soil solution concentration are also important for uncertainty of earthworm concentration.

Table 14. Ranking of uncertainty sources for Cd conc. in earthworms at different loading scenario's in 2015.

Scenario	Present load		0.5 load		0.125 load	
parameter	RTU	SRC	RTU	SRC	RTU	SRC
hXUpW	0.49 (1)	-0.51 (1)	0.46 (1)	-0.47 (1)	0.39 (2)	-0.40 (2)
kXExcrW	0.39 (2)	-0.41 (2)	0.36 (3)	-0.38 (3)	0.30 (3)	-0.31 (3)
RhoSIM	0.37 (3)	-0.27 (3)	0.34 (4)	-0.34 (4)	0.27 (4)	-0.27 (4)
cXTotSoilIn	0.34 (4)	0.34 (4)	0.41 (2)	0.41 (2)	0.44 (1)	0.43 (1)
cXAdsSIMIn	0.30 (5)	-0.29 (6)	0.29 (5)	-0.27 (6)	0.21 (7)	-0.20 (6)
kDMortW	0.30 (6)	-0.32 (5)	0.29 (6)	-0.30 (5)	0.23 (6)	-0.25 (5)
kXUpW	0.23 (7)	0.27 (7)	0.22 (8)	0.25 (7)	0.16 (8)	0.19 (7)
cXAdsSOMIn	0.22 (8)	0.01(33)	0.25 (7)	0.00(90)	0.27 (5)	0.00(90)
hDEatW	0.17 (9)	-0.22 (8)	0.17 (9)	-0.21 (8)	0.14(10)	-0.18
kDAssW	0.16(10)	-0.15 (9)	0.16(10)	-0.15 (9)	0.16 (9)	-0.13 (9)
R^2	0.96		0.92		0.72	

Table 15. Basic statistics for Cd conc. in earthworms for all loading scenario's in 2015 and 2050.

	2015				2050			
	1/1	1/2	1/4	1/8	1/1	1/2	1/4	1/8
average	13.33	10.67	9.31	8.63	15.69	10.56	7.86	6.49
standard deviation	3.62	3.04	2.75	2.60	3.82	2.68	2.09	1.79
coeff. of variation	0.27	0.28	0.30	0.30	0.24	0.25	0.27	0.28

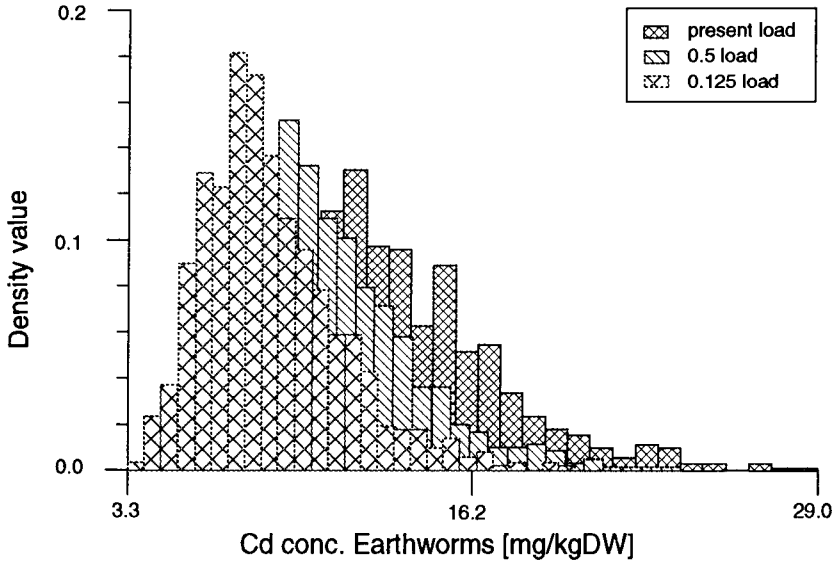

Fig. 26. Distribution of the Cd concentration in earthworms in 2015, at different Cd loading scenario's.

7.2.3.8 Cadmium concentration Mice

Cadmium concentrations in mice are shown because mice are the sole prey for the raptorial birds in this food web. An environmental standard has been derived for the maximum allowed concentration in their food, therefore we study uncertainty for this particular model output.

In general, cadmium concentrations in Mice are low, and strongly skewed to the right (fig. 27). Uncertainty is reduced by range checks, applied on the BAF crop, but also on BAF Mice. Cadmium concentrations in mice are low, since crop concentrations are moderately high and the average BAF for mice is about 0.45. Average cadmium concentrations in herbivorous mice are therefore lower than the soil concentrations at the same Cd load. The pattern of decreasing standard deviation and increasing relative uncertainty (coeff. of variation) is repeated once more (table 17). Compared to other model outputs, relative uncertainty in the mice concentration is larger, indicating the accumulation of uncertainty for higher trophic levels.

Since the concentration in Mice can be predicted by the soil concentration multiplied by BAF crop, multiplied by BAF soil, we expect uncertainty to be influenced by these sources. The fit of the regression model decreased strongly with decreasing Cd loads. Because of the consistency of the ranking of uncertainty measures, we decided to use the linear model even when R^2 was 0.7.

The strongest source of uncertainty is the cadmium assimilation efficiency of mice, and this does not change with different Cd loads (Table 16). Initial cadmium concentration is important too, as predicted. With decreasing Cd loads, the uptake rate of Cd from soil solution of the crop (kXUpCr) becomes less important, and excretion rate (kXExcrMi) becomes more important. All other listed sources are also strong sources for the bioaccumulation factors mentioned, thus the usefulness of the BAF formula has been confirmed.

The kidney concentration of mice has been calculated by multiplying the overall body concentration with a bioaccumulation factor. The predicted kidney level is compared with an NOEC for kidney damage, based on internal concentrations. The uncertainty of this model output shows the same sources as presented in table 16, but uncertainty in the bioaccumulation factor for the kidney is the strongest source (results not shown).

Table 16. Ranking of uncertainty sources for Cd conc. in Mice at different loading scenario's in 2015.

Scenario	Present load		0.5 load		0.125 load	
parameter	RTU	SRC	RTU	SRC	RTU	SRC
fXAssMi	0.68 (1)	0.73 (1)	0.65 (1)	0.70 (1)	0.58 (1)	0.62 (1)
cXTotSoilIn	0.23 (2)	0.22 (4)	0.27 (2)	0.25 (2)	0.30 (2)	0.29 (2)
kXUpCr	0.23 (3)	0.25 (3)	0.20 (5)	0.22 (4)	0.17 (6)	0.18 (5)
kDRespMi	0.23 (4)	0.28 (2)	0.20 (4)	0.25 (3)	0.19 (4)	0.24 (3)
kXExcrMi	0.22 (5)	-0.22 (5)	0.20 (3)	-0.20 (5)	0.21 (3)	-0.21 (4)
RhoSIM	0.21 (6)	-0.20 (6)	0.19 (6)	-0.18 (7)	0.16 (7)	-0.16 (7)
hXUpCr	0.18 (7)	-0.18 (8)	0.18 (7)	-0.18 (8)	0.14 (9)	-0.14(10)
fDAssMi	0.16 (8)	-0.20 (7)	0.16 (9)	-0.19 (6)	0.14 (8)	-0.18 (6)
cXAdsSIMIn	0.16 (9)	-0.17(10)	0.14(10)	-0.15(10)	0.13(10)	-0.14 (9)
kDMortMi	0.16(10)	-0.18 (9)	0.14(11)	-0.15 (9)	0.13(11)	-0.15 (8)
R^2	0.88		0.82		0.70	

Table 17. Basic statistics for Cd conc. in Mice for all loading scenario's in 2015 and 2050.

	2015				2050			
	1/1	1/2	1/4	1/8	1/1	1/2	1/4	1/8
average	0.159	0.126	0.109	0.101	0.190	0.124	0.091	0.075
standard deviation	0.073	0.059	0.051	0.048	0.082	0.054	0.034	0.033
coeff. of variation	0.460	0.470	0.472	0.476	0.432	0.436	0.440	0.446

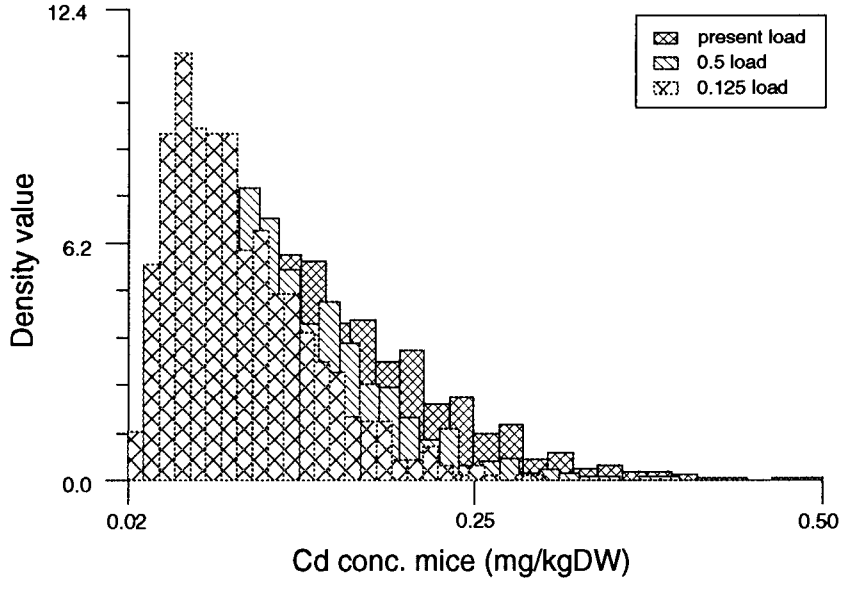

Fig. 27. Distribution of the Cd concentration in Mice in 2015, at different loading scenario's.

7.2.3.9 Cd in food of meadow birds.

Food of meadow birds mainly consists of earthworms and Diptera larvae. Concentration in the food is the weighed average of the concentrations in the food items. Cadmium concentration in food of meadow birds is clearly skewed to the right for all three scenario's depicted (fig. 28). No direct range check was applied to this output, but it is influenced by the allowed BAF for earthworms, which in its turn is influenced by other range checks. Load reductions are not very effective yet in 2015, but this improves with time. A reduction of one eighth of the present load reduces food concentrations with one third in 2015, and food concentrations are reduced with one half in 2050 (table 19). Absolute uncertainty is reduced when loads are reduced, but relative uncertainty (coeff. of variation) increases.

The fit of the regression model used for uncertainty analysis deteriorates with load reductions, up to the limit where we can still use the linear model (table 18). The strongest source is the half saturation constant for earthworms. Clearly earthworms are the most important source of cadmium in food of meadow birds, since other parameters such as kDMortW and kXExcrW are also important sources of uncertainty. The density of soil inert matter (RhoSIM) shows an inverse relation with meadow bird food, so soil properties can influence concentrations in the secondary trophic level too. The initial cadmium concentration (cXTotSoilIn) is fifth in rank for the present load, but its importance increases to become the strongest source at the highest load reduction.

The RTU and the SRC differ for the sorption constant for soil organic matter (cXAdsSOMin). The SRC ranking is very low, indicating a very weak source. The RTU ranking is much higher, because cXAdsSOMIn is correlated with cXTotSoilIn, a very strong source.

Table 18. Ranking of uncertainty sources for Cd conc. in food of meadow birds at different loading scenario's in 2015.

Scenario	Present load		0.5 load		0.125 load	
parameter	RTU	SRC	RTU	SRC	RTU	SRC
hXUpW	0.45 (1)	-0.47 (1)	0.43 (1)	-0.45 (1)	0.36 (2)	-0.38 (2)
kDMortW	0.41 (2)	-0.43 (2)	0.38 (3)	-0.40 (3)	0.32 (3)	-0.33 (3)
kXExcrW	0.38 (3)	-0.40 (3)	0.35 (4)	-0.37 (4)	0.29 (4)	-0.30 (4)
RhoSIM	0.34 (4)	-0.35 (4)	0.39 (5)	-0.33 (5)	0.25 (5)	-0.25 (5)
cXTotSoilIn	0.32 (5)	0.33 (5)	0.27 (2)	0.40 (2)	0.42 (1)	0.42 (1)
cXAdsSIMIn	0.29 (6)	-0.27 (6)	0.21 (6)	-0.25 (6)	0.20 (7)	-0.19 (6)
kXUpW	0.23 (7)	0.27 (7)	0.24 (8)	0.25 (7)	0.17 (8)	0.19 (7)
cXAdsSOMIn	0.20 (8)	0.01(50)	0.14 (7)	0.00(90)	0.26 (5)	0.01(58)
hDEatW	0.13 (9)	-0.18 (8)	0.14 (9)	-0.18 (8)	0.12 (9)	-0.15 (8)
fDEnvCr	0.11(10)	-0.11 (9)	0.11(10)	-0.11 (9)	0.11(10)	-0.11 (9)
R^2	0.93		0.90		0.71	

Table 19. Basic statistics for Cd conc. in food of meadowbirds for all loading scenario's in 2015 and 2050.

	2015				2050			
	1/1	1/2	1/4	1/8	1/1	1/2	1/4	1/8
average	6.60	5.21	4.54	4.21	7.66	5.16	3.84	3.17
standard deviation	1.87	1.57	1.41	1.33	2.01	1.41	1.09	0.93
coeff. of variation	0.29	0.30	0.31	0.32	0.26	0.27	0.28	0.29

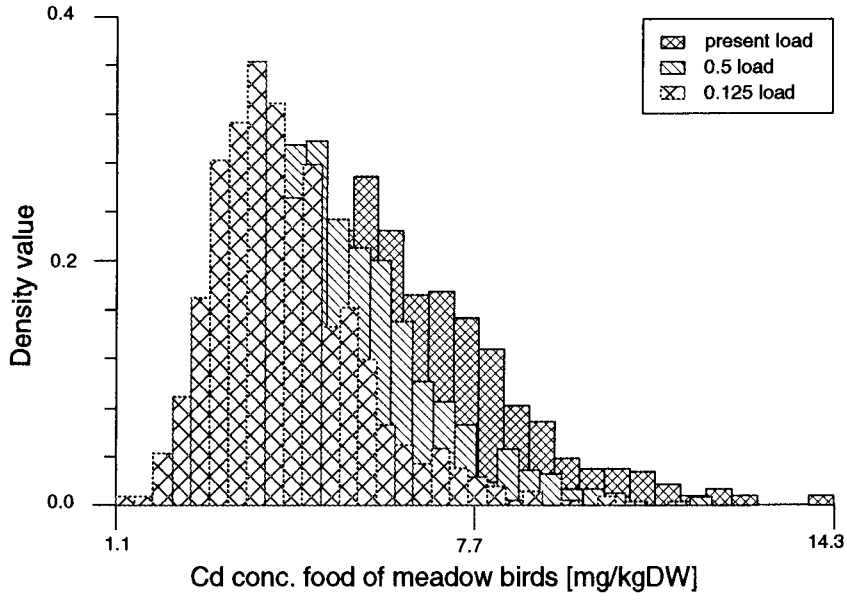

Fig. 28. Distribution of the Cd concentration in food of meadow birds in 2015, at different Cd-loading scenario's.

7.2.3.10 Cd concentration in kidney of moles

The uncertainty in the prediction of the Cd concentration in the kidney of moles is studied because an NOEC is available cd concentrations in kidney. This NOEC has been used before to assess whether small vertebrates are experiencing detrimental effects from cadmium. The kidney concentration is predicted by multiplying the earthworm concentration with an empirical bioaccumulation factor (Ma 1987).

The probability distributions for cadmium concentrations in mole kidney are also skewed to the right (fig. 29), since this is also true for earthworm concentrations. Load reductions show the same dynamics as in other compartments. Halving the present load causes a slight decrease of the average concentration in 2050, compared to 2015 (table 21). The standard deviation of all runs decreases and relative uncertainty (coeff. of variation) decreases with a decrease in loading.

RTU and SRC usually have the same ranking of parameters, except for cXAdsSOMIn, which is a weak source according to the SRC, but correlated with the strong source cXTotSoilIn. The bioaccumulation factor for the kidney (cBCFMoKidWorm) is the strongest source of uncertainty (table 20). However, the variation in this parameter is very well known from field data. The half saturation constant for cadmium uptake (hXUpW) by earthworms from pore water is a very strong source The density if the bulk of the top soil, RhoSIM, is important in the calculation of the dissolved concentration, which shows in the ranking of sources. When cd loading decreases, initial soil concentration (cXTotSoilIn) becomes more important and the soil density becomes less important. All other important sources of uncertainty follow the same ranking as those for the concentration in earthworms.

Table 20. Ranking of uncertainty sources for Cd conc. in the kidney of moles at different loading scenario's in 2015.

Scenario	Present load		0.5 load		0.125 load	
parameter	RTU	SRC	RTU	SRC	RTU	SRC
cBCFMoKidWorm	0.58 (1)	0.59 (1)	0.53 (1)	0.54 (1)	0.47 (1)	0.48 (1)
hXUpW	0.38 (2)	-0.41 (2)	0.36 (2)	-0.39 (2)	0.32 (3)	-0.35 (3)
kXEXcrW	0.33 (3)	-0.34 (3)	0.30 (4)	-0.31 (4)	0.27 (4)	-0.27 (4)
cXTotSoilIn	0.28 (4)	0.28 (5)	0.33 (3)	0.33 (3)	0.37 (2)	0.37 (2)
RhoSIM	0.28 (5)	-0.29 (4)	0.26 (5)	-0.27 (5)	0.23 (5)	-0.24 (5)
cXAdsSIMIn	0.25 (6)	-0.24 (7)	-0.24 (6)	-0.23 (7)	0.19 (8)	-0.17 (7)
kDMortW	0.25 (7)	-0.25 (6)	0.24 (7)	-0.24 (6)	0.21 (7)	-0.21 (6)
kXUpW	0.18 (8)	0.21 (8)	0.17 (9)	0.20 (8)	0.12(10)	0.14 (8)
cXAdsSOMIn	0.18 (9)	0.01(39)	0.21 (8)	0.01 (61)	0.16 (9)	-0.02(46)
kDAssW	0.15(10)	-0.13(10)	0.15(10)	-0.14(10)	0.16 (9)	-0.14(10)
R^2	0.96		0.90		0.74	

Table 21. Basic statistics for Cd conc. in kidney of moles for all loading scenario's in 2015 and 2050.

