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Link to publication

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Abstract

A catchment-scale mass-balance model of linked carbon and nitrogen cycling in ecosystems has been developed for simulating leaching losses of inorganic nitrogen. The model (MERLIN) considers linked biotic and abiotic processes affecting the cycling and storage of nitrogen. The model is aggregated in space and time and contains compartments intended to be observable and/or interpretable at the plot or catchment scale. The structure of the model includes the inorganic soil, a plant compartment and two soil organic compartments. Fluxes in and out of the ecosystem and between compartments are regulated by atmospheric deposition, hydrological discharge, plant uptake, litter production, wood production, microbial immobilization, mineralization, nitrification, and denitrification. Nitrogen fluxes are controlled by carbon productivity, the C:N ratios of organic compartments and inorganic nitrogen in soil solution. Inputs required are: 1) temporal sequences of carbon fluxes and pools; 2) time series of hydrological discharge through the soils, 3) historical and current external sources of inorganic nitrogen; 4) current amounts of nitrogen in the plant and soil organic compartments; 5) constants specifying the nitrogen uptake and immobilization characteristics of the plant and soil organic compartments; and 6) soil characteristics such as depth, porosity, bulk density, and anion/cation exchange constants. Outputs include: 1) concentrations and fluxes of NO_3 and NH_4 in soil solution and runoff; 2) total nitrogen contents of the organic and inorganic compartments; 3) C:N ratios of the aggregated plant and soil organic compartments; and 4) rates of nitrogen uptake and immobilization and nitrogen mineralization. The behaviour of the model is assessed for a combination of land-use change and nitrogen deposition scenarios in a series of speculative simulations. The results of the simulations are in broad agreement with observed and hypothesized behaviour of nitrogen dynamics in growing forests receiving nitrogen deposition.

Introduction

Forested ecosystems are commonly nitrogen deficient and retention of nitrogen within the ecosystems is usually essentially complete (e.g. Likens *et al.* 1977, Bormann *et al.* 1977, Vitousek and Howarth 1991, Johnson 1992). Although periodic or random disturbances can cause losses of inorganic nitrogen from forested ecosystems (e.g. Vitousek *et al.* 1979), these responses are generally transient, and nitrogen retention resumes when the disturbance is removed. Long-term inputs of inorganic nitrogen from atmospheric deposition may, however,

produce 'nitrogen saturation' (e.g. Nilsson 1986, Ågren and Bosatta 1988, Aber *et al.* 1989, Brandon and Hüttl 1990, Stoddard 1994), a condition characterized by increased and persistent leaching losses of inorganic nitrogen from forests in streamflow or groundwater discharge (e.g. Aber *et al.* 1989, van Miegroet *et al.* 1992, van Miegroet and Johnson 1993). It is generally thought that the increased leaching associated with 'saturation' occurs when the combined inputs of inorganic nitrogen from internal sources (such as nitrogen mineralization and fixation) and external sources (such as atmospheric

deposition and fertilization) exceed the nitrogen uptake requirements of plants and soil microorganisms (Stoddard 1994).

Nitrogen leaching can produce adverse effects on catchment resources. Inorganic nitrogen is usually lost from forests as nitrate, although in some cases ammonium is also leached. Nitrate is a strong acid anion and, if released to soils and surface waters, is effective as an acidifying agent and can mobilize toxic aluminium (Henriksen *et al.* 1988, Brown 1988). Assimilation of ammonium in soils or water can also have an acidifying effect. High concentrations of nitrate and ammonium in soils have been implicated in forest die-back in central Europe (van Breemen and van Dijk 1988). Nitrate and ammonium are also important nutrients for aquatic plants and decreased retention in catchment soils can result in elevated concentrations of these nutrients in surface waters which in turn can lead to eutrophication (National Academy of Sciences 1969). Leaching of nitrate to groundwater can lead to concerns for human health if the groundwater resource is exploited for water supply (National Research Council 1991).

There are indications that current levels of nitrogen deposition are resulting in increased mobilization of nitrogen in terrestrial and aquatic ecosystems (e.g. Emmett *et al.* 1993, Stoddard 1994, Dise and Wright 1995). Experimental manipulations of forested ecosystems have shown that inorganic nitrogen leaching can be induced or alleviated rather quickly with only modest changes in inorganic nitrogen inputs (Kahl *et al.* 1993, Wright and van Breemen 1995). Given that deposition of inorganic nitrogen has been projected to increase by at least 25% in the next 25 years in North America and Europe (Galloway *et al.* 1994), there is cause for concern that nitrogen leaching from forested ecosystems may increase .