	2015				2050			
	1/1	1/2	1/4	1/8	1/1	1/2	1/4	1/8
average	59.88	47.91	4.18	38.73	70.47	47.42	35.31	29.11
standard deviation	19.92	16.51	14.80	13.91	21.80	15.11	11.60	9.85
coeff. of variation	0.33	0.34	0.35	0.36	0.31	0.32	0.33	0.34

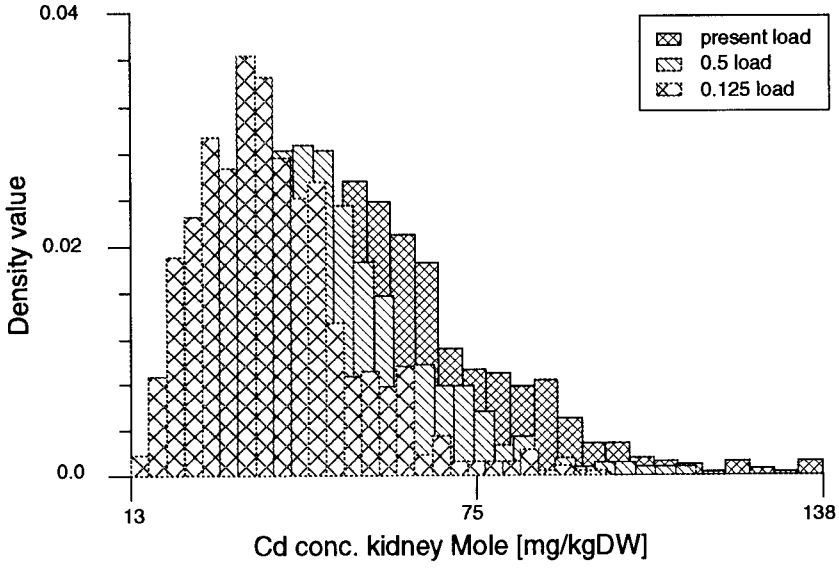

Fig. 29. Distribution of the Cd concentration in kidney of moles in 2015, at different loading scenario's.

7.3 Evaluation of environmental standards.

Probability distributions of model output have been generated for the uncertainty analysis. These distributions are also used to calculate the probability that NOECs or other environmental standards are exceeded. We collected suitable environmental standards, and calculated the probability that they will be exceeded in 2015 or 2050. In the tables, different cadmium load reductions, indicated by 1/1, 1/2, 1/4 and 1/8 times the present Cd input, are printed in bold.

An extrapolation procedure has been used to calculate a soil cadmium concentration at which 95% of all species are protected (Aldenberg & Slob 1991). The Maximum Permissible Concentration (MPC) is calculated from a set of NOEC values (Van de Meent et al. 1990), at a 95 % species protection level with 50% confidence. The value resulting from this, is corrected for the type of soil in our case study area, assuming an organic matter content of 30% and a lutum content of 5%. The present Cd load leads to a 100% exceedance of the MPC (table 22), indicating that the probability that more than 5% of the species are unprotected, is 100%. Load reductions of up to one quarter of the present load do not lead to a lower probability. Only the strongest load reduction of one eighth offers an improvement but we must look beyond 2050 before the MPC can be achieved. The level at which detrimental effect of cadmium on soil species are negligible, is defined as 1% of the MPC (VROM 1991), which for this type of soil is 0.004 mg/kgDW. In case the background value is higher than this level, the background level should be used as a negligible risk level. The background value for Cd is 0.05 mg/kgDW (CCRX 1985) and this standard is exceeded in 2015 and 2050, regardless of the scenario.

Table 22. Probability that the MPC for peaty soils or the background level for cadmium is exceeded at different loading scenarios, in 2015 and 2050. HC5 = hazardous concentration for 5% of the species.

Maximum permissible concentration (MPC) for Cd in peaty soils (at which 95% of species is protected) is 0.4 mg/kgDW, background level is 0.05 mg/kgDW.				
	1/1	**1/2**	**1/4**	**1/8**
MPC 2015 (HC5-50)	100%	100%	100%	99.7%
MPC 2050 (HC5-50)	100%	100%	100%	93.0%
2015 background level	100%	100%	100%	100%
2050 background level	100%	100%	100%	100%

Table 23. Probability that water quality standards and cattle feedstuff standards are exceeded for different Cd loading scenarios, in 2015 and 2050.

ground water quality standard derived from drinking water standard (1.5 µg/l) and cattle feedstuff quality standard (1.2 mg/kg).				
	1/1	**1/2**	**1/4**	**1/8**
Cd dissolved 2015 and 2050	0%	0%	0%	0%
Cd Conc. grass 2015 and 2050	0%	0%	0%	0%

The concentration of the interstitial water is used to assess whether the quality of water that seeps down to deeper layers, conforms to drinking water quality standards since ground water is often used for drinking water. The present quality standard for the preparation of drinking water from surface water is 1.5 µg/l (CCRX 1990) and the probability that it is exceeded for any scenario up to 2050 is zero (table 23).

Romijn et al. (1991b) determined an NOEC for cadmium in food of birds and mammals, extrapolated from existing toxicological data according to Aldenberg & Slob (1991). The NOEC in food is a value only for birds and mammals, at which 95% of these species do not experience a sublethal effect of cadmium. Table 24 shows the probability that the cadmium concentration in food of birds is exceeded, as determined from model calculations for average food concentrations. The probability that the NOEC for food is exceeded, is very small for raptorial birds in 2015, and becomes zero after reducing the cadmium load to a quarter. In 2050, the probability is already zero at half the present load. The food of meadow birds contains much more cadmium, and the probability that more than 5% of meadow bird species are unprotected, is 100% for all scenario's and times studied. This situation is disconcerting, since meadow birds are considered to be important indicators of ecosystem quality.

Table 24. Probability that the environmental standard for food of birds is exceeded at different Cd loading scenarios, in 2015 and 2050.

Environmental standard for Cd in food of birds: 0.35 mg/kg (calculated with an extrapolation procedure).				
	1/1	**1/2**	**1/4**	**1/8**
Cd conc. in food of raptors 2015	2.2%	0.4%	0%	0%
Cd conc. in food of raptors 2050	4.7%	0%	0%	0%
Cd conc. in food of meadow birds 2015 and 2050	100%	100%	100%	100%

Table 25. Probability that the environmental standard for food of mammals is exceeded at different Cd loading scenarios, in 2015 and 2050.

Environmental standard for Cd in food of mammals: 0.35 mg/kg (calculated with an extrapolation procedure).				
	1/1	**1/2**	**1/4**	**1/8**
Cd. conc. in food of moles 2015 and 2050	100%	100%	100%	100%
Cd conc. in food of herbivores 2015	45.1%	13.9%	4.7%	2.4%
Cd conc. in food of herbivores 2050	84.3%	6.7%	0%	0%

The same NOEC value for food of 0.35 mg/kg is used for mammals (Table 25). The probability that animals that mostly feed on earthworms, such as moles, are less than 95% protected, is 100% for all scenario's and times studied. In the present model, herbivores are exposed through grass. Therefore, we cannot make a distinction between large and small herbivores with respect to this NOEC. The probability that more than 5% of herbivores experience sublethal effects of cadmium, is about 45% at the present load and is rising fast to 84% in 2050. Clearly, the present load will soon be detrimental to herbivores at the present cadmium input. Halving the input drastically improves this situation, with only a 7% probability that more than 5% of the species is unprotected.

Table 26. Probability that the NOEC for kidney damage is exceeded at different Cd loading scenarios, in 2015 and 2050.

NOEC for kidney damage: 150 mgCd/kgDW				
	1/1	**1/2**	**1/4**	**1/8**
Cd in kidney of mole 2015	0%	0%	0%	0%
Cd in kidney of mole 2050	0.5%	0%	0%	0%
Cd in kidney of mice 2015	0%	0%	0%	0%
Cd in kidney of mice 2050	0%	0%	0%	0%

Empirical bioaccumulation factors were used to predict vertebrate kidney levels. An NOEC for kidney damage of 150 mg/kgDW has been used, but values as low as 120 mg/kgDW have been suggested (Ma et al. 1991). Mole kidney levels have a very small probability of exceeding the NOEC for kidney damage in 2050 (table 26). This indicates that after 2050, this probability will soon increase. Halving the Cd load reduces this probability to zero. The prediction for kidney levels of mice are no cause for concern, since all probabilities are zero.

Quality standards from different disciplines can be evaluated with model predictions. Since concentrations are based on dry weight, the concentration in harvested crop for winter fodder can be compared with cattle feedstuff quality. This standard of 1.2 mg kg/DW (Vreman et al. 1986) is rather high, and the probability that it is exceeded is zero for all scenario's (table 23).

In conclusion, we can state that functional groups with earthworms in their diet have a high probability at experiencing sublethal effects for more than 5% of the species in a functional group. For moles however, this does not yet lead to unacceptable kidney levels. The probability that raptorial birds with a diet of herbivorous animals will suffer sublethal effects, is very low. Herbivores themselves, however, can experience sublethal effects for more than 5% of the species with a high probability at the present Cd load, especially in 2050. Soil standards are exceeded with a probability of 100%, indicating that soil fauna in general is affected at present cadmium concentrations in this area, and that a strong reduction of Cd input is required to bring protection levels back to 95% of the species. The high degree of cadmium contamination is transferred selectively up the food chain with higher risks for carnivorous vertebrates than for herbivorous vertebrates.

8. Discussion and conclusions

The model presented in the preceding chapters is used to study the response of a meadow ecosystem to a continued loading with a persistent contaminant, such as cadmium. The probabilistic treatment of the model resulted in probability distributions of all relevant model output. Hence, it was possible to calculate the probabilities to exceed environmental standards or 'maximum permissible concentrations' (MPCs).
An integrated ecotoxicological model will always be relatively complex. This does not mean that its results are more difficult to use or interpret, only more considerations have to be made in the building of the model. This chapter examines some of these considerations in more detail, followed by conclusions.

8.1 General model behaviour

The overall behaviour of the model is determined to a large extent by the biomass cycle. The dynamics of the biomass of functional groups in their turn are determined by the type of growth equation employed. Much uncertainty still exists about the exact composition of functional groups in abundant ecotope types such as meadows. Therefore, a detailed description of seasonal food abundance and seasonal activity of animals was not included in the model, even though these processes are at least partly responsible for patterns in contaminant accumulation by invertebrates (Janssen 1991).

Model simulations show that a steady state of biomass is reached very fast within three years (fig. 16a-c). This is the consequence of the strong stabilizing properties of the logistic growth equation. It is obvious that in the real world such a steady state does not exist, but we are primarily interested in the long-term average abundance of groups. Since we want to use the model with wide parameter ranges due to biological variability and uncertainty, we accept this discrepancy, in return for robust model behaviour.

The uncertainty and variability associated with the biomass cycle has been used to calculate the probability distributions for the biomass of all functional groups (fig. 18a-h). Most of these distributions are skewed to the left, which can be explained by the use of carrying capacities in the modelformulations. If a functional group is not limited by food supply, the population tends to grow towards its carrying capacity K. The closer K is approached by the growing population, the stronger the growth will be slowed down, explaining the sudden drop in the probability distributions near the carrying capacity. The skewness to the left is therefore an indication that most functional groups in the present model tend to grow towards their carrying capacity, rather than be limited by food supply or predation.

The reference run shows that concentrations in all functional groups follow the same accumulation pattern as total Cd concentration in the top soil (fig. 17a-f). An unchanged Cd load causes a rise of cadmium concentrations which continues far into the next century. A load reduction of more than one half is needed to stabilize concentrations at the present level. The slow but steady cadmium accumulation in top soil determines the dynamics of cadmium accumulation in all other compartments. Since the biomass is in

steady state within three years, the slow rise in cadmium concentrations in the top soil is the cause of the pseudo steady-state of the concentrations in all other compartments. The implication of this prediction for monitoring networks (as proposed by Tolsma et al. 1991) is, that a continued monitoring of a few species would suffice.
For this purpose, model predictions should first be validated on a larger array of species, implying a large effort at the start of the monitoring network, to be replaced later by a much smaller effort if predictions are confirmed. This is the more necessary, since time series of concentration measurements are hardly available for the terrestrial environment. Even the large scale project in the province of South-Holland (PIMM 1989, 1991) can return to the same location only once every ten years. Consequently, a combined modelling-monitoring network is much needed.

The same pattern of bioaccumulation throughout the foodweb suggests that the ratio between accumulation in different trophic levels, i.e. the bioaccumulation factor, is more or less constant. This ratio can be predicted with the formula from page 37:

$$BAF = fXDass \cdot \frac{kDResp + kDMort}{kXExcr + kDMort}$$

It was confirmed in appendix D that this formula predicts the average of the simulated bioaccumulation factor for whole functional groups adequately. When little physiological information is available, BAFs are often used to predict bioaccumulation (Romijn et al. 1991b, Luttik et al. 1992). The formula makes it possible to estimate the average bioaccumulation by the population if physiological information is available, or inversely to estimate physiological parameters if a suitable BAF is available. Therefore, the BAFs can be used to do a quick assessment of the expected average concentration in a functional group exposed through food.

8.2 Uncertainty analysis

Uncertainty analysis shows that elaborate details of the model, such as cadmium sorption equilibria, and earthworms feeding from different layers, hardly influence uncertainty of model outputs. This does not necessarily mean that these model details are superfluous, if we want to preserve a general modelstructure applicable to different ecosystems on different types of soil.
Cadmium sorption by soil organic matter (SOM) is hard to distinguish from the older, parent peat material since both are highly organic and can be expected to show the same sorption behaviour. In a sandy soil, with a much greater difference between sorption of SOM and the parent material, the influence of SOM may prove larger.
The litter layer also hardly influences model behaviour, which is the way it should be. In a meadow, the litter layer is hardly present as such, and the turnover is high. In forests with a mor type of soil, with a slow degradation of pine needles, much higher Cd concentrations are found in litter (Janssen 1991). When we model such an ecosystem, a much higher influence of litter parameters on model behaviour can be expected.

A great deal of model uncertainty is determined by cadmium sorption of the parent soil material (SIM), which represents the bulk of cadmium in the system. The dissolved concentration calculated from the cadmium sorption equilibrium, turns out to be very sensitive to the density of the soil. Measurements of dissolved cadmium concentrations were not available, thus no calibration could take place. This uncertainty is transmitted to all plants and animals exposed directly to soil pore water, and animals dependent on these food sources. More attention needs to be paid to formulation of sorption equilibria because of these consequences for bio-availability.
Other important parameters that determine model uncertainty to a great extent are rates of uptake, assimilation and excretion of cadmium, immediately followed by respiration and mortality rates. Parameters for uptake by the biota from the soil solution are not known, but have been calibrated on empirical bioaccumulation factors. More research on uptake from soil solution is required to improve modeling of bio-availability.

8.3 Evaluation of environmental standards

The probability distributions of model outputs such as concentrations allows the simultaneous evaluation of environmental standards or NOECs. Thus it is possible to compare environmental standards for ground water quality, the soil ecosystem, human food quality etc.
The evaluation of the standard for drinking water quality (Table 23) is straightforward, since the standard is derived from negative effects on humans.
To evaluate whether the ecosystem might be damaged, we always deal with large arrays of species, with sometimes widely differing sensitivities. Statistical methods have been devised to estimate Maximum Permissible Concentrations (MPCs) on the basis of a limited number of toxicity experiments (Van Straalen & Denneman 1989, Aldenberg & Slob 1991). In the original concept, 5% of all species are unprotected against detrimental effects of toxicants at the MPC. Romijn et al. (1991b) modified the same methodology to calculate an MPC for a specific group of animals. For vertebrate functional groups, we calculated the probability that the MPC for mammals and birds is exceeded (Table 24,25). A probability of 100% that MPCs are exceeded, indicates that it is certain that more than 5% of the species of that functional group are unprotected. How many species of a functional group are unprotected, can be calculated in future versions according to Van Straalen (1990). This will require the collection of toxicity data per functional group, and will be dealt with in future versions of CATS models.

8.4 Future model developments and applications

The results of the model can be used for setting environmental standards in a number of ways:

- To assess whether load reductions are necessary to prevent harmful effects on the ecosystem, and if so, how great the reduction should be. Load reductions appear to be necessary in the present case.
- To compare different environmental standards in an integrated model in order to identify the most sensitive part(s) of the ecosystem. In this case, this proved to be worm-eating animals and soil fauna in general. The standard for drinking water was not exceeded, underlining the fact that ecosystems can be damaged when human health supposedly is not.
- To assess whether concentrations increase with each successive trophic level (i.e. if biomagnification occurs), and if so, does this lead to unacceptable concentrations according to some environmental standard or NOEC. The present case shows that no biomagnification occurs, but earthworms accumulate cadmium to high levels which is considered harmful for worm-eaters.

The present model has been used for the prediction of cadmium accumulation in meadows on peaty soils. This is the first of possible applications of CATS models. The expansion of the model's application range is possible in different directions:

- Expand into different classes of toxicants, such as polycyclic aromatic hydrocarbons or dibenzodioxines\dibenzodifuranes. Priority toxicants are those toxicants for which a monitoring programme exists (CCRX 1990). The next toxicant to be considered is lindane.
- Expand into different soil types, such as clay or sand. An application of CATS-1 to meadows on different soil types is presently being undertaken.
- Expand the number of ecosystem models for different eco-series. Aquatic CATS models are being developed for shallow freshwater lakes and large rivers. New terrestrial CATS models will be developed for arable land and forests.
- Expand into effect models (Type IV, Douben & Aldenberg 1990).

Apart from these applications for toxicants only, two other possible applications of CATS are suggested:

- The impact of changing land use and soil acidification on bioaccumulation in the food web has become a topic in the Chemical Time Bombs project. Model simulations with and adaptation of the precursor model NMPCulty have shown, that the drop in pH causes the mobilization of sorbed cadmium, thereby increasing the dissolved cadmium concentration which is reflected in the food web (Knoop & Traas 1992). The present model can be linked to a more elaborate soil acidification module, as in SMART (de Vries & Kros 1991) to pursue the study of joint effects of acidification and cadmium loading on ecosystems.

- The MOVE project is concerned with the derivation of ecological standards for nutrient concentrations in ecosystems. The statistical methodology of the derivation of this standard is under development, but is related to the methodology of deriving standards for toxicants. A project will start to evaluate these methodologies and to propose an integrated approach for deriving standards for both nutrients and toxicants (cf. Latour et al. 1992). Since CATS models can contain both nutrients and toxicants, an integrated approach is feasible.

8.5 Conclusions.

- *Cadmium accumulation in meadow ecosystems on peaty soil will continue at the present cadmium load. A load reduction of about one half is needed to halt the increase of cadmium accumulation. The maximum permissible concentration (MPC) in soil with respect to protecting 95% of all species, is still exceeded in 2050 at this reduction of cadmium load. A reduction to about one-eighth of the cadmium load is needed to achieve this protection level in soil in 2050.*

- *The model predicts that the maximum permissible concentration (MPC) in food of animals feeding on earthworms, such as moles and meadow birds, is still exceeded at a load reduction of one-eighth in 2050. This is a cause for concern, since meadow birds are considered important indicators for ecosystem quality.*

- *In meadow ecosystems, it is more likely that meadow birds are exposed to a harmful cadmium concentration in their food than raptorial birds. This conclusion is based on the fact that raptorial birds in this foodweb mainly prey on herbivorous mice.*

- *The probability that more than 5% of the vertebrate herbivore species are unprotected against detrimental effects of toxicants, is small. Only if the present cadmium load is unchanged up to 2050 could this protection level be exceeded. The model predicts that a load reduction of one half is enough to bring this risk down to a negligible level. Model calculations predict a negligible low probability that raptorial birds feeding on small herbivores experience sublethal effects of cadmium at the present load.*

- *Uncertainty analysis shows that model uncertainty with respect to bioaccumulation and bioaccumulation factors depends primarily on a number of parameters from both the toxicant* and *the biomass cycle:*

    - *Important sources of uncertainty from the soil subsystem are initial soil cadmium concentrations, soil density and soil sorption constants.*

    - *Important sources of uncertainty from the food web are parameters for cadmium uptake from the soil solution, and rates for mortality, respiration and excretion.*

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Appendix A. Nomenclature

The ease of use of large models is greatly enhanced by a consistent nomenclature. If this nomenclature is well designed, the source code is to a large extent self-explanatory and can be more easily re-used. In this report, nomenclature as explained below, is used throughout the text.
Nomenclature of constants, derived constants, state variables, derivatives and auxiliaries is based on the conventions as documented by Wortelboer & Aldenberg (1991) and Janse & Aldenberg (1990). Below, the composition of an identifier is treated systematically from the first to the last letter. To improve legibility, nomenclature is case-sensitive even though the simulation software ACSL does not distinguish between upper and lower case. Units are written between square brackets: [unit].

First part: type of expression

The first letter (lower case) indicates the type of the identifier, which could be a constant, a derivate, a state variable or an auxiliary variable.

k . . . . . rate constant	[y^{-1}]
h . . . . . half saturation constant	[different units]
f . . . . . fraction	[-]
c . . . . . other declared constants	
- . . . . . all derived constants	
d . . . . . derivative	[$gD \cdot m^{-2} \cdot y^{-1}$] or [$gX \cdot m^{-2} \cdot y^{-1}$]
s . . . . . state variable	[gD/m2] or [gX/m2]
a . . . . . auxiliary variable whose value is calculated with an equation	
. . . . . containing at least one state variable	[different units]

Second part: type of cycle

The second part (upper case) after the first letter (lower case) indicates to which cycle the term belongs. Three options exist:

D . . . . . Dry weight (organic material)	[gD/m2]
X . . . . . Pollutant mass, which is cadmium in this model	[gX/m2]
XD . . . . . Ratio of *X* and *D*, which is the concentration of cadmium	
. . . . . in a specific biotic compartment	[gX/gD]

Third part: type of process
The third part relates to the *D* and *X* processes or constants, like growth, predation, mortality. Apart from these general processes mentioned below, less general constants or auxiliary expressions exist for the calculation of soil equilibria, soil and litter density, and concentrations, etc. We do not state those below.

D and *X* processes:
Cons . . . relates to consumption
Pr . . . . . relates to predation
Gr . . . . . relates to growth of plants or crops
Ass . . . . . relates to assimilation
Eges . . . . relates to egestion
Resp . . . . relates to respiration
Env relates to environmental limitations of populations not explicitly modelled
Mort . . . . relates to mortality
Carr . . . . relates to the carrying capacity of populations
Pre . . . . relates to precipitation

X processes:
Excr . . . . relates to excretion
Up . . . . . relates to uptake of pollutant from the soil solution
Sat . . . . . relates to Monod saturation kinetics
Ads . . . . relates to soil equilibria of pollutants or nutrients
Diss . . . . relates to dissolved pollutants or nutrients
Leach . . . relates to leaching of excess water
Slow . . . . relates to slow cadmium fluxes [1/y]
Fast . . . . relates to fast cadmium fluxes (equilibria)
Tot(al) . . average concentration in total dried soil or litter

Fourth Part: flux identification

The fourth part (if present) shows to which compartment the flux belongs, like fluxes associated with mortality, respiration etc. Fluxes associated with predation and consumption usually occur between two compartments. In those cases, the first part mentions the compartment that is consumed or predated on, and the second part mentions the consumer or predator. In order to prevent identifiers from becoming too long, abbreviations are used as listed below in the second column.

Crop . . . *Cr* . the crop
Cow . . . . *C* . . large herbivores, cows
Litt . . . . . *L* . . litter, 100% organic
Soil . . . . . soil, SOM and SIM together
Worm . . . *W* . saprophages, worms
Tip . . . . . *T* . . soil herbivores, larvae of Tipulidae and Bibionidae
Mole . . . *M* . soil predators, moles
Mice . . . . *Mi* . small herbivores, mice
Bird . . . . *B* . . meadow birds
Rapt . . . . *R* . . free roaming raptorial birds, mainly kestrels
SOM . . . . . organic matter in the soil
SIM . . . . . inert or inorganic matter in the soil

Fifth part: Input or Output

The fifth part (if present) shows whether the term is an input or an output. Model inputs and outputs usually have user-friendly units. So, in the initial section of the model inputs are transformed to model units (*gD/m2* or *gX/m2*). In the terminal section of the model, model outputs are given in user-friendly units.
In . . . . . model input (constants) in user-friendly units
Out . . . . model output in user-friendly units

Examples

aDRespMole
a . . . . . auxiliary variable
D . . . . . dry weight
Resp . . . . respiration
Mole . . . The compartment 'mole'loses dryweight by respiration

kDMortT
k . . . . . rate constant [y^{-1}]
D . . . . . dry weight
Mort . . . . mortality
T . . . . . the compartment Tipulidae dies at a certain rate

aXDRaptOut
a . . . . . auxiliary variable
XD . . . . . concentration cadmium in compartment
Rapt . . . . the compartment raptorial birds
Out . . . . concentration is a model output in a pleasant unit.

Appendix B. Model equations and parameters

B.1 Overview

B1.1 State Variables

The model describes biomass and toxicant mass flow through a grassland agro-ecosystem. Biotic compartments or dead organic matter pools are represented twice, in biomass and in toxicant mass. Symbols and dimensions of state variables are given in table B.1.

Table B.1 state variables in the model.

Biomass variable	Toxicant variable	Description
sDLitt [gDW/m^2]	*sXLitt* [gX/m^2]	Litter
	sXDissLitt [gX/m^2]	Dissolved pollutant in litter interstitial water
	XSIM [gX/m^2]	Pollutant associated with Soil Inert Matter
	XDissLitt [gX/m^2]	Dissolved pollutant is soil interstitial water
sDWorm [gD/m^2]	*sXWorm* [gX/m^2]	Annelid worms
sDTip [gD/m^2]	*sXTip* [gX/m^2]	Larvae of Diptera
sDMole [gD/m^2]	*XMole* [gX/m^2]	Moles
sDCrop [gD/m^2]	*sXCrop* [gX/m^2]	Crop (grass)
sDMice [gD/m^2]	*sXMice* [gX/m^2]	Small vertebrate herbivores like mice, hares
sDCow [gD/m^2]	*sXCow* [gD/m^2]	Large herbivores, cows
sDBird [gD/m^2]	*sXBird* [gX/m^2]	Meadow birds like lapwing, godwit etc.
sDRapt [gD/m^2]	*sXRapt* [gX/m^2]	Raptorial birds
sDTotExtFl [gD/m^2]	*sXTotExtFl* [gX/m^2]	Summation of fluxes for checking mass balance

B1.2 Processes

This section gives an overview of processes incorporated in the model. Corresponding *D* and *X* processes are stated together (table B.2)

Table B.2 Overview of processes in the model

Abiotic processes:	
XDryDep, XManure [gX·m^{-2}·y^{-1}]	external loading by dry deposition or by manure
XLeach [gX·m^{-2}·y^{-1}]	pollutant percolation

Table B.2 Overview of processes in the model (continued)

Crop processes:		
DPrimProd [gD·m^{-2}·y^{-1}]		primary production
	XupCrop [gX·m^{-2}·y^{-1}]	pollutant uptake by crop from soil interstitial water
DLittFall [gD·m^{-2}·y^{-1}]	*XLittFall* [gX·m^{-2}·y^{-1}]	detritus to litter layer
DRootFall [gD·m^{-2}·y^{-1}]	*XRootFall* [gX·m^{-2}·y^{-1}]	detritus to soil layer
DRespCrop [gD·m^{-2}·y^{-1}]		crop respiration
DHarvest [gD·m^{-2}·y^{-1}]	*XHarvest* [gX·m^{-2}·y^{-1}]	crop harvesting
Processes by microorganisms:		
DRespSOM	*DRespLitt*[gD·m^{-2}·y^{-1}]	respiration by microorganisms
Processes occuring in functional groups, where *P,Q* can be any of the functional groups:		
DConsPQ [gD·m^{-2}·y^{-1}]	*XConsPQ* [gX·m^{-2}·y^{-1}]	consumption of *P* by *Q*
DAssPQ [gD·m^{-2}·y^{-1}]	*XAssPQ* [gX·m^{-2}·y^{-1}]	assimilation of consumed food and pollutant from *P* by *Q*
DEgesQ [gD·m^{-2}·y^{-1}]	*XEgesQ* [gX·m^{-2}·y^{-1}]	egestion of unassimilated food and pollutant by *Q*
DRespQ [gD·m^{-2}·y^{-1}]	*XExcrQ* [gX·m^{-2}·y^{-1}]	respiration and pollutant excretion by *Q*
DMortQ [gD·m^{-2}·y^{-1}]	*XMortQ* [gX·m^{-2}·y^{-1}]	mortality of *Q*
DEnvQ [gD·m^{-2}·y^{-1}]		logistic correction on production and mortality of *Q* due to environmental limitation
	XUpQ [gX·m^{-2}·y^{-1}]	pollutant uptake from interstitial water by soft bodied soil organisms *Q*
pollutant equilibria:		
	XSlowQ [gX·m^{-2}·y^{-1}]	pollutant fluxes to and from *Q*
	XFastPQ [gX·m^{-2}·y^{-1}]	equilibrating fluxes (fast) from *P* to *Q*

B.2. abiotic processes

B2.1 external cadmium loading

External cadmium loading is by three sources: Cd in manure (*cXManScen*), Cd as particulate fall out (*cXDryDep*) and by wet deposition:

$$XWetDep = \frac{cXPre \cdot cPre}{mmPm}$$

with

XWetDep	cadmium input by wet deposition	[gX·m^{-2} ·y^{-1}]
cXPre	cadmium dissolved in rain water	[mgCd/l]
mmPm	conversion of precipitation per 10 cm^2 to m^2	[mmPm]

B.2.2 percolation of precipitation surplus

Leaching of cadmium from litter to soil and from soil to layers outside system boundary is described with:

$$aXLeachLittSoil = XDissLitt \cdot fPreLittSoil \cdot \frac{cPre}{mmPm}$$

$$aXLeachSoil = XDissSoil \cdot fPreSoilDeep \cdot fPreLittSoil \cdot \frac{cpre}{mmPm}$$

with

aXDissSoil, aXDissLitt	dissolved cadmium in pore water
fPreLittSoil	fraction of water surplus leached from litter to soil
fPreSoilDeep	fraction of water leached from litter that leaches further down
mmPm	conversion (see above)
cPre	rainfall (mm/y)

B.3 Litter & Soil processes

B.3.1. Derivation of differential equations for soil and litter organic matter.

We consider two layers with densities:

Rho_{litt}	litter density, constant [gDW$_{litt}$/m^3]
Rho_{soil}	soil density, variable [gDW$_{soil}$/m^3]

We express organic matter in soil and in litter in standard model units:

$$sD_{litt} = Rho_{litt} \cdot H_{litt} \quad [gD_{litt}/m^2]$$
$$sD_{soil} = Rho_{soil} \cdot H_{soil} \quad [gD_{soil}/m^2]$$

with H_{litt} Litter depth (m)
H_{soil} Soil depth (m)

Litter fall is a source of organic matter and soil fauna converts litter to soil organic matter. The differential equations for biomass of litter and soil organic matter become:

$$\frac{dDLitt}{dt} = DLittFall - DConsLitt$$
$$\frac{dDSOM}{dt} = k \cdot DConsLitt$$

with *dDLitt/dt* change of litter biomass [gDW/m²/y]
dDSOM/dt change of soil organic matter [gDW/m²/y]
k fraction of litter consumed not assimilated by soil fauna

Depth *H* of the litter layer and the soil density are calculated dynamically:

$$H_{litt} = D_{litt} / Rho_{litt} \quad [m]$$
$$Rho_{soil} = D_{soil} / H_{soil} \quad [gDW/m^3]$$

B.3.2 Turnover of soil organic matter

Since the amount of organic matter is very important for pollutant binding, we need to derive an expression for soil density. The model keeps track of the SOM mass and specific SOM density is calculated:

$$RhoSOM = \frac{DSOM}{Depth} \cdot \frac{kgDWPgDW}{lPm^3}$$

with *RhoSOM* dynamic density of soil organic matter [kgDW/lT]
Depth soil depth [m]
kgDPgD unit conversion [kgDW/gDW]
lPm³ unit conversion [l/m³]

To calculate overall soil density, we determine the density of soil organic matter. The remaining volume will be filled with soil inert matter:

$$RhoSOMFrac = \frac{RhoSOM}{RhoSOMMax}$$
$$RhoSoil = RhoSOM + (1 - RhoSOMFrac) \cdot RhoSIM$$

with		
	RhoSOMFrac	fraction of maximal SOM density [-]
	RhoSOMMAx	maximal SOM density [kgDW/lT)
	RhoSoil	overall soil density, dynamic [kgDW/lT]

B.3.3 Litter and soil cadmium equilibria

For litter and soil we describe cadmium equilibria:

$$XLittIn = cXAdsLitt \cdot XDissLittIn$$
$$XSimIn = cXAdsSIM \cdot XDissSoilIn$$
$$XSOMIn = cXAdsSOM \cdot XDissSoilIn$$

with		
	XDissLittIn	dissolved Cd concentration in litter, input [mg Cd/l]
	XDissSoilIn	dissolved Cd concentration in soil, input [mg Cd/l]
	cXAdsQ	sorption constant for compartment Q [lLiquid/kgDW]
	XQIn	sorbed Cd to fraction Q [mg Cd/kgDWQ]

Dissolved cadmium concentrations or sorbed amounts are estimated. For this we need total cadmium content of dried soil or litter and the equilibria. We take litter as an example, and first we define initial litter depth (*DepthLitt0*) and water content of soil (*ThetaLitt*):

$$DepthLitt0 = \frac{DLitt0}{RhoLitt \cdot gDPkgD \cdot lPm3}$$
$$ThetaLitt = EpsLitt \cdot MoistLitt$$

with		
	DLitt0	initial litter mass [gDW/m^2]
	RhoLitt	litter density [kgDW/l Litt]
	gDPkgD	unit conversion [gDW/kgDW]
	lPm3	unit conversion [l/m^3]
	EpsLitt	pore volume fraction [l/l]
	MoistLitt	moisture, fraction of pore volume filled with water [l/l]

With this, we can calculate equilibrium concentrations from the total cadmium content:

$$XLittIn = \frac{cXTotLittIn}{1 + \frac{ThetaLitt}{cXAdsLitt \cdot RhoLitt}}$$

$$XDissLittIn = \frac{XLittIn}{cXAdsLittIn}$$

$$XDissLitt0 = XDissLittIn \cdot ThetaLitt \cdot DepthLitt0$$

$$XLitt0 = XLittIn \cdot RhoLitt \cdot DepthLitt0$$

with

cXTotLittIn	total cadmium in litter (input) [mgCd/kgDW]
XDissLittIn	dissolved cadmium [mgCd/l]
XLittIn	sorbed cadmium [mgCd/kgDW]
XDissLitt0	initial mass of dissolved Cd [gCd/m2]
XLitt0	initial mass of sorbed Cd [gCd/m2]

The sorption constant after conversion to model units is without dimension, since we have

$$XAdsLitt = \frac{sXLitt}{sXDissLitt}$$

with

XAdsLitt	equilibrium constant for litter [-]
sXLitt, sXDissLitt	state variables for dissolved and sorbed Cd in litter [gCd/m^2]

Since the amount of SOM is dynamic, the overall binding capacity of the soil, which is derived from both SIM and SOM, is a dynamic variable. Because of model units, a conversion to the original unit of sorption constant is needed:

$$XAdsTot = \frac{XSIM + XSOM}{XDissSoil} \cdot \frac{ThetaSoil}{RhoSoil}$$

with

XSIM, XSOM, XDissSoil	toxicant mass [gCd/m^2]
ThetaSoil	water content of soil [lLiquid/lT]
RhoSoil	soil density, dynamic [kgDW/lT]
XAdsTot	overall binding constant [lLiquid/kgDW]

The equilibria are implemented using Clasen's mechanism (1976). Fast fluxes are subtracted from the dissolved phase and added to the sorbing fractions:

$$\frac{dXSOM}{dt} = XSlowSOM + XFastDissSOM$$

$$\frac{dXSIM}{dt} = XSlowSIM + XFastDissSIM$$

$$\frac{dXDissSoil}{dt} = XSlowDissSoil - XFastDissSOM - XFastDissSIM$$

B.4 Vegetation processes

The general vegetation growth model is represented by

$$\frac{dDCrop}{dt} = DPrimProd - DHarvest - DRespCrop - DDetrFall$$

with	*DPrimProd*	primary production	[gDW/m²/y]
	DHarvest	harvested biomass	,,
	DRespCrop	respired biomass	,,
	DDetrFall	all detritus fluxes	,,

The quadratic environmental correction term *DEnvCr* should be associated with one of the fluxes mentioned above. For a full derivation of this extension of the logistic growth equation, see appendix C. We chose to divide *DEnvCr* between a reduction of production and an increase of detritus fluxes:

$$DPrimProd = kDGrCrop - fDEnvCr \cdot DEnvCr$$
$$DDetrFall = kDFallCr \cdot sDCrop + (1 - fDEnvCr) \cdot DEnvCr$$
$$DLittFall = fDFallL \cdot DDetrFall$$
$$DRootFall = (1 - fDFallL) \cdot DDetrFall$$

with	*kDGrCr*	growth rate of crop [1/y]
	kDFallCr	loss rate of detritus [1/y]
	fDEnvCr	fraction of environmental correction [-]
	fDFallL	fraction of litter production [-]
	sDCrop	vegetation biomass [gDW/m²]
	DDetrFall	total detritus flux [gD·m^{-2}·y^{-1}]
	DLittFall	litter fall [gD·m^{-2}·y^{-1}]
	DRootFall	root senescence[gD·m^{-2}·y^{-1}]

The fraction *fDEnvCr* determines how much of *DEnvCr* is allocated to a decrease of production or an increase of detritrus losses, and can be used to tune the size of detritus fluxes. Detritus losses are divided over litter fall and root senescence by the use of the fraction *fDFall*.