There is a need, therefore, to develop an integrated scientific understanding of the many processes responsible for nitrogen retention and loss in forested ecosystems. In addition, the development of sound emissions control and resource management policies will require the ability to predict the onset and effects of nitrogen leaching. Mathematical models of nitrogen dynamics in terrestrial ecosystems are needed for both tasks. In particular, there is a need for a model that focuses on the retention and loss of inorganic nitrogen at the catchment scale, while maintaining sound process representations of biotic and abiotic interactions occurring within the catchment. In order to be most useful in the context of transboundary atmospheric pollution and deposition, the model should be applicable in regional as well as site specific analyses, and should rely on data readily obtainable at the catchment or landscape level.

The Model of Ecosystem Retention and Loss of Inorganic Nitrogen (MERLIN) was developed to meet these needs and this paper describes the conceptual basis, the mathematical structure and the implementation of MERLIN and describes a series of simulation exercises to demonstrate the potential use and range of response inherent in the model structure.

Structure of the model

BACKGROUND

Nitrogen dynamics within terrestrial ecosystems have been investigated by a variety of models focused primarily on nitrogen but formulated with different levels of complexity or for different applications. Dise and Wright (1995) constructed a simple empirical relationship describing catchment-scale nitrogen leaching from forest systems as a function of atmospheric deposition. Soil profile and field-scale models such as SOIL/SOILN have been developed for use on agricultural land cultivated for crops (Bergstrom and Jarvis 1991), and more recently have been applied to forest stands (Eckersten *et al.* 1995). Aber *et al.* (1991) constructed a lumped parameter model (VEGIE) linking organic matter turnover, nutrient dynamics, and forest productivity. More detailed process models linking nitrogen dynamics to carbon productivity have been constructed by Aber and Federer (1992; Pnet-CN), Running and Gower (1991; FOREST-BGC), and Thornley and Cannell (1992). Models linking nutrient cycling, nitrogen dynamics and the effects of atmospheric anthropogenic deposition on biogeochemical cycling have been formulated by Li *et al.* (1991; NuCM), and Groenenberg *et al.* (1995; NUCSAM). Catchment-scale models such as MAGIC-WAND (Ferrier *et al.* 1995, Jenkins *et al.* in press) have been used to examine the interactive effects of sulphur and nitrogen deposition on catchment soils and drainage waters. At the most detailed scale, complex nitrogen cycling models such as NICCCE (van Dam and van Breemen 1995) have been developed to interpret results of tracer experiments using a stable isotope of nitrogen (^{15}N), as well as simulating the turnover of stable isotopes of carbon (^{12}C and ^{13}C).

Nitrogen dynamics are often included in models developed primarily for other purposes such as simulation of forest productivity, forest vitality or ecosystem succession. Productivity models have been developed to examine the consequences for forest growth of changes in environmental conditions such as meteorology or air quality, management actions such as thinning or treatment of disease, climate change and CO_2 enhancement (Ågren *et al.* 1991, Landsberg *et al.* 1991). Although focused on carbon productivity, these models usually contain some level of detail about effects of nitrogen availability. Concern about the condition of forest health in Europe and North America has resulted in the development of ecophysiological models to assess forest vitality and nutritional imbalances especially in relation to nitrogen availability and magnesium deficiency, such as

FIWALD (Schall 1991), and NAP (van Oene 1992), and exposure to pollutants such as ozone (Weinstein *et al.* 1991; TREGRO). Interest in the effects of climate change and nutrient availability on forest succession have been modelled in detail by Shugart (1984; FORET) and more recently Krauchi (1995; FORSUM). Eco-regional responses have been examined by Rastetter *et al.* (1991; GEM) in a generalized modelling approach examining the effects of increased global CO_2 concentrations, temperature, and nitrogen inputs on carbon storage.

These existing models of nitrogen dynamics in terrestrial systems are in general focused on details of nitrogen cycling within the biotic community as a whole or within individual organisms. The mobility of nitrogen in the abiotic environment is usually not considered in detail. Agricultural runoff models are a notable exception, but these are limited in application and not intended for forested ecosystems. Yet it is the mobility of nitrogen in the abiotic environment that is of primary concern for acidification of soils and acidification and eutrophication of surface waters.

CONCEPTUAL BASIS OF THE MODEL

MERLIN is a model of linked biotic and abiotic processes affecting the cycling and storage of nitrogen in an ecosystem (Fig. 1). The conceptual representation of the ecosystem is highly aggregated in space and time. The compartments and processes included in the model are intended to be observable and/or interpretable at the plot or catchment scale (rather than at the scale of individual

organisms or soil pedons). The time steps are monthly to yearly and the intended periods of simulation are decadal (50 to 100 years or more). The processes and fluxes in the model can be grouped roughly as transformations and transport of inorganic nitrogen species (unshaded left side of Fig. 1); and translocation, transport and storage of organic nitrogen (shaded right side of Fig. 1). The organic processes are further subdivided into those mediated by plants and those mediated by soil microorganisms. The fluxes of nitrogen (open arrows in Fig. 1) through the abiotic and biotic pathways are controlled or affected by hydrological processes, the physical characteristics of the soil matrix and the fluxes of organic carbon (closed arrows in Fig. 1) through the biotic compartments.