Respiration and harvest are considered first order processes, with rate constants *kDResp* and *kDHarvest* [1/y]:

$$DHarvest = kDHarvest \cdot sDCrop$$
$$DRespCrop = kDRespCr \cdot sDCrop$$

If we assume saturating kinetics for uptake from the soil solution, Cd uptake is modelled as follows:

$$XUptakeCr = kXUpCr \cdot \frac{XDissSoil}{lXUpCr + XDissSoil} \cdot sDCrop$$

with

XDissSoil	Cd conc in soil solution [gX/m^3]
kXUpCr	specific uptake rate [gCd· gDW^{-1}·y^{-1}]
hXUpCr	Cd concentration in soil at which *kXUpCr* is half-maximal [gX/m^3]
sDCrop	crop biomass [gDW/m^2]

The uptake parameters (*kXUpCr, hXUpCr*) are calibrated on a Bioaccumulation Factor (BAF) determined in the same soil type. The same mechanism is used for uptake by earthworms from the soil solution.
The biomass losses due to harvest and detritus carry with them an amount of cadmium, determined by the cadmium content of the crop *XDCrop*, so we can write

$$XLittFall = XDCrop \cdot DLittFall$$
$$XRootFall = XDCrop \cdot DRootFall$$
$$XHarvest = XDCrop \cdot DHarvest$$

with

XLittFall	Cd flux to litter due to litter fall [gX·m^{-2} ·y^{-1}]
XRootFall	Cd flux to SOM due to root senescence [gX·m^{-2} ·y^{-1}]
XHarvest	Cd removal from the system due to harvest[gX·m^{-2} ·y^{-1}]
XDCrop	Cd concentration of crop [gX/gDW]

B.5 Microorganisms

Respiration of soil and litter by microorganisms is modelled as a first order process:

$$DRespLitt = kDRespL \cdot sDLitt$$
$$DRespSOM = kDRespSOM \cdot sDSOM$$

with *kDRespL, kDRespSOM* respiration rates of microorganisms [1/y]

B.6 growth and food limitation

B.6.1 Logistic growth

The generic population growth equation for a predator group Q is given by:

$$\frac{dDQ}{dt} = (kDAssQ \cdot sDQ - DEnvQ) \cdot DSatQ - kDRespQ \cdot DQ - (kDMortQ \cdot sDQ + DEnvQ \cdot (1 - DSatQ))$$

with

	kDAssQ	maximal assimilation rate [1/y]
	kDRespQ	respiration rate [1/y]
	kDMortQ	natural mortality rate [1/y]
	DEnvQ	environmental correction [1/y]
	DSatQ	Monod food saturation function
	sDQ	biomass (state variable) of functional group Q [[gDW/m^2]

It should be noted that the environmental correction *DEnvQ* is effective at the level of assimilated biomass (net production), and not at the level of consumed biomass. *DEnvQ* is divided over production and mortality (Appendix C). Firstly, net production is calculated, secondly the amount of biomass consumed and egested:

$$DConsQ = DAssQ \cdot \frac{1}{fDAssQ}$$
$$DEgesQ = DConsQ - DAssQ$$

with

	fDAssQ	assimilation efficiency of biomass [-]
	DConsQ	consumed biomass [gD·m^{-2} ·y^{-1}]
	DEgesQ	egested biomass[gD·m^{-2} ·y^{-1}]

Calculation of total net production of food is a little more complicated using separate food saturation functions, taking meadow birds as an example:

$$DAssWB = (kDAssB \cdot sDBird - DEnvBird) \cdot dSatWB$$
$$DAssTB = (kDAssB \cdot sDBird - DEnvBird) \cdot dSatTB$$
$$DConsWB = DAssWB \cdot \frac{1}{fDAssB}$$
$$DConsTB = DAssWB \cdot \frac{1}{fDAssB}$$
$$DConsBird = DConsWB + DConsTB$$

with

DAssWB, DAssTB	production from separate food sources [gD·m^{-2} ·y^{-1}]
DSatWB, DSatTB	food saturation functions for two food sources [-]
DConsWB, DConsTB	consumption of separate food sources [gD·m^{-2} ·y^{-1}]
DConsBird	total bird consumption [gD·m^{-2} ·y^{-1}]

B6.2 Food limitation

The Monod function for food saturation has been used. The half-saturation parameter *hDPrQ* determines at which food density *kDAssQ* is half maximal:

$$DSatQ = \frac{sDPrey}{hDPrQ + sDPrey}$$

Several functional groups have more than one food source. The food limitation function then becomes (taking meadow birds as an example):

$$aDSatBird = \frac{sDTip + sDWorm}{hDPrB + sDWorm + sDTip}$$
$$aDSatWB = \frac{sDWorm}{hDPrB + sDWorm + sDTip}$$
$$aDSatTB = \frac{sDTip}{hDPrB + sDWorm + sDTip}$$

with

hDPrB	half saturation constant for bird consumption [gDW/m^2]
DSatBird	food saturation function for bird [-]
DSatWB	specific saturation function for predation of birds on worms
DSatTB	specific saturation function for predation of birds on diptera larvae

B6.3 Derivation of food filtering function of earthworms.

Filtration rate can be modelled as follows (Janse & Aldenberg 1990):

$$DFilt = GMax \cdot \frac{h}{h + DFood}$$

with

	DFilt	filtration of organic material [1/y]
	GMax	maximum specific filtration rate [l/mgC/y]
	h	half saturating food concentration [mgC/l]

The units in this equation are not compatible with the terrestrial environment, but the saturating effect seems appropriate (Daniel 1991). Worms do consume a certain amount of soil per gDW per unit time, which means that *GMax* should have the unit [m^3/gDWworm-/y].To match units, the concentration of food (i.e. *sDSOM* and *sDLitt*) should be expressed in [gDW/m^3] by dividing soil and litter biomass by their layer depth :

$$DFilt = GMax \cdot \frac{h}{h + \frac{Dsoil + DLitt}{H1 + H0}}$$

with

	H1	soil layer depth [m]
	H0	litter layer depth [m]
	h	half saturation constant [gDFood/m^3]
	GMax	filtered volume per unit worm biomass per unit time [$m^3 \cdot gDWworm^{-1} \cdot y^{-1}$]

the unit of the second part of the right side of the equation is now [m3(soil + litter layer) · $gD^{-1} \cdot y^{-1}$]. However, we would like to express filtration in terms of gDFood/ gDWorm/y. To achieve this, we expand the equation thus:

$$DFilt = GMax \cdot \frac{h \cdot \frac{sDSoil + sDLitt}{H1 + H0}}{h + \frac{sDSoil + sDLitt}{H1 + H0}}$$

now, the 2nd part of the right hand side of the equation has unit [gDFood · $gDworm^{-1} \cdot y^{-1}$].

We can simplify the equation to

$$DFilt = GMax \cdot \frac{h \cdot (sDSoil + sDLitt)}{h \cdot (H1 + H0) + sDSoil + sDLitt}$$

The consumption fluxes for litter and soil separately are found by separating the equation in their component parts:

$$DFiltSoil = GMax \cdot \frac{h \cdot sDSoil}{h \cdot (H1 + H0) + sDSoil + sDLitt}$$

and for litter

$$DFiltLitt = GMax \cdot \frac{h \cdot sDLitt}{h \cdot (H1 + H0) + sDSoil + sDLitt}$$

For brevity, we used symbols which are different from the model source:

FMax = *kDAssW* [m3 $\cdot y^{-1} \cdot y^{-1}$]
H1 = *cDepthSoil* [m]
H0 = *DepthLitt*, dynamic [m]

B6.4 Estimation of respiration and assimilation rates

Body size relationships were used (Peters 1983) to estimate respiration and maximal consumption rates (Table B3)

B6.5 Natural mortality

Natural mortality is modelled as as a first order process, for any functional group *Q*:

$$DMortQ = kDMortQ \cdot sDQ$$

with *dMortQ* natural mortality [gDW/m2/y]
kDMortQ natural mortality rate constant [1/y]

Table B3. respiration and maximal assimilation rates.

	average body weight	kDResp [1/y]	kDCons [1/y]
sDMice	20 gFW (Ma et al. 1991)	50	156
sDMole	85 gFW (Haeck 1969)	20	115
sDCow	550 kg FW (m.m. CA-BO)	3	10
sDRapt	300 gFW (Koning & Bayens 1990)	25	80
sDBird	250 gFW (estimate)	20	80
sDTip	0.4 gFW (Olsthoorn et al 1984)	4.4	20
sDWorm	0.3 gFW (Olsthoorn et al 1984)	4.8	different unit

B7. Cadmium processes

Cadmium in food is assimilated and the non-assimilated part is egested:

$$XConsQ = DConsQ \cdot XDFoodQ$$
$$XAssQ = XConsQ \cdot fXAssQ$$
$$XEgesQ = XConsQ - XAssQ$$

with
- *fXAssQ* cadmium assimilation efficiency [-]
- *XConsQ* consumed amount of cadmium [gX/m^2/y]
- *XDFoodQ* Cd concentration of the food
- *XAssQ* Cd assimilation [gX/m^2/y]
- *XEgesQ* Cd egestion [gX/m^2/y]

A functional group loses toxicant by excretion, mortality and predation.

$$XMortQ = XDQ \cdot DMortQ$$
$$XExcrQ = kXExcrQ \cdot sXQ$$

with
- *XMortQ* cadmium loss by natural mortality [gX/m^2/y]
- *XExcrQ* excretion of cadmium [gX/m^2/y]
- *kXExcrQ* excretion constant [1/y]

Cadmium processes for functional groups with more food sources do not differ from those described above, except that Cd intake consists of two sources, worms (W) and Diptera larvae (T), as in this example for meadow birds:

$$XConsWB = DConsWB \cdot XDWorm$$
$$XConsTB = DConsTB \cdot XDTip$$
$$XConsBird = XConsTB + XConsWB$$

with *XConsTB,XConsWB* cadmium intake from separate food sources
XConsBird total cadmium intake of bird [gX/m²/y]

Cadmium uptake from the soil solution by earthworms is modelled with the same mechanism that was used for cadmium uptake of the vegetation (section B4).

B8. Model parameters

The model CATS-meadows consists of 105 modelinputs, initial conditions and model parameters. Cadmium input scenario's are specified below (table B4). Parameters and initial conditions are listed (Table B5) with their nominal value, the range we used for uncertainty analysis and references. The distribution of the parameters for uncertainty analysis with the UNCSAM package (Janssen et al. 1992) is uniform in all cases but one. The only normal distribution is specified for initial total cadmium in soil, according to UNCSAM formats. Average, variance, minimum and maximum are given. Carrying capacities were held constant. The remaining model source is given in Table B6.

Table B4. Cadmium input scenario's

	Manure	**Deposition** (wet and dry)
First scenario: present Cd loading (Langeweg 1989)	2.7 [gX·m^{-2}·y^{-1}]	1.9 [gX·m^{-2}·y^{-1}]
Second scenario: 0.5 · present load	1.35 [gX·m^{-2}·y^{-1}]	0.95 [gX·m^{-2}·y^{-1}]
Third scenario: 0.25 · present load	0.675 [gX·m^{-2}·y^{-1}]	0.475 [gX·m^{-2}·y^{-1}]
Fourth scenario: 0.125 · present load	0.3375 [gX·m^{-2}·y^{-1}]	0.2375 [gX·m^{-2}·y^{-1}]

Table B5. Specification of inputs, initial conditions and parameters.

name	nominal value	range	reference
Initial biomass and organic matter			
cDSOM0	100 [gD·m^{-2}]	80-120	
cDLittIn	0.4 [tDW/ha]	0.3-0.5	IBP 19
cDCropIn	8 [tDW/ha]	6-10	Boxem & Leusink 1978
cDCow0	50 [gDW/m^2]	45-70	m.m. v.d. Ven, CABO
cDWorm0	10 [gDW/m^2]	5-15	Oudshoorn et al. 1984
cDTip0	10 [gDW/m^2]	5-20	Oudshoorn et al. 1984
cDMole0	0.01 [gDW/m^2]	0.001-0.05	Haeck 1969
cDBird0	0.005 [gDW/m^2]	0.001-0.01	SOVON 1987
cDMice0	0.03 [gDW/m^2]	0.01-0.1	Stoddart 1979
cDRapt0	1.0E-3 [gDW/m^2]	1.0E-4-2.0E-3	Koning & Bayens 1990
Initial Cd concentrations			
cXTotSoilIn	0.35 [!mgCd/lTSoil]	0.35 0.0044 0.2 0.6	CCRX 1985
cXTotLittIn	2.0 [mgCd/kgDW]	1.0-3.0	
cXDCowIn	0.15 [mgCd/kgDW]	0.008-1.0	estimated from Vreman et al. 1986
cXDWormIn	12.0 [mgCd/kgDW]	5-25	Van Rooij et al. 1988
cXDTipIn	7.0E-2 [mgCd/kgDW]	0.05-25	
cXDMoleIn	2.3 [mgCd/kgDW]	1.0-4.0	estimated from Ma 1987
cXDBirdIn	1.5 [mgCd/kgDW]	0.01-5.0	estimated from Weyers et al. 1985
cXDMiceIn	0.3 [mgCd/kgDW]	0.01-3.0	Andrews et al. 1984.
cXDRaptIn	0.15 [mgCd/kgDW]	0.01-2	
Litter and soil parameters			
cXAdsSIMIn	1500 [kg/l]	1200-1800	Chardon 1984
cXAdsSOMIn	1500 [kg/l]	1200-1800	Chardon 1984
cXAdsLittIn	1000 [kg/l]	800-1200	Somers 1978
cRhoSIM	0.4 [kg/l]	0.3-0.5	
cRhoSOM	0.2 [kg/l]	0.2-0.4	
cEpsSoil	0.8 [l/l]	0.8-0.9	
cMoistSoil	0.8 [l/l]	0.7-0.9	
cRhoLitt	0.2 [kg/l]	0.15-0.25	
cEpsLitt	0.9 [l/l]	0.8-0.9	
cMoistLitt	0.4 [l/l]	0.2-0.6	
fPreLittSoil	0.7 [-]	0.6-0.8	
fPreSoilDeep	0.4 [-]	0.3-0.4	
cPre	775 [mm/y]		
Max. assimilation /growth rate			
kDAssR	40 [1/y]	32-50	Peters 1983, Koning & Bayens 1990
kDAssB	40.0 [1/y]	30-50	Peters 1983
kDAssC	10 [1/y]	8-12	Peters 1983
kDAssM	75 [1/y]	70-90	Haeck 1969

Table B5. Specification of inputs, initial conditions and parameters, continued.

name	nominal value	range	reference
kDAssT	10 [1/y]	8-12	Peters 1983
kDAssW	6.0E-3 [$m^3 \cdot gDW y^{-1}$]	4.9E-3-7.0E-3	estimated from Edwards & Lofty 1979
kDAssMi	78 [1/y]	65-100	IBP 1980
kDGrCr	12.0 [1/y]	11-13	
Half saturation constants			
hDConsCrC	100 [gDW/m^2]	50-180	
hDEatW	2000 [gDW/m^3]	1200-2500	
hDConsT	20 [gDW/m^2]	15-25	
hDPrWM	5.0 [gDW/m^2]	2-8	
hDPrB	5.0 [gDW/m^2]	4-11	
hDConsCrMi	60.0 [gDW/m^2]	40-100	
hDPrMiR	1.0E-3 [gDW/m^2]	0.5E-3-1.5E-3	
Respiration rate			
kDRespMi	50.0 [1/y]	40-60	Peters 1983
kDRespR	25.0 [1/y]	20-30	Peters 1983
kDRespC	3.0 [1/y]	2.6-4.0	Peters 1983
kDRespM	25.0 [1/y]	25-32	Peters 1983
kDRespT	2.5 [1/y]	2.0-3.0	Peters 1983
kDRespW	4.8 [1/y]	1.0-3.0	Peters 1983
kDRespCr	3.0 [1/y]	2.5-3.5	Peters 1983
kDRespL	2.6 [1/y]	2.0-3.0	Smith 1982
kDRespSOM	2.6 [1/y]	2.0-3.0	Smith 1982
kDRespB	20.0 [1/y]	16-24	Peters 1983
Mortality rate			
kDMortMi	2.0 [1/y]	0.7-4.0	
kDMortR	3.0 [1/y]	1.0-5.0	Koning & Bayens 1990
kDMortC	0.2 [1/y]	0.05-0.25	
kDMortM	12.0 [1/y]	8-16	estimated from Haeck 1969
kDMortT	2.0 [1/y]	1.0-3.0	
kDMortW	2.0 [1/y]	1.0-3.0	
kDMortB	2.0 [1/y]	1.0-4.0	
Biomass assimilation efficiency			
fDAssC	0.4 [-]	0.4-0.6	IBP 1980
fDAssW	0.45 [-]	0.35-0.55	Daniel 1991
fDAssT	0.5 [-]	0.4-0.6	
fDAssM	0.5 [-]	0.4-0.6	
fDAssB	0.5 [-]	0.4-0.6	
fDAssMi	0.6 [-]	0.5-0.7	Hayward & Phillipson 1979
fDAssR	0.5 [-]	0.4-0.6	

Table B5. Specification of inputs, initial conditions and parameters, continued

name	nominal value	range	reference
Crop parameters			
kDHarvest	0.5 [-]	0.4-0.6	
kDFallCr	0.3 [1/y]	0.25-0.30	
fDEnvCr	0.96 [-]	0.93-0.97	
fDFallL	0.5 [-]	0.4-0.6	
Bird immigration			
cDBirdImm	1.0E-3 [gDW/m2/y]	9.0E-4-1.1E-3	
cXDBirdImm	0.05 (mgCd/gDW]	0.01-0.1	
Toxicant assimilation efficiency			
fXAssC	0.05 [-]	0.01-0.10	Ros & Slooff 1987
fXAssW	0.05 [-]	0.01-0.2	Ros & Slooff 1987, Janssen 1991
fXAssT	0.05 [-]	0.01-0.2	Ros & Slooff 1987, Janssen 1991
fXAssM	0.05 [-]	0.01-0.07	Ros & Slooff 1987
fXAssB	0.05 [-]	0.01-0.10	Ros & Slooff 1987
fXAssMi	0.05 [-]	0.01-0.07	Ros & Slooff 1987
fXAssR	0.05 [-]	0.01-0.10	Ros & Slooff 1987
Toxicant uptake from pore water			
kXUpCr	6.0E-5 [gCd·gDW^{-1}·y^{-1}]	4.0E-5-6.5E-5	
kXUpW	7.5E-4 [gCd·gDW^{-1}·y^{-1}]	7.7E-4-1.0E-3	
hXUpCr	5.0E-2 [gCd/m^3]	5.0E-2-7.0E-2	
hXUpW	1.0E-2 [gCd/m^3]	6.5E-3-1.1E-2	
Toxicant excretion rate			
kXExcrC	0.25	0.02-0.2	
kXExcrW	2.5	2.0-3.0	
kXExcrT	2.5	2.0-3.0	
kXExcrM	1.3	0.7-4.0	
kXExcrB	1.95	1.0-4.0	
kXExcrMi	2.5	0.5-4.0	Ros & Slooff 1987
kXExcrR	1.95	1.0-4.0	
Bioaccumulation factors			
cBAFMoKidWorm	4.4[-]	3-6	Ma 1989
cBAFMiKidTot	3.0 [-]	2-4	Andrews et al. 1984
cBCFCropIn	0.36 [l/kg]		Knoop & Aldenberg 1989

Table B5. Specification of inputs, initial conditions and parameters, continued

name	nominal value	range	reference
Carrying capacity (K)			
cDCarrCr	1000 [gDW/m²]		IBP 1980, m.m. van de Ven
cDCarrC	70 [gDW/m²]		Proefstat. Rundveehouderij, m.m.
cDCarrW	36 [gDW/m²]		Cotton & Curry, in Tamis 1992
cDCarrT	20 [gDW/m²]		Oudshoorn et al. 1984
cDCarrM	0.14 [gDW/m²]		Haeck 1969
cDCarrB	0.04 [gDW/m²]		estimated from SOVON 1987
cDCarrMi	0.015 [gDW/m²]		Denneman 1989, Stoddart 1979
cDCarrR	1.0E-3 [gDW/m²]		estimated from SOVON 1987
cDepthSoil	0.05 [m]		

Table B6. **PROGRAM CATS-1, listing**

```
! Last changes: 13 august, FRI, Version 2.28
! Accumulation of Cd in Soil, Litter, Rootdetr, Worms, Tipulidae,
! Crop, Cows, Moles, Meadowbirds, Mice, Bird of Prey (Rapt)
! Area: 'Peat-West', Crop: 'Grass'.
! By Theo Traas & Tom Aldenberg, RIVM/LWD

!  INTEGRATION ROUTINE SETUP

  ALGORITHM  IALG = 2                    ! Gear's Stiff
  CINTERVAL  OutputStep = 1              ! y
  NSTEPS     NSTP = 1000

  VARIABLE Time, BeginTime = 1990.0      ! y
  CONSTANT EndTime         = 2050.0      ! y

  MERROR sXSIM = 1.0D-06                 ! Rel. error
  XERROR sXSIM = 1.0D-09                 ! Absolute error in sXSIM

INITIAL
  ! In the initial, all constants all declared. Since Table B5 lists
  ! these constants, only derived constants are listed here.
  ! UNIT CONVERSION CONSTANTS

  ! ------- Cannot be changed at runtime for safety---------
   m2Pha           = 10000.0             ! m2/ha
   dPy             = 365.25              ! d/y
   mmPm            = 1000.0              ! mm/m
   kgDPtD          = 1000.0              ! kgDW/tDW
   gDPkgD          = 1000.0              ! gDW/kgDW
   mgXPgX          = 1000.0              ! mgCd/gCd
   lPm3            = 1000.0              ! l/m3

  ! SOIL AND SOM CONSTANTS

   RhoSOM0       = cDSOM0 /cDepthSoil/lPm3/gDPkgD     ! kgDW/lTSoil
   ThetaSoil     = cEpsSoil * cMoistSoil              ! lLSoil/lTSoil
   ! ------------ XDissSoil calculated from totalsoilconc.
   ! ------------ with known soilequilibria. See separate notes
   XDissSoilIn   = cXTotSoilIn / &
   (ThetaSoil+cRhoSIM*cXAdsSIMIn+RhoSOM0 *cXAdsSOMIn)! mgCd/lLSoil
   ! ------------ All soil X quantities calculated in gCd/m2
   XSIMIn        = XDissSoilIn * cXAdsSIMIn           ! mgCd/kgSIM
   XSIM0         = XSIMIn  * cRhoSIM  * cDepthSoil    ! gCd/m2
   XDSOMIn       = XDissSoilIn * cXAdsSOMIn           ! mgCd/kgDW
   XSOM0         = XDSOMIn * RhoSOM0 * cDepthSoil     ! gCd/m2
   XDissSoil0    = XDissSoilIn * ThetaSoil * cDepthSoil! gCd/m2
   XTotalSoil0   = (XDissSoil0+XSOM0 + XSIM0) / &
                   (cRhoSIM + RhoSOM0)/cDepthSoil       ! mgCd/kgSSoil

  ! CROP CONSTANTS

   kDIncrCr      =  kDGrCr - kDRespCr - kDFallCr              ! 1/y
   DCrop0        =  cDCropIn * kgDPtD * gDPkgD / m2Pha        ! gDW/m2
   XDCropIn       =   cBCFCrop * XTotalSoil0                          !
mgCd/kgDW
   XCrop0        =  XDCropIn / mgXPgX / gDPkgD * DCrop0       ! gCd/m2

  ! LITTER CONSTANTS

   DLitt0        =  cDLittIn * kgDPtD * gDPkgD / m2Pha     ! gDW/m2
   DepthLitt0    =  DLitt0 / cRhoLitt / gDPkgD / lPm3      ! m
   ThetaLitt      =  cEpsLitt * cMoistLitt                   ! lLLitt/l
TLitt
   XDLittIn        =   cXTotLittIn /(1+ ThetaLitt/ cXAdsLittIn/ cRho-
Litt)
                                                            ! mgCd/kgDW
   XLitt0        =  XDLittIn * cRhoLitt * DepthLitt0       ! gCd/m2
   XDissLittIn   =  XDLittIn / cXAdsLittIn                   ! mgCd/lL-
Litt
   XDissLitt0    =  XDissLittIn * ThetaLitt * DepthLitt0   ! gCd/m2


  ! COW CONSTANTS

   kDIncrC       =  kDAssC - kDRespC - kDMortC             ! gDW/m2
   XCow0         =  cXDCowIn /mgXPgX / gDPkgD * DCow0      ! gCd/m2

  ! WORM CONSTANTS

   kDIncrW       =  kDAssW*hDEatW - kDMortW - kDRespW      ! 1/y
   XWorm0        =  cXDWormIn * cDWorm0 / mgXPgX / gDPkgD  ! gCd/m2

  ! TIPULIDAE CONSTANTS

  kDIncrT     = kDAssT - kDMortT - kDRespT          ! 1/y
  XTip0       = cXDTipIn * cDTip0/ mgXPgX/ gDPkgD ! gCd/m2

  ! MOLE CONSTANTS

  kDIncrM  =  kDAssM - kDRespM - kDMortM             ! 1/y
  XMole0   =  cXDMoleIn / mgXPgX / gDPkgD * DMole0   ! gCd/m2

  ! MEADOWBIRD CONSTANTS
```

```
  kDIncrB      =  kDassB - kDMortB - kDRespB                    ! 1/y
  XBird0       =   cXDBirdIn / mgXPgX / gDPkgD * DBird0          !
gCd/m2
  XBirdImm     =   cXDBirdImm / mgXPgX / gDPkgD * cDBirdImm      !
gCd/m2/y

  ! MICE CONSTANTS

  kDIncrMi =  kDAssMi - kDRespMi - kDMortMi          ! 1/y

  XMice0   =  cXDMiceIn / mgXPgX / gDPkgD * DMice0   ! gCd/m2

  ! OWL CONSTANTS

  kDIncrR      =  kDassR - kDMortR - kDRespR                  ! 1/y
  XRapt0       =  cXDRaptIn / mgXPgX / gDPkgD * DRapt0        ! gCd/m2

  ! PRECIPITATION and LEACH CONSTANTS

   XWetDep     =  cXPre * cPre * dPy       ! gCd/m2/y

  ! CADMIUM DEPOSITION CONSTANTS
  ! Table B4.

  !---------  INPUT  CONSTRAINTS  CHECKING  ------------------------
----

  IF  (kDIncrCr .LE. 0.0D0)       THEN
                  GrChkOUT  = .TRUE.
    ELSE IF (kDINcrC  .LE. 0.0D0) THEN
                  GrChkOUT  = .TRUE.
    ELSE IF (kDINcrW  .LE. 0.0D0) THEN
                  GrChkOUT  = .TRUE.
    ELSE IF (kDINcrT  .LE. 0.0D0) THEN
                  GrChkOUT  = .TRUE.
    ELSE IF (kDINcrM  .LE. 0.0D0) THEN
                  GrChkOUT  = .TRUE.
    ELSE IF (kDINcrB  .LE. 0.0D0) THEN
                  GrChkOUT  = .TRUE.
    ELSE IF (kDINcrMi .LE. 0.0D0) THEN
                  GrChkOUT  = .TRUE.
    ELSE IF (kDINcrR  .LE. 0.0D0) THEN
                  GrChkOUT  = .TRUE.
  END  IF  ! ------------------------------------------------------
----

END !  Of Initial


DYNAMIC

 DERIVATIVE

  ! SOILFLUXES & AUX. SIM AND SOM
  ! ------------------ D Soil ----------------------------
  aDRhoSom        = sDSOM / cDepthSoil / lPm3 / gDPkgD   ! kgDW/lT-
Soil
  ! --------------- fraction of max. SOM density
  afDRhoSOM       = aDRhoSom/cRhoSOM                     ! -
  !---------------- overall soil density
  aDRhoSoil       = aDRhoSom + (1-afDRhoSOM)*cRhoSIM     ! kgDW/lT-
Soil
  aDRespSOM       = sDSOM * kDRespSOM                    ! gDW/m2/y
  ! ------------------ X Soil ----------------------------
  aXSIM            = sXSIM / cRhoSIM/ cDepthSoil          ! mgCd/k-
gSIM
  aXDSOM          = sXSOM/sDSOM                          ! gCd/gDW
  aXDissSoil      = sXDissSoil /ThetaSoil /cDepthSoil    ! gCd/m3
  aXLeachSoil     = aXDissSoil * fPreSoilDeep            &
                    * fPreLittSoil * cPre / mmPm         ! gCd/m2/y

  ! CROP FLUXES & AUX.
  ! ------------------ D Crop ----------------------------
  aDGrMaxCr     = kDGrCr * sDCrop                        ! gDW/m2/y
  !-------------- Intraspecific competition term
  aDEnvCr       = kDIncrCr/cDCarrCr * sDCrop * sDCrop     ! gDW/m2/y
  aDPrimProd    = aDGrMaxCr  - aDEnvCr * fDEnvCr         ! gDW/m2/y
  ! -------------- Intraspecific competition term
  aDEnvDetr     = (1 - fDEnvCr) * aDEnvCr                ! gDW/m2/y
  aDDetrFall    = kDFallCr * sDCrop  + aDEnvDetr         ! gDW/m2/y
  ! -------------- Partitioning total detritus over litter & roots
  aDLittFall    = fDFallL * aDDetrFall                   ! gDW/m2/y
  aDRootFall    = (1- fDFallL) * aDDetrFall              ! gDW/m2/y
  aDRespCrop    = kDRespCr * sDCrop                      ! gDW/m2/y
  aDHarvest     = kDHarvest * sDCrop                     ! gDW/m2/y

  ! ------------------ X Crop ----------------------------
  aXDCrop     = sXCrop /sDCrop                           ! gCd/gDW
  aXLittFall  = aXDCrop * aDLittFall                     ! gCd/m2/y
  aXRootFall  = aXDCrop * aDRootFall                     ! gCd/m2/y
  aXHarvest   = aXDCrop * aDHarvest                      ! gCd/m2/y
  aXUpCrop    = kXUpCr*aXDissSoil/(hXUpCr+aXDissSoil) &
                * sDCrop                                 ! gCd/m2/y

  ! LITTERFLUXES & AUX.
  ! ----------------- D Litter -----------------------
  aDRespLitt  = kDRespL * sDLitt                         ! gDW/m2/y
  aDepthLitt  = sDLitt / cRhoLitt / gDPkgD / lPm3        ! m
  ! ----------------- X Litter -----------------------
  aXDLitt     = sXLitt /sDLitt                           ! gCd/gDW
  aXDissLitt  = sXDissLitt /ThetaLitt/aDepthLitt         ! gCd/m3
  aXLeachLittSoil = aXDissLitt*fPreLittSoil*cPre/ mmPm   ! gCd/m2/y

  ! COW FLUXES & AUX
```