Model structure

Two species of inorganic nitrogen (NO_3 and NH_4) are considered in the model. Both have a dissolved phase in soil solution and the model provides the potential for both to have an adsorbed phase (cation and anion exchange) on the soil matrix. Both forms of inorganic nitrogen can be incorporated into organic matter. The incorporation of inorganic nitrogen into the organic compartments is regulated by aggregated plant and soil microbial processes and by availability of inorganic nitrogen in the abiotic environment (Fig. 1). The conceptualization is that uptake and immobilization are: 1) directly proportional to concentrations of inorganic nitrogen in soil solution (i.e., substrate limited at some level); 2) directly proportional to carbon fluxes through each organic compartment (i.e., a function of carbon produc-
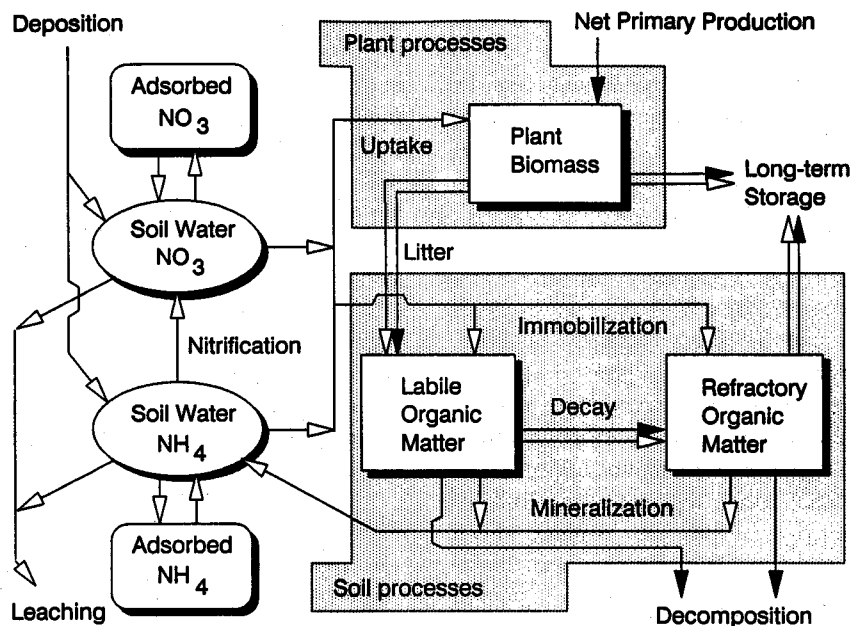

Fig. 1 *A diagram of the conceptual basis of the MERLIN model.*

tivity); and 3) inversely proportional to the nitrogen status of each organic compartment (i.e., negative feedback for regulation to a 'preferred' nitrogen content). Each of the rectangular boxes in Fig. 1 represents a pool of organic material containing both carbon and nitrogen. The fluxes of nitrogen through these organic compartments are linked to the fluxes of carbon, which are specified as inputs to the model.

The plant compartment is an aggregated pool of carbon and nitrogen representing the 'active' portion of the ecosystem. This pool conceptually includes, for example, foliage and fine roots for forests and perhaps whole plants for grasslands. Long-term storage losses from this · pool (Fig. 1) can be thought of as wood production in forests, or production of any plant structure that removes carbon and nitrogen from the ecosystem for the duration of the simulation. The litter flux represents the sum of all organic material transferred to the soil compartments and includes leaf litter, fine-root death, and woody debris. Carbon mass balance for this compartment requires that the difference between inputs and outputs equals the rate of change of the compartment. Thus, specified time sequences of plant biomass, litter production and long-term storage determine the net primary productivity of the system for that period of simulation (Fig. 1). For forested systems, time sequences of standing crop, litter production and wood production are well (or at least approximately) known, and obtaining these input sequences for a model application is relatively straightforward.