Table B6. **PROGRAM CATS-1, listing, continued**

```
! -------------- D Cow ---------------------------------
! ---------- Saturating cow consumption
aDSatCow   = sDCrop/(hDConsCrC+sDCrop)                          ! -
!----------- Intraspecific competition term
aDEnvCow   = kDIncrC/cDCarrC * sDCow * sDCow                    ! gDW/m2/y
aDAssCow   = (kDAssC * sDCow - aDEnvCow) * aDSatCow             ! gDW/m2/y
aDConsCow  = aDAssCow / fDassC                                  ! gDW/m2/y
aDEgesCow  = aDConsCow - aDAssCow                               ! gDW/m2/y
aDRespCow  = kDRespC * sDCow                                    ! gDW/m2/y
aDMortCow  = kDMortC*sDCow + aDEnvCow * (1 -aDSatCow)           ! gDW/m2/y

! -----------------X Cow ---------------------------------
aXDCow     = sXCow / sDCow                                      ! gCd/gDW
aXConsCow  = aDConsCow * aXDcrop                                ! gCd/m2/y
aXAssCow   = fXAssC * aXConsCow                                 ! gCd/m2/y
aXEgesCow  = aXConsCow - aXAssCow                               ! gCd/m2/y
aXMortCow  = aXDCow * aDMortCow                                 ! gCd/m2/y
aXExcrCow  = kXExcrC * sXCow                                    ! gCd/m2/y

! WORM FLUXES & AUX.
!---------------- D Worm -----------------------------
!---------- Saturating wormcons. functions
aDSatWormS= sDSOM/(hDEatW*(aDepthLitt+cDepthSoil)+sDSOM+sDLitt)
aDSatWormL= sDLitt/(hDEatW*(aDepthLitt+cDepthSoil)+sDSOM+sDLitt)
aDSatWorm = (sDLitt+sDSOM) &
    /(hDEatW*(aDepthLitt+cDepthSoil)+sDSOM+sDLitt)              ! -
!---------------- Intraspecific competition term
aDEnvWorm       = kDIncrW/cDCarrW * sDWorm * sDWorm             ! gDW/m2/y
aDAssSOMWorm    = (kDAssW *hDEatW * sDWorm - aDEnvWorm) &
                  * aDSatWormS                                  ! gDW/m2/y
aDAssLittWorm   = (kDAssW *hDEatW  * sDWorm - aDEnvWorm)&
                  * aDSatWormL                                  ! gDW/m2/y

aDAssWorm       = aDAssSOMWorm + aDAssLittWorm                  ! gDW/m2/y
aDConsSOMWorm   = aDAssSOMWorm / fDAssW                         ! gDW/m2/y
aDConsLittWorm  = aDAssLittWorm / fDAssW                        ! gDW/m2/y
aDConsWorm      = aDConsSOMWorm + aDConsLittWorm                ! gDW/m2/y
aDEgesWorm      = aDConsWorm - aDAssWorm                        ! gDW/m2/y
aDRespWorm      = kDRespW * sDWorm                              ! gDW/m2/y
aDMortWorm      = kDMortW  * sDWorm +                          &
                  aDEnvWorm * (1-aDSatWorm)                     ! gDW/m2/y

!---------------- X Worm -----------------------------
aXConsLittWorm  = aDConsLittWorm * aXDLitt                      ! gCd/m2/y
aXConsSOMWorm   = aDConsSOMWorm * aXDSOM                        ! gCd/m2/y
aXConsWorm      = aXConsSOMWorm + aXConsLittWorm                ! gCd/m2/y
aXUpWorm        = kXUpW * sDWorm                               &
                  * aXDissSoil / (hXUpW + aXDissSoil)           ! gCd/m2/y
aXDWorm         = sXWorm / sDWorm                               ! gCd/gDW
aXAssWorm       = fXAssW * aXConsWorm                           ! gCd/m2/y
aXEgesWorm      = aXConsWorm - aXAssWorm                        ! gCd/m2/y
aXMortWorm      = aXDWorm * aDMortWorm                          ! gCd/m2/y
aXExcrWorm      = kXExcrW * sXWorm                              ! gCd/m2/y


! TIPULIDAE FLUXES & AUX

! -------------- D Tip ---------------------------------
! -------------- Saturating Tipulidae consumption
aDSatTipCr  = sDCrop/(hDConsT +sDCrop+sDSOM)                    ! -
aDSatTipSOM = sDSOM /(hDConsT +sDCrop+sDSOM)                    ! -
aDSatTip    = (sDCrop + sDSOM)/(hDConsT +sDCrop+sDSOM)          ! -
!--------------- Intraspecific competition term
aDEnvTip    = kDIncrT/cDCarrT * sDTip * sDTip                   ! gDW/m2/y
aDAssCrT    = (kDAssT * sDTip - aDEnvTip)                      &
                  * aDSatTipCr                                  ! gDW/m2/y
aDAssSOMT   = (kDAssT * sDTip - aDEnvTip)                      &
                  * aDSatTipSOM                                 ! gDW/m2/y
aDAssTip    = aDAssCrT + aDAssSOMT                              ! gDW/m2/y
aDConsCrT   = aDAssCrT / fDAssT                                 ! gDW/m2/y
aDConsSOMT  = aDAssSOMT / fDAssT                                ! gDW/m2/y
aDConsTip   = aDConsCrT +  aDConsSOMT                           ! gDW/m2/y
aDEgesTip   = aDConsTip - aDAssTip                              ! gDW/m2/y
aDRespTip   = kDRespT * sDTip                                   ! gDW/m2/y
aDMortTip   = kDMortT  * sDTip +                               &
                  aDEnvTip * (1-aDSatTip)                       ! gDW/m2/y

!---------------- X Tip -----------------------------
aXConsCrT   = aDConsCrT * aXDCrop                               ! gCd/m2/y
aXConsSOMT  = aDConsSOMT * aXDSOM                               ! gCd/m2/y
aXConsTip   = aXConsCrT + aXConsSOMT                            ! gCd/m2/y
aXDTip      = sXTip / sDTip                                     ! gCd/gDW
aXAssTip    = fXAssT * aXConsTip                                ! gCd/m2/y
aXEgesTip   = aXConsTip - aXAssTip                              ! gCd/m2/y
aXMortTip   = aXDTip * aDMortTip                                ! gCd/m2/y
aXExcrTip   = kXExcrT * sXTip                                   ! gCd/m2/y

! MOLE FLUXES & AUX

! ---------------- D MOLE -----------------------------
! ---------- Saturating mole consumption
aDSatMole   = sDWorm/(hDPrWM+sDWorm)                            ! -
!----------- Intraspecific competition term
aDEnvMole   = kDIncrM/cDCarrM * sDMole * sDMole                 ! gDW/m2/y
```

```
aDAssMole  = (kDAssM * sDMole -aDEnvMole) * aDSatMole  ! gDW/m2/y
aDConsMole = aDAssMole / fDAssM                        ! gDW/m2/y
aDEgesMole = aDConsMole - aDAssMole                    ! gDW/m2/y
aDRespMole = kDRespM * sDMole                          ! gDW/m2/y
aDMortMole = kDMortM*sDMole + aDEnvMole * (1-aDSatMole)! gDW/m2/y

!--------------- X Mole --------------------------------
aXDMole        = sXMole/sDMole                         ! gCd/gDW
aXConsMole     = aDConsMole * aXDWorm                  ! gCd/m2/y
aXAssMole      = fXAssM * aXConsMole                   ! gCd/m2/y
aXEgesMole     = aXConsMole - aXAssMole                ! gCd/m2/y
aXMortMole     = aXDMole * aDMortMole                  ! gCd/m2/y
aXExcrMole     = kXExcrM * sXMole                      ! gCd/m2/y

! BIRD FLUXES & AUX , eat worms and jack

!---------------- D Bird -------------------------------
!---------------- Saturating birdcons. functions
aDSatBirdW = sDWorm/(hDPrB + sDWorm + sDTip)           ! -
aDSatBirdT = sDTip/(hDPrB + sDWorm + sDTip)            ! -
aDSatBird  = (sDTip + sDWorm)/(hDPrB + sDWorm + sDTip) ! -
!--------------- Intraspecific competition term
aDEnvBird      = kDIncrB/cDCarrB * sDBird * sDBird     ! gDW/m2/y
aDAssWormBird  = (kDAssB * sDBird - aDEnvBird)         &
                 * aDSatBirdW                          ! gDW/m2/y
aDAssTipBird   = (kDAssB * sDBird - aDEnvBird)         &
                 * aDSatBirdT                          ! gDW/m2/y
aDAssBird      = aDAssWormBird + aDAssTipBird          ! gDW/m2/y
aDConsWormBird = aDAssWormBird / fDAssB                ! gDW/m2/y
aDConsTipBird  = aDAssTipBird / fDAssB                 ! gDW/m2/y
aDConsBird     = aDConsWormBird + aDConsTipBird        ! gDW/m2/y
aDEgesBird     = aDConsBird - aDAssBird                ! gDW/m2/y
aDRespBird     = kDRespB * sDBird                      ! gDW/m2/y
aDMortBird     = kDMortB  * sDBird +                   &
                 aDEnvBird * (1-aDSatBird)             ! gDW/m2/y

!---------------- X Bird -------------------------------
aXConsWormBird  = aDConsWormBird * aXDWorm             ! gCd/m2/y
aXConsTipBird   = aDConsTipBird * aXDTip               ! gCd/m2/y
aXConsBird      = aXConsWormBird + aXConsTipBird       ! gCd/m2/y
aXDBird         = sXBird / sDBird                      ! gCd/gDW
aXAssBird       = fXAssB * aXConsBird                  ! gCd/m2/y
aXEgesBird      = aXConsBird - aXAssBird               ! gCd/m2/y
aXMortBird      = aXDBird * aDMortBird                 ! gCd/m2/y
aXExcrBird      = kXExcrB * sXBird                     ! gCd/m2/y

! RAPTORIAL BIRD FLUXES & AUX.

!--------------- D Rapt -------------------------------
! ----------- Saturating owl consumption
aDSatRapt    = sDMice/(hDPrMiR + sDMice)               ! -
!------------ Intraspecific competition term
aDEnvRapt    = kDIncrR/cDCarrR * sDRapt * sDRapt       ! gDW/m2/y
aDAssRapt    = (kDAssR * sDRapt -aDEnvRapt) * aDSatRapt ! gDW/m2/y
aDConsRapt   = aDAssRapt / fDAssR                      ! gDW/m2/y
aDEgesRapt   = aDConsRapt - aDAssRapt                  ! gDW/m2/y
aDRespRapt   = kDRespR * sDRapt                        ! gDW/m2/y
aDMortRapt   = kDMortR*sDRapt + aDEnvRapt *(1-aDSatRapt)! gDW/m2/y

!--------------- X Rapt -------------------------------
aXDRapt        = sXRapt/sDRapt                         ! gCd/gDW
aXConsRapt     = aDConsRapt * aXDMice                  ! gCd/m2/y
aXAssRapt      = fXAssR * aXConsRapt                   ! gCd/m2/y
aXEgesRapt     = aXConsRapt - aXAssRapt                ! gCd/m2/y
aXMortRapt     = aXDRapt * aDMortRapt                  ! gCd/m2/y
aXExcrRapt     = kXExcrR * sXRapt                      ! gCd/m2/y

! MICE FLUXES & AUX.

! --------------- D Mice ---------------------------------
! ---------- Saturating Mice consumption
aDSatMice  = sDCrop/(hDConsCrMi+sDCrop)                ! -
!----------- Intraspecific competition term
aDEnvMice  = kDIncrMi/cDCarrMi * sDMice * sDMice       ! gDW/m2/y
aDAssMice  = (kDAssMi*sDMice -aDEnvMice) * aDSatMice   ! gDW/m2/y
aDConsMice = aDAssMice / fDAssMi                       ! gDW/m2/y
aDEgesMice = aDConsMice - aDAssMice                    ! gDW/m2/y
aDRespMice = kDRespMi * sDMice                         ! gDW/m2/y
aDMortMice = kDMortMi*sDMice + aDEnvMice *(1-aDSatMice)! gDW/m2/y

! ----------------X Mice ---------------------------------
aXDMice      = sXMice / sDMice                         ! gCd/gDW
aXConsMice   = aDConsMice * aXDcrop                    ! gCd/m2/y
aXAssMice    = fXAssMi * aXConsMice                    ! gCd/m2/y
aXEgesMice   = aXConsMice - aXAssMice                  ! gCd/m2/y
aXMortMice   = aXDMice * aDMortMice                    ! gCd/m2/y
aXExcrMice   = kXExcrMi * sXMice                       ! gCd/m2/y

! CADMIUM DEPOSITION

aXDryDep    = cXDepScen / m2Pha                        ! gCd/m2/y
aXManure    = cXManScen / m2Pha                        ! gCd/m2/y

! SLOW DERIVATIVES

! ----------------- D DERIVATIVES ----------------------
dDSOM        =  aDEgesWorm + aDMortWorm + aDEgesTip    &
                + aDMortTip + aDEgesMole + aDMortMole  &
                + aDRootFall - aDConsSOMWorm - aDRespSOM &
                - aDConsSOMT                           ! gDW/m2/y
dDLitt       =  aDLittFall + aDEgesCow + aDEgesBird    &
                + aDMortMice + aDEgesMice + aDEgesRapt &
                +  aDMortRapt  -  aDConsLittWorm -aDRespLitt ! gDW/-
m2/y
```

Table B6. **PROGRAM CATS-1, listing, continued**

```
dDCrop      =  aDPrimProd - aDHarvest - aDConsCow       &
               - aDRespCrop - aDConsMice - aDConsCrT    &
               - aDLittFall - aDRootFall                ! gDW/m2/y
dDWorm      =  aDAssWorm - aDRespWorm - aDMortWorm      &
               - aDConsMole - aDConsWormBird            ! gDW/m2/y
dDTip       =  aDAssTip - aDRespTip - aDMortTip         &
               - aDConsTipBird                          ! gDW/m2/y
dDCow       =  aDAssCow  - aDRespCow - aDMortCow        ! gDW/m2/y
dDMole      =  aDAssMole - aDRespMole - aDMortMole      ! gDW/m2/y
dDBird      =  cDBirdImm + aDAssBird - aDRespBird       &
               - aDMortBird                             ! gDW/m2/y
dDMice      =  aDAssMice - aDRespMice - aDMortMice      &
               - aDConsRapt                             ! gDW/m2/y
dDRapt       = aDAssRapt - aDRespRapt - aDMortRapt      ! gDW/m2/y

! ------------------ X DERIVATIVES ---------------------
dXCrop      =  aXUpCrop -aXHarvest-aXConsCow- aXConsCrT &
               - aXConsMice - aXLittFall - aXRootFall   ! gCd/m2/y
dXWorm      =  aXAssWorm + aXUpWorm - aXExcrWorm        &
               -aXMortWorm - aXConsMole - aXConsWormBird! gCd/m2/y
dXTip       =  aXAssTip - aXExcrTip - aXMortTip         &
               - aXConsTipBird                          ! gCd/m2/y
dXCow       =  aXAssCow - aXExcrCow - aXMortCow         ! gCd/m2/y
dXMole      =  aXAssMole - aXExcrMole - aXMortMole      ! gCd/m2/y
dXBird      =  XBirdImm + aXAssBird - aXExcrBird        &
               - aXMortBird                             ! gCd/m2/y
dXMice      =  aXAssMice - aXExcrMice - aXMortMice      &
               - aXConsRapt                             ! gCd/m2/y
dXRapt       =  aXAssRapt - aXExcrRapt - aXMortRapt     ! gCd/m2/y

! ------------   SLOW FLUXES TO/FROM LITT. & SOIL -------
aXSlowLitt    = aXDryDep +aXManure+aXEgesCow+aXExcrCow &
                +aXEgesBird+aXExcrBird+aXLittFall     &
                + aXExcrMice+aXEgesMice+aXExcrRapt    &
                +aXEgesRapt+aXMortMice + aXMortRapt   &
                -aXConsLittWorm                       ! gCd/m2/y
aXSlowDissLitt = XWetDep - aXLeachLittSoil            ! gCd/m2/y
aXSlowSOM      = aXEgesWorm + aXExcrWorm + aXMortWorm  &
                + aXEgesTip+ aXExcrTip+ aXMortTip     &
                +aXEgesMole + aXRootFall+ aXExcrMole  &
                + aXMortMole-aXConsSOMT-aXConsSOMWorm ! gCd/m2/y
aXSlowSIM      = 0
aXSlowDissSoil = aXleachLittSoil-aXLeachSoil-aXUpCrop &
                 - aXUpWorm                           ! gCd/m2/y

! CLASENEQUATION FOR LITTER AND SOIL CADMIUM EQUILIBRIUM

  ! ------------ FAST FLUXES TO/FROM LITT. & SOIL ---------
  aXFastLitt =(-aXSlowLitt*sXDissLitt+aXSlowDissLitt*sXLitt)&
                  / (sXDissLitt + sXLitt)                 ! gCd/m2/y

  aXFastDissSOM =  ((sXDissSoil * sXSOM *aXSlowDissSoil) - &
                     (sXDissSoil**2 * aXSlowSOM)        -  &
                     (sXDissSoil * sXSIM * aXSlowSOM) +    &
                     (sXDissSoil * sXSOM * aXSlowSIM))     &
  / (sXDissSoil**2  +  sXDissSoil  *  sXSIM  +  sXDissSoil  *  sXSOM)!
gCd/m2/y

  aXFastDissSIM   = ((sXDissSoil * sXSIM *aXSlowDissSoil)- &
                     (sXDissSoil**2 * aXSlowSIM)        -   &
                     (sXDissSoil * sXSOM * aXSlowSIM)  +    &
                     (sXDissSoil * sXSIM * aXSlowSOM))      &
  / (sXDissSoil**2 + sXDissSoil*sXSIM + sXDissSoil * sXSOM)! gCd/-
m2/y

  !--- TOTAL OF FAST AND SLOW FLUXES  FOR SOIL AND LITT -----
  dXSOM       = aXSlowSOM + aXFastDissSOM                   ! gCd/-
m2/y
  dXSIM       = aXSlowSIM + aXFastDissSIM                   ! gCd/-
m2/y
  dXDissSoil  = aXSlowDissSoil-aXFastDissSIM-  aXFastDissSOM ! gCd/-
m2/y
  dXLitt      = aXSlowLitt + aXFastLitt                     ! gCd/-
m2/y
  dXDissLitt = aXSlowDissLitt - aXFastLitt                  ! gCd/-
m2/y

  !  DERIVATIVES FOR CHECKING MASS BALANCE

  dDTotExtFl  = aDPrimProd +cDBirdImm -aDMortCow-aDMortBird &
                -aDRespLitt-aDRespWorm-aDRespTip            &
                -aDRespCow-aDRespMole-aDRespBird-aDRespMice &
                 -aDRespCrop-aDRespRapt-    aDRespSOM-aDHarvest    !
gDW/m2/y
  dXTotExtFl  = XWetDep + aXDryDep + aXManure + XBirdImm    &
                - aXLeachSoil                               &
                - aXHArvest  -  aXMortCow  -  aXMortBird            !
gCd/m2/y

  !   INTEGRATION
  !------------------ D STATES -----------------------
  sDSOM       = INTEG(dDSOM, cDSOM0)                    !  gDW/m2
  sDLitt      = INTEG(dDLitt, DLitt0)                   !  gDW/m2
```

```
  sDCrop      = INTEG(dDCrop, DCrop0)                    !  gDW/m2
  sDCow       = INTEG(dDCow, DCow0)                      !  gDW/m2
  sDWorm      = INTEG(dDWorm, cDWorm0)                   !  gDW/m2
  sDMole      = INTEG(dDMole, DMole0)                    !  gDW/m2
  sDTip       = INTEG(dDTip, cDTip0)                     !  gDW/m2
  sDBird      = INTEG(dDBird, DBird0)                    !  gDW/m2
  sDMice      = INTEG(dDMice, DMice0)                    !  gDW/m2
  sDRapt      = INTEG(dDRapt, DRapt0)                    !  gDW/m2
  sDTotExtFl  = INTEG(dDTotExtFl, DTotExtFl0)            !  gDW/m2

  ! ------------------ X STATES -----------------------
  sXSOM       = INTEG(dXSOM, XSOM0)                      !  gCd/m2
  sXSIM       = INTEG(dXSIM, XSIM0)                      !  gCd/m2
  sXLitt      = INTEG(dXLitt, XLitt0)                    !  gCd/m2
  sXDissLitt  = INTEG(dXDissLitt, XDissLitt0)            !  gCd/m2
  sXDissSoil  = INTEG(dXDissSoil, XDissSoil0)            !  gCd/m2
  sXCrop      = INTEG(dXCrop, XCrop0)                    !  gCd/m2
  sXCow       = INTEG(dXCow, XCow0)                      !  gCd/m2
  sXWorm      = INTEG(dXWorm, XWorm0)                    !  gCd/m2
  sXMole      = INTEG(dXMole, XMole0)                    !  gCd/m2
  sXTip       = INTEG(dXTip, XTip0)                      !  gCd/m2
  sXBird      = INTEG(dXBird, XBird0)                    !  gCd/m2
  sXMice      = INTEG(dXMice, XMice0)                    !  gCd/m2
  sXRapt      = INTEG(dXRapt, XRapt0)                    !  gCd/m2
  sXTotExtFl  = INTEG(dXTotExtFl, XTotExtFl0)            !  gCd/m2

 END  ! Of Derivative

  ! GENERATION OF OUTPUT, USER-FRIENDLY UNITS AND CHECKS.

  ! SOIL OUTPUT

  aXDissSoilOut    = sXDissSoil / ThetaSoil /cDepthSoil  ! mgCd/l
  aXSIMOut         = sXSIM / cRhoSIM /cDepthSoil          ! mgCd/kgS-
Soil
  aXSoilTotOut     = (sXSIM +sXDissSoil + sXSOM )        &
                     /aDRhoSoil/ cDepthSoil               ! mgCd/kgS-
Soil
  aXAdsSIM        = sXSIM /sXDissSoil                    !  -
  aXAdsSIMOut     = aXAdsSIM * ThetaSoil / cRhoSIM       ! lLSoil/k-
gSIM


  ! SOIL ORGANIC MATTER OUTPUT

  aXDSOMOut        = sXSOM / aDRhoSom / cDepthSoil      ! mgCd/kgDW
  aXAdsSOM         = sXSOM/sXDissSoil                   ! -
  aXAdsTot         = (sXSIM + sXSOM)/sXDissSoil         &
                     * ThetaSoil / aDRhoSoil             ! lLSoil/kg-
SSoil

  ! LITTER OUTPUT

  aXDissLittOut    = sXDissLitt / ThetaLitt /aDepthLitt  ! mgCd/l
  aXDLittOut       = sXLitt / cRhoLitt /aDepthLitt       ! mgCd/kgDW
  aXLittTotOut     = (sXLitt +sXDissLitt )  &
                       / cRhoLitt / aDepthLitt           ! mgCd/kgDW
  aXAdsLitt        = sXLitt /sXDissLitt                  ! -
  aXAdsLittOut     = aXAdsLitt * ThetaLitt / cRhoLitt    ! lLSoil/kg-
SSoil

  ! CROP OUTPUT

  aDCropOut       = sDCrop / gDPkgD * m2Pha              ! kgDW/ha
  aXDCropOut      = aXDCrop * mgXPgX * gDPkgD            ! mgCd/kgDW
  aBCFCropOut     = aXDCropOut /aXSoilTotOut             ! kgSSoil/-
kgDW
  aDHarvestOut  = aDHarvest / gDPkgD * m2Pha             ! kg DW/ha
  aXDHArvestOut = aXHArvest/aDHarvest * mgXPgX * gDPkgD ! mgCd/kgDW

  ! WORM OUTPUT
  aXDWormOut      = sXWorm / sDWorm * mgXPgX *gDPkgD     ! mgCd/kgDW
  aBCFWormOut     = aXDWormOut / aXSoilTotOut            ! l/kgDW
  aPBWormOut      = aDAssWorm/sDWorm                     ! 1/y

  ! TIPULIDAE OUTPUT
  aXDTipOut     = sXTip / sDTip * mgXPgX * gDPkgD       ! mgCd/kgDW

  ! COW OUTPUT
  aXDCowOut       = sXCow / sDCow * mgXPgX * gDPkgD      ! mgCd/kgDW
  aBCFCowOut      = aXDCowOut / aXDCropOut               ! -

  ! MOLE OUTPUT

  CONSTANT   cBCFMoKidWorm = 4.4                !

  aXDMoleOut      = sXMole / sDMole * mgXPgX * gDPkgD    ! mgCd/kgDW
  aXDMoKidOut     = aXDWormOut * cBCFMoKidWorm
  aXDFoodM        = aXConsMole/aDConsMole * mgXPgX * gDPkgD! mgCd/kgDW
  aBCFMoleOut     = aXDMoleOut/aXDWormOut                ! -

  ! BIRD OUTPUT
  aXDBirdOut      = sXBird / sDBird * mgXPgX * gDPkgD    ! mgCd/kgDW
  aXDFoodB        = aXConsBird/aDConsBird * mgXPgX * gDPkgD! mgCd/kgDW

  ! MICE OUTPUT
  CONSTANT cBCFMiKidTot = 3.0D0

  aXDMiceOut      = sXMice / sDMice * mgXPgX * gDPkgD    ! mgCd/kgDW
  aXDMiKidOut     = aXDMiceOut * cBCFMiKidTot            ! mgCd/kgDW
  aBCFMiceOut     = aXDMiceOut / aXDCropOut              ! kgDW/kgDW

  ! RAPTORAIL BIRDS OUTPUT
  aXDRaptOut      = sXRapt / sDRapt * mgXPgX * gDPkgD    ! mgCd/-
kgDW
```

Table B6. **PROGRAM CATS-1, listing, continued**

```
  aXDFoodR       = aXConsRapt/aDConsRapt * mgXPgX * gDPkgD   ! mgCd/-
kgDW

! ---------------- TERMINATION OF RUN ----------------------------
----
 TERMT (( Time .GE. EndTime ) .OR. ( RChkOUT ).OR.(GrChkOUT))

 END  ! Of Dynamic
END ! Of Program Peis2
```

B9. Calibration procedure files

The calibration procedure as described in chapter 6 made use of an UNCSAM sample file, almost as specified for the uncertainty analysis, with one exception: all distributions are uniform and no correlations between parameters were specified. The calibration made use of a file with acceptable ranges (table B7) and and a file with measurements (table B9). The run with the best fit was used to study general model behaviour. The parameter values for this run are specified in table B8, as incorporated in a settings file (.CMD file) for the simulation language ACSL.

Table B7. Range Check file as used for both calibration and uncertainty analysis

VarName	Low bound	High bound	Reference
sDMice	1.0D-4	5.0D-1	Stodart 1979, Denneman 1989
aBCFCropOut	2.0D-1	4.6D-1	Knoop & Aldenberg 1989, PIMM 1986
sDRapt	1.0D-7	2.5D-3	SOVON 1987, Koning & Bayens 1990
sDTip	2.0D0	3.0D1	Oudshoorn et al. 1984
aBCFWormOut	7.0D0	4.0D1	Van Rooij et al. 1988, Ma 1982
sDBird	1.0D-6	1.0D-1	SOVON 1987
sDMole	5.0D-4	2.0D-1	Haeck 1969
sDCow	1.25D1	7.0D1	m.m. Proefstation Lelystad
sDCrop	6.0D2	1.5D3	m.m. CABO-DLO
sDWorm	2.0D0	3.6D1	Tamis 1992
aBCFCowOut	5.0D-3	6.0D-1	Vreman et al. 1986, van de Ven et al. 1977
aBCFMiceOut	2.0D-1	1.0D0	Andrews et al. 1984, Hunter et al. 1987.
aBCFMoleOut	1.0D-2	3.0D-1	Ma 1987
aDHarvest	3.0D2	6.0D2	Boxem & Leusink 1978

Table B8. Settings file for ACSl, with parameter values for best run according to BACT

```
! Parameter values of best run, output of BACT with
measurements file (table B9).

 set  cXTotSoilIn        =  0.2202435781800002
 set  cXTotLittIn        =   2.431731316900003
 set  cXDCowIn           =  0.3111880887800003
 set  cXDWormIn          =   21.64284024200002
 set  cXDJackIn          =   21.83198360700002
 set  cXDMoleIn          =   2.538147681200003
 set  cXDBirdIn          =   2.934916513400003
 set  cXDMiceIn          =  0.8402812608200008
 set  cXDOwlIn           =  0.3327273703000003
 set  fXAssC             =  7.9892897783000115E-02
 set  fXAssW             =  4.0146078134000049E-02
 set  fXAssJ             =  4.8049862373000067E-02
 set  fXAssM             =  8.0764826403000107E-02
 set  fXAssB             =  1.6293601410000023E-02
 set  fXAssMi            =  1.9722590583000024E-02
 set  fXAssO             =  9.4120307657000133E-02
 set  kXExcrC            =   17.69535034900002
 set  kXExcrW            =   2.296044045100003
 set  kXExcrJ            =   2.606338563500003
 set  kXExcrM            =   2.894663260000003
 set  kXExcrB            =   2.135381292500002
 set  kXExcrMi           =   2.056981368300002
 set  kXExcrO            =   2.374818419900002
 set  cXAdsSIMIn         =   1363.606383900001
 set  cXAdsSOMIn         =   1658.357121400001
 set  cXAdsLittIn        =   978.4169637900009
 set  cXDBirdImm         =  6.8723181874000083E-02
 set  kDAssMi            =   81.35103995700008
 set  kDAssO             =   41.97392956000004
 set  kDAssB             =   34.51973904200003
 set  kDAssC             =   8.065475649600009
 set  kDAssM             =   82.43293372600007
 set  kDAssJ             =   10.24695740000001
 set  kDAssW             =  5.9682476979000084E-03
 set  kDGrCr             =   11.85306022300001
 set  kDRespMi           =   58.77509401900006
 set  kDRespO            =   27.41908611100003
 set  kDRespC            =   3.824164461700004
 set  kDRespM            =   27.09786907700003
 set  kDRespJ            =   2.855259255300003
 set  kDRespW            =   2.643307992300003
 set  kDRespCr           =   3.167399206800003
 set  kDRespL            =   2.436090964800003
 set  kDRespSOM          =   2.963479425500003
 set  kDRespB            =   20.41348094000002
 set  kDMortMi           =   3.396280463000004
 set  kDMortO            =   3.884890413700004
 set  kDMortC            =  0.1736125967600002
 set  kDMortM            =   15.29712307200001
 set  kDMortJ            =   2.696035420600003
 set  kDMortW            =   1.914256368500002
 set  kDFallCr           =  0.2695411687100004
 set  kDHarvest          =  0.5125371472000006
 set  kDMortB            =   1.012740251300001
 set  hDConsCrC          =   164.6826656500001
```

```
 set  hDEatW              =   1882.874132400001
 set  hDConsRJ            =   15.53659684000001
 set  hDPrWM              =   7.566710042600008
 set  hDPrB               =   7.355942116400008
 set  hDConsCrMi          =   82.60929056600007
 set  hDPrMiO             =  5.5245923838000093E-04
 set  cDSOM0              =   118.5241878200001
 set  cDCropIn            =   6.494678643200007
 set  cDLittIn            =  0.4058020492700004
 set  cDCowIn             =  0.6774836264400008
 set  cDWorm0             =   9.735293194700009
 set  cDJack0             =   17.72786518400002
 set  cDMoleIn            =  3.8934066074000055E-05
 set  cDBirdIn            =  4.7930548342000070E-05
 set  cDBirdImm           =  9.6431948925000164E-06
 set  cDMiceIn            =  9.9132184466000140E-03
 set  cDOwlIn             =  1.0418525057000017E-06
 set  fDAssC              =  0.4590350128500004
 set  fDAssW              =  0.5629742755300006
 set  fDAssJ              =  0.5908263402400007
 set  fDAssM              =  0.5899784764500006
 set  fDAssB              =  0.4232308941100005
 set  fDAssMi             =  0.4986884463100005
 set  fDAssO              =  0.5229425970700006
 set  cRhoSIM             =  0.3497132781800004
 set  cRhoSOM             =  0.3159815633300003
 set  cEpsSoil            =  0.8067067758200007
 set  cMoistSoil          =  0.8973373358700011
 set  cRhoLitt            =  0.1629408550600002
 set  cEpsLitt            =  0.8612396732600010
 set  cMoistLitt          =  0.3621070135900004
 set  fDEnvCr             =  0.9592345012400010
 set  fPreLittSoil        =  0.6299691122900008
 set  fPreSoilDeep        =  0.3371479516800004
 set  kXUpCr              =  6.3857230596000096E-05
 set  hXUpCr              =  6.6894624820000085E-02
 set  kXUpW               =  8.1137141376000112E-04
 set  hXUpW               =  8.0385991364000112E-03

! Settings after equilibrium (2 jr).
! XStates recalculated towards XDIn's

s     cDBirdIn =  0.01962474027D-02
s      cDCowIn =  4.75602553416D-01
s     cDCropIn =  8.52241145046D+00
s     cDJack0  =  1.95288871071D+01
s     cDLittIn =  1.73597569288D+00
s     cDMiceIn =  0.00694082826D-02
s     cDMoleIn =  0.02538617416D-02
s      cDOwlIn =  3.54962247579D-06
s       cDSOM0 =  1.27588083108D+02
s   SDTOTEXTFL =  0
s      cDWorm0 =  1.12108658709D+01
s    cXDBirdIn =  6.4053D-01
s    cXDCowIn  =  1.0693D-02
s    cBCFCrop  =  3.75D-01
s    cXDJackIn =  2.7468D-02
s  cXTotLittIn =  1.1D+00
s    cXDMiceIn =  7.0563D-02
s    cXDMoleIn =  2.6121D+00
s    cXDOwlIn  =  5.9025D-02
s   SXTOTEXTFL =  0
s    cXDWormIn =  8.8673D+00
```

Table B9. **Measurement file for BACT calibration, as used for the study of general model behaviour.**

```
#1  4 august 1992
#2  BAYESIAN CALIBRATION TECHNIQUE, BY RIVM-LWD-MM (BACT.EXE)
#3  Copyright (C) RIVM/CWM, 1992
#4  Measurements file  (0, nr outputs, nr msr, -1)
0        15         9       -1
```

	sDWorm	sDTip	sDMole	sDMice	sDCow	sDRapt	sDBird	aBCFCowOut	aBCFCropOut	aBCFWormOut	aXSoilTotOut	aBCFMiceOut	aBCFMoleOut	sDCrop	aDHarvest
1)	17.55	7.9	0.066	0.015	36.0	1.4E-4	0.024	0.10	0.36	14	1.19	0.40	0.029	800	4000
2)	7.75	3.0	0.034	0.010	54.0	2.8E-4	0.005	0.31	0.20	11	0.55	0.72	0.029	800	4500
3)	15.75	16.0	0.100	*	40.0	1.0E-4	0.04	0.45	0.40	13	0.87	0.61	0.016	900	5000
4)	2.75	*	0.14	*	50.0	*	*	0.05	*	10	0.55	0.86	0.18	1000	3500
5)	8.65	*	0.066	*	*	*	*	0.028	*	*	0.70	*	0.08	*	*
6)	7.50	*	0.06	*	*	*	*	0.02	*	*	*	*	*	*	*
7)	*	*	*	*	*	*	*	0.016	*	*	*	*	*	*	*
8)	*	*	*	*	*	*	*	0.028	*	*	*	*	*	*	*
9)	*	*	*	*	*	*	*	0.02	*	*	*	*	*	*	*

References

sDWorm:	Tamis 1992 (1,2,3,4); Oudshoorn et al. 1984 (5); Edwards & Lofty 1979 (6)
sDTip	Oudshoorn et al. 1984 (1,2,3)
sDMole	Haeck 1969 (1,2,3,4,6)
sDMice	estimated from territorium sizes, 400 m2 and 600 m2, Denneman 1989 (1,2)
sDCow	stocking densities of between 2, 2.4, 2.7 and 3 cows per hectare
sDRapt	SOVON 1987 (1,2); Koning & Bayens 1990 (3)
sDBird	SOVON 1987 (1,2,3)
aBCFCowOut	van de Ven et al. 1977 (1,2,3); Vreman et al. 1986 (4,5,6,7,8,9)
aBCFCropOut	Knoop & Aldenberg 1989 (1); PIMM 1986 (2,3)
aBCFWormOut	Van Rooij et al. 1988 blz 49 (1,2,3,4)
aXSoilTotOut	Van Rooij et al. 1988, Aldenberg & Knoop 1989, CCRX 1985, Cd database LBG-RIVM
aBCFMiceOut	Andrews et al. 1984 (1,2); Hunter et al. 1987 (3,4)
aBCFMoleOut	Ma 1987 (1,2,3,4,5)
sDCrop	m.m. CABO-DLO, Boxem & Leusink 1978
aDHarvest	m.m. CABO-DLO

Appendix C. Logistic population growth modelling and implications for biomass turnover.

Ecosystem modelling within the CATS model concept is based on a thorough bookkeeping of both nutrient and pollutant cycles. Consequently, all biomass fluxes and the pollutant associated with these, should be accounted for. Below we will discuss what the implications of the way we combined the logistic growth equation for populations are on modelling of biomass fluxes.

1. The logistic population growth equation

First, we will consider the bookkeeping of biomass per biotic compartment. We can write the general biomass balance equation for the biotic compartment as:

$$\frac{dD}{dt} = DAss - DResp - DMort - DConsPred \qquad [gDW/m2/y] \tag{1}$$

with biomass D [gDW/m^2]. The fluxes *DAss, DResp*, etc are written as functions of constants, auxiliary variables and state variables. These processes determine the dynamics of the model. Usually, we cannot describe all mechanisms acting on populations in their environment. Consequently, the dynamics of the model do not have to be a true representation of the dynamics in the field. Moreover, the dynamic behaviour of the model could be caused by a certain combination of parameter values. Because the goal of our model is not to predict true population field dynamics, but to study the impact of emission reduction, we choose to embed mechanisms in the more phenomenological approach of logistic population growth. Since in our model concept, compartments represent functional groups and not single populations, we feel that this justifies the use of a simple population model.
The much used logistic growth equation according to Verhulst (1838) can be written as

$$\frac{dx}{dt} = r \cdot x \cdot \left(1 - \frac{x}{K}\right) = r \cdot x - \frac{r}{K} \cdot x^2 \tag{2}$$

with r the intrinsic rate of increase and K the carrying capacity. This equation offers important dynamic advantages. For small x the population will grow exponentially and eventually stabilises at K by negative feedback. Following Hallam et al. (1986) and Smith (1982), we propose to combine mechanisms considered limiting with the logistic growth equation. Other limitations not explicitly modelled are represented by the environment (*Env*) as set by the carrying capacity K. The result of this type of dynamics is, that the population is persistent between *0* and K for every biotic compartment. It also leads to general overall stability of the ecosystem model, which is of great importance because we want to use the model with widely varying parameter values. We will consider K as the maximum observed density that occurs naturally. The local ecosystem determines which limitation mechanisms should be modelled to bring the density to a realistic value.In the

next derivation, we will not consider predation losses for the sake of clarity. Afterwards, predation can be added easily without affecting nutrient balance.

Food availability for the population is given by the Monod equation (type II saturation kinetics):

$$DSat = \frac{DFood}{hFood + DFood}$$

with hFood the half saturation constant. This equation can be modified to incorporate several food sources, with an overall half saturation constant.
If we rewrite the first equation in full, without predation, we get

$$dD/dt = kDAss \cdot DSat \cdot D - kDResp \cdot D - kDMort \cdot D$$

with rate constants identified by *kD...*[y^{-1}]. If there is no food limitation, exponential growth in *D* results. The limitation of growth to reach a stable population size depends on realistic modelling of food availability and the limitation mechanism. Food limitation is not the only mechanism to keep biomass *D* in check.

For *DSat =1* (no food limitation whatsoever), logistic growth (meaning growth limitation by the environment) can be brought into the equation:

$$dD/dt = kDIncr \cdot D - kDIncr/cDCarr \cdot D^2.$$

where

$$kDIncr\ [y^{-1}] = kDAss - kDResp - kDMort$$

is the intrinsic rate of increase. *kDIncr* is the sum of rate constants for assimilation (production) and the inevitable losses by respiration and mortality, i.e. net production. No losses by predation are accounted for, since a population need not be predated on. In the absence of the predator, the population density is set by the environment with *cDCarr* as the carrying capacity [gDW/m^2]. The equilibrium population density is

$$D\ [gDW/m^2] = cDCarr$$

which is a stable equilibrium. Now we can define the environmental correction term, where *Env* means environment:

$$DEnv\ [gDW/m^2/y] = kDIncr/cDCarr \cdot D^2 \qquad (3)$$

This term is equal to the quadratic part of the logistic equation (2). With the introduction of this correction (feedback) term two problems arise, that must be solved. Fluxes are associated with *DResp, DMort* and *DAss*. Biomass can be respired (*DResp*), or it can be added to soil or litter by mortality (*DMort*). Where does the biomass flux *DEnv* [$gDW/m^2/y$] come from and where does it go to? The second problem arises when *DSat* < *1*, which conforms to a limited food supply.

If we see *DEnv* solely as a production correction term, the production is reduced by *DEnv*:

$$DAss \ [\text{gDW/m}^2\text{/y}] = kDAss \cdot DSat \cdot D - DEnv$$

For small *DSat* the first term of the expression is also small and hence the expression could become negative. It is not allowed that *DAss* is less than 0. Therefore, we chose to divide *DEnv* between production and mortality, like Hallam et al. (1986). Production is reduced and mortality increased, which conforms to the original derivation of the quadratic feedback. To prevent negative production, we propose to reduce the correction on production as well, if food supply is limiting:

$$DAss \ [\text{gDW/m}^2\text{/y}] = (kDass \cdot D - DEnv) \cdot DSat \qquad (4)$$

When we compare (4) and (3), it is apparent that $DEnv \cdot DSat$ falls short of (3), and we are left with $DEnv \cdot (1 - DSat)$. This is added to population mortality:

$$DMort \ [\text{gDW/m2/y}] = kDMort \cdot D + DEnv(1 - DSat)$$

Since we now have new expressions for *DAss* en *DMort*, we can rewrite equation (1) as a derivation of the logistic growth equation. We now have a generic population growth equation which we will use for every biotic functional group:

$$\frac{dD}{dt} = ((kDAss \cdot D - DEnv) \cdot DSat) - kDResp \cdot D - (kDMort \cdot D + DEnv \cdot (1 - DSat)) \qquad (5)$$

2. Consequences of logistic growth for P/B ratio and biomass turnover.

With equation (3) for logistic population growth, we can express equilibrium density and and production efficiency as a function of food availability.
After some manipulations and substituting (3) in (5), the equilibrium density D^* of the functional group becomes:

$$D^* = \frac{kDAss \cdot DSat - kDResp - kDMort}{kDAss - kDResp - kDMort} \cdot cDCarr \qquad (6)$$

We find that if $DSat \rightarrow 1$, the density *D* will approach the carrying capacity. As an example, we can use the nominal parameter values from the 'Mice' group to calculate the equilibrium densities for progressive food limitation (table C1).

It is clear that the equilibrium density comes down from the carrying capacity (0.01 g DW/m^2) to 0. No existence is possible below the food limitation where

$$DSat = (kDResp + kDMort) / kDAss = 0.671$$

At equilibrium we can also calculate relative assimilation (comparable to the P/B ratio), relative respiration and relative mortality as a function of food availability (table C2).

Table C1. Equilibrium density of Mice in relation to food availability calculated from equation (6).

DSat	D^*
1	0.01000
0.9	0.00696
0.8	0.00392
0.7	0.00088
0.671	0.00000

Table C2. Relative DAss, Resp and DMort as a function of food availability

DSat	*RelDAss*	*RelDResp*	*RelDMort*
1	52.00	50	2.00
0.9	53.78	50	3.78
0.8355	54.10	50	4.10
0.8	54.00	50	4.00
0.7	52.68	50	2.68
0.671	52.00	50	2.00

From table C2 we observe that the assimilation optimum is at *DSat* = 0.8355, which is a mild food limitation. At equilibrium, the relative assimilation hardly changes at different food availability, while the density is strongly affected (table C1). It appears that the relative assimilation is equal at total food saturation and minimal existence saturation, and is calculated as follows:

$$RelDAss = kDResp + kDMort \quad = 52 \text{ [1/y]}$$

Since we have an expression for relative production in a convenient unit, we can calculate the residence time of biomass in the mice compartment. Using table 2 we can see that the residence time is between

$$1/54.1 \cdot 365.25 = 6.75 \text{ [d] and}$$
$$1/52 \cdot 365.25 = 7.02 \text{ [d]}$$

which is about a week. If we can also calculate the residence time of the pollutant, we can calculate the equilibrium pollutant concentration using the quotient of these two residence times. This matter will be dealt with in Appendix D.

Appendix D. Bioaccumulation Factors

In this appendix, we will derive a formula for the bioaccumulation factor, taking into account both biomass and pollutant turnover. In Appendix C, we paid attention to the turnover of biomass, which was shown to depend on food availability. Here we will show that bioaccumulation also depends on food availability.

CATS ecosystem models are based on a thorough bookkeeping of both nutrient and pollutant cycles. Consequently, all biomass fluxes and the pollutant associated with these, should be accounted for. Below we will discuss what the implications of the choice of the logistic growth equation for populations are on modelling of biomass fluxes.

Bioaccumulation of pollutants in compartments of ecosystem models can be studied by bookkeeping both the biomass and the toxic mass of the compartments (fig 6). Two generic mass balances are made per biotic compartment, where X is toxic mass, and D is biomass:

$$\frac{dD}{dt} = DAss - DResp - DMort - DConsPred \quad [gDW \cdot m^{-2} \cdot y^{-1}] \tag{1}$$

$$\frac{dX}{dt} = XAss - XExcr - XMort - XConsPred \quad [gX \cdot m^{-2} \cdot y^{-1}] \tag{2}$$

It is easy to see the parallel between the two terms. They can be, but do not necessarily have to be indepent from each other. Turnover of pollutant and biomass is not necessarily the same. Some loss processes do not change the ratio of pollutant and toxicant while others do. Biomass and pollutant mass leaving the compartment by mortality have a fixed ratio, equal to the ratio in the (living) compartment:

$$XMort / DMort = X/D \quad [gX/gD] \tag{3}$$

Consequently, mortality does not influence bioaccumulation of the biotic compartment. The same holds true for predation; the ratio of the biomass and toxic mass leaving (cf. eq. 3) is not different from the ratio of the compartment. Equations (1) and (2) also show that different processes are responsible for the loss of only biomass or pollutant mass:

carbon respiration	*DResp*
toxicant excretion	*XExcr*

The assimilation of food demonstrates that pollutant and biomass enter the compartment at different rates. The concentration of pollutant in the food is expressed as *XDFood* [gX/gD]. The assimilation efficiencies of X and D (resp. [gX/gX] en [gD/gD] can be different, thus changing the assimilated ratio *X/D*.

To derive a formula for the Bioaccumulation Factor (*sensu* Walker 1987), we need to rewrite a number of expressions, ignoring predation for the time being:

$$XAss = fXAss \cdot XCons \quad (4)$$

X assimilation is a fraction of the cadmium consumed by the animal

$$XCons = DCons \cdot XDFood \quad (5)$$

X consumed is the amount of biomass consumed times the concentration of *X* in the food

$$DCons = DAss / fDAss \quad (6)$$

D consumed is the assimilated biomass divided by the biomass assimilation efficiency

$$fXDAss = fXAss / fDAss \quad (7)$$

The assimilation ratio is the ratio of the two efficiencies

Substituting (5) and (7) and then (6) in (1) we obtain

$$XAss = fXDAss \cdot fDAss \cdot DCons \cdot XDFood =$$

$$= fXDAss \cdot XDFood \cdot DAss \quad (9)$$

We define excretion and respiration as a first order process, and rewrite the expression for the amount of pollutant leaving the compartment by mortality:

$$XExcr = kXExcr \cdot X = kXExcr \cdot XD \cdot D \quad (10)$$

$$DResp = kDResp \cdot D \quad (11)$$

and $$XMort = XD \cdot DMort \quad (12)$$

The massbalance for *X* can now be rewritten by substituting (9), (10) and (12) in (2):

$$\frac{dX}{dt} = fXDAss \cdot XDFood \cdot DAss - kXExcr \cdot XD \cdot D - XD \cdot DMort \quad (13)$$

We now want to derive a simple formula for the concentration *XD* in the compartiment. The equations for *DAss* and *DMort* both contain correction terms for environmental limitation, resp. *DEnv* and *Denv · (1 - DSat)*, and the food saturation function *DSat*. At equilibrium dD/dt=0, thus equation (1) becomes (ignoring predation):

$$DMort = DAss - DResp \quad (14)$$

Also, dX/dt = 0 so we can rewrite equation (13), substituting (14) in (13):

$$XD = fXDAss \cdot XDFood \cdot \left(\frac{DAss}{DAss + kXExcr \cdot D - DResp} \right) \quad (15)$$

The relative assimilation of carbon (*RelDAss*) is defined as *DAss/D* at equilibrium. If we devide by D, and substitute (11) in (15) we find

$$XD = fXDAss \cdot XDFood \cdot \frac{RelDAss}{RelDAss + kXExcr\text{-}kDResp} \tag{16}$$

With this formula, we can derive an equation for the bioaccumulation factor. If the respiration of *D* and excretion of *X* occur at the same rate, then *kXExcr* = *kDResp* and the pollutant concentration can be written as

$$XD = fXDAss \,.\, XDFood \tag{17}$$

In general, the bioaccumulation factor (*BAF*) for terrestrial organisms can be defined as the ratio of the concentration in a biotic compartment and its food:

$$BAF = XD/XDFood \tag{18}$$

Consequently, the bioaccumulation factor for this specific case is equal to *fXDAss* which is the ratio of the assimilation efficiencies:

$$BAF = fXDAss = fXAss \,/\, fDAss \tag{19}$$

However, if the excretion rate differs significantly from the respiration rate, the *BAF* becomes

$$BAF = fXDAss \cdot \frac{RelDAss}{RelDAss + kXExcr\text{-}kDResp} \tag{20}$$

It is now possible to calculate the *BAF*, taking *Mice* as an example. The next nominal values are taken from an earlier version of the model:

kXExcrMi = 2.5 [1/y]
kDRespMi = 50 [1/y]
fXAssMi = 0.05 [-]
fDAssMi = 0.50 [-]
fXDAssMi = 0.1 [-]

The relative *DAss* depends on the food saturation function *DSat*, which has been shown in Appendix 4. We can now show that the Bioaccumulation Factor depends on food availability (table D1):

Table D1. The bioaccumulation factor as a function of food availability

DSat (food saturation)	BAF (bioaccumulation factor)
1	1.156
0.9	0.857
0.8355	0.820
0.8	0.831
0.7	1.018
0.6710	1.156

For *Mice*, the bioaccumulation factor is less than 1 at moderate food limitation. When no food limitation is present (DSat=1) or at severe food limitation (DSat=0.671), the BAF is more than 1. Earlier, we have shown (Appendix C) that for these cases the relative assimilation becomes

$$RelDAss = kDResp + kDMort \tag{21}$$

This 'worst case' BAF can be calculated if we substitute (21) in (20):

$$BAF = fXDass \cdot \frac{kDResp + kDMort}{kXExcr + kDMort} \tag{22}$$

This equation can be used to predict the worst case bioaccumulation factor from model parameters, without the actual running of the model. If BAFs are known from field studies and general physiological and ecological knowlegde can be used to estimate the biomass parameters, the toxicant assimilation efficiency and excretion rate constant can be estimated.

As shown before in Appendix 4, we can express the relative assimilation, excretion and mortality at equilibrium, and here we do this for the pollutant:

$$RelXExcr = (kXExcr \cdot X)/X = kXExcr \tag{23}$$

with *kXExcr* an excretion constant. The relative cadmium loss by mortality is written as

$$RelXMort = XD \cdot DMort/X = DMort/D = RelDMort \tag{24}$$

As we now see, the relative (per capita) cadmium loss by mortality is not constant, and equal to *RelDMort.* It is tabulated as a function of food availability in Appendix C, table C2.

From (2) it can be shown that at equilibrium

$$RelXAss = RelXExcr + RelXMort \tag{25}$$

Consequently, RelXAss also depends on food availability, tabulated in table D2.

Table D2. Relative Cadmium Assimilation of *Mice* as a function of food availability

DSat	RelXAss	RelXExcr	RelXMort
1.0	4.500	2.5	2.0
0.9	6.275	2.5	3.775
0.835	6.598	2.5	4.098
0.8	6.500	2.5	4.000
0.7	5.175	2.5	2.675
0.671	4.500	2.5	2.000

When food conditions are either saturating or extremely limiting at the survival limit, the relative cadmium assimilation, i.e the turnover of pollutant *RelXAss,* is at its lowest:

$$RelXass = kXExcr + kDMort = 4.5 \text{ [1/y]} \tag{26}$$

If we compare this with the turnover of biomass:

$$RelDAss = kDResp + kDMort = 52 \text{ [1/y]} \tag{27}$$

we see that these turnovers are quite different. The mean residence time of cadmium, which is the inverse of turover, is expressed in days. At these specific parameter values of *Mice* the residence time is

$$(1/4.5) \cdot 365.25 = 81.2 \text{ [d]}$$

which is almost three months, while the residence time of biomass is a week (Appendix C). At suboptimal food conditions, the relative cadmium assimilation is highest (table D2) and the mean residence time shorter:

$(1/6.598) \cdot 365.25 = 55.4$ [d] , almost two months.

Since equations (26) and (27) define the relative cadmium assimilation at equilibrium, we can rewrite equation (22) in terms of mass turnovers, by substituting (26) and (27) in (22):

$$BAF_{worstcase} = fXDAss \cdot \frac{RelDAss}{RelXass} = fXDAss \cdot \frac{Turnover\ D}{Turnover\ X} \tag{28}$$

Because of the inverse relation turnover - residence time we can also write

$$BAF_{worstcase} = \frac{fXAss}{fDAss} \cdot \frac{residencetime\ X}{residencetime\ D} \tag{29}$$

This definition of the BAF shows that the bioaccumulation factor is the product of the ratio of the assimilation efficiencies (*fXDAss*) and the ratio of the residence times.

Appendix E: Sorption equilibria according to Clasen

In the CATS model, equilibrating cadmium fluxes are considered as 'fast' reactions (Clasen 1976), relative to 'slow' cadmium fluxes like cadmium input by plant litter, manure, dead animals etc. We consider an equilibrium between dissolved and sorbed cadmium:

$$P_{diss} \rightleftharpoons P_{sorb} \qquad \textit{equilibrium equation}$$

$$\frac{P_s(t)}{P_d(t)} = k$$

$$\frac{dP_d}{dt} = S_d \qquad \textit{slow processes}$$

$$\frac{dP_s}{dt} = S_s \qquad \textit{slow processes}$$

with P_s = sorbed cadmium [gCd/m^2]
P_d = dissolved cadmium [gCd/m^2]
dP_d/dt = change in dissolved cadmium [gCd/m^2/y]
dP_s/dt = change in sorbed cadmium [gCd/m^2/y]
S_s, S_d = slow processes [gCd/m^2/y]

We can differentiate the equilibrium equation to time, yielding

$$\frac{dP_s}{dt} \cdot \frac{1}{P_d} - \frac{P_s}{(P_d^2)} \cdot \frac{dP_d}{dt} = 0 \quad \Rightarrow$$

$$\frac{dP_s}{dt} \cdot \frac{k}{P_s} - \frac{k}{P_d} \cdot \frac{dP_d}{dt} = 0$$

if we now divide by k, we find

$$\frac{dP_s}{dt} \cdot \frac{1}{P_s} - \frac{dP_d}{dt} \cdot \frac{1}{P_d} = 0 \qquad (1)$$

The fast, equilibrating fluxes are represented by $R = R(t)$:

$$\frac{dP_d}{dt} = S_d - R$$

$$\frac{dP_s}{dt} = S_s + R \qquad (2)$$

We can substitute the expanded equations (2) in (1) if we keep in mind that P_g and P_o cannot be zero:

$$\frac{S_s + R}{P_s} - \frac{S_d - R}{P_d} = 0 \tag{3}$$

Because we need an expression for the fast fluxes R to solve equations (2) in the model, we solve for R:

$$R = \frac{P_s \cdot S_d - P_d \cdot S_s}{P_d + P_s} \tag{4}$$

In the CATS model, equations (2) and (4) are used to describe cadmium equilibrium in litter. However, in soil we have two sorbing fractions, soil inert matter (SIM) and soil organic matter (SOM). This is a more complex equilibrium, with X_0 the dissolved fraction, X_1 the organic fraction and X_2 the inert fraction

$$\begin{aligned} X_1 &\rightleftharpoons X_0 \rightleftharpoons X_2 \\ \frac{dX_o}{dt} &= S_o - F_{01} - F_{02} \\ \frac{dX_1}{dt} &= S_1 + F_{01} \\ \frac{dX_2}{dt} &= S_2 + F_{02} \end{aligned}$$

With F_{01} = equilibrating cadmium flux from dissolved to soil organic matter
F_{02} = equilibrating cadmium flux form dissolved to soil inert matter
S_q = slow processes of compartment q

We can solve this set of equations in the same way as before, for the two fast reactions F_{01} and F_{02}, representing equilibrating fluxes to both sorbing fractions. The solutions are rather lengthy, and are given in Appendix B. Because of the amount of work involved in an analytical solution, the integration software FAME contains an operator for numerical solutions of complex equilibria (Wortelboer & Aldenberg 1991).

Appendix F: Latin and common names of species

Latin name	English name	Dutch name
Anas penelope	wigeon	smient
Anas platyrhynchos	mallard	wilde eend
Falco tinnunculus	kestrel	torenvalk
Fulica atra	coot	meerkoet
Hirundo rustica	swallow	boerenzwaluw
Limosa limosa	black-tailed godwit	grutto
Microtus arvalis	continental field vole	veldmuis
Tipula palidosa		emelt
Vanellus vanellus	lapwing	kievit

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