Soil organic material (Fig. 1) is divided into labile organic matter (LOM) and refractory organic matter (ROM). Each compartment is a highly aggregated pool of carbon and nitrogen representing accumulated non-living organic compounds in the ecosystem. These materials provide the energy substrate for growth of soil microorganisms, and this microbial activity results in the carbon and nitrogen fluxes of interest in ecosystem soils (Fig. 1). In fact, these pools contain live microorganisms, and thus the compartments are not strictly 'non-living'. However, field measurements are typically not capable of distinguishing living microbial biomass from detrital material, so the distinction is not maintained in the model. The LOM pool may be most readily identified with the forest floor in forested systems. Alternately, it may represent an accumulation of a number of years (cohorts) of litter. The soil A and O horizons may also comprise part of the LOM compartment. The LOM is intended to provide a soil organic matter compartment that can respond rather quickly to changing external conditions and inputs. The ROM pool, on the other hand, represents the bulk of carbon and nitrogen present in soil profiles down through the B and C horizons. It might also include the accumulation of humic materials higher in the soil profile. In general, the interpretation of each aggregated compartment will vary with application depending on the quality and quantity of data available from the site.

Labile organic matter is conceived of as relatively 'fresh' material, and thus the litter flux from the plant compartment enters this pool. Carbon leaves this pool by two pathways: decomposition and decay. Decomposition is defined as transformation of organic carbon to inorganic carbon (CO_2). Decay is defined as degradation of the quality of the organic matter (i.e., transformation from labile to refractory material). Carbon mass balance for the LOM compartment requires that the difference between inputs and outputs equals the rate of change of the compartment. For instance, specifying time sequences of LOM standing crop, litter production and decomposition (Fig. 1) determines the time series of decay for the compartment. Litter production is determined by the carbon balance for the plant biomass compartment so the additional carbon inputs required for LOM dynamics in a model application are time sequences of LOM standing crop and decomposition.

Refractory organic matter is conceived of as the bulk of slowly decomposing organic material in the soil. Carbon enters this pool by the decay pathway. Decomposition of this material is conceived of as occurring more slowly than in the LOM compartment, but the larger amount of material in the compartment may result in a mineralization flux as large or larger than that from the LOM compartment. Long-term storage losses from the ROM represent losses of organic matter to peat formation or losses through leaching of dissolved organic compounds in drainage waters. This flux might well be ignored for many upland forested systems and grasslands. Carbon mass balance for the ROM compartment requires that the difference between inputs and outputs equals the rate of change of the compartment. For this compartment, specifying time sequences of ROM standing crop and long-term storage losses would determine the time sequence of decomposition because the sequence of decay is determined by the carbon mass balance on the LOM compartment (Fig. 1).

Three characteristics of MERLIN can be identified that distinguish this conceptual approach from other models of nitrogen cycling in ecosystems: 1) the emphasis on the coupling and interaction of hydrological and abiotic processes affecting nitrogen with the biotic cycling of nitrogen within the ecosystem; 2) the focus on aggregated carbon dynamics as forcing functions for biotic transformations of nitrogen; and 3) ، the identification of organic compartments and fluxes in the model with readily observable or measurable characteristics of ecosystems.

Model application.

To apply MERLIN, a number of inputs must be specified for the model. Firstly, the sequences of carbon fluxes and pools described above must be provided (i.e., time series of: plant standing crop; litter and wood production; forest floor standing crop and decomposition;

and the amount of organic matter in the bulk soil and its decomposition). The intention is that some reasonable values for these carbon sequences can be derived for a given site simply by observing the landscape at the site. Knowledge that the current ecosystem contains a 60 year old temperate, mixed hardwood forest on an inceptisol in Virginia or a 30 year old plantation of Sitka spruce on a spodosol in Wales should provide a good deal of information about the required carbon pools and fluxes (and their recent history) even in the absence of measurements at the site in question. Secondly, the current nitrogen status of the ecosystem is needed. This will require measurements of the current nitrogen content of the important biotic and abiotic pools at the site. Thirdly, information is needed about the soil and hydrological properties at the site. Finally, the history of nitrogen inputs (primarily from the atmosphere, but also any history of nitrogen manipulation such as fertilization, etc.) must be specified.

The procedure is then to run the model (with the assumed historical carbon sequences and nitrogen inputs driving the simulation) for several decades of the recent past, arriving at the present day with the 'correct' nitrogen content of each organic compartment and the 'correct' leaching losses of the catchment or plot. 'Correct' in this case means that the simulated C:N ratios of the organic compartments match those measured for the system and the simulated leaching losses also match the observed. If a 'correct' match is not obtained, the parameters of the model are adjusted and the hindcast run again. If this iterative procedure converges to a 'correct' match, then the model is considered calibrated for the site. The emphasis on running a hindcast as part of the calibration procedure (rather than just using current observed nitrogen status as initial conditions for the model and running forward from the present) stems from the belief that the future behaviour of a system depends not only on its present status but is also strongly conditioned by the pathway followed to reach the present status. The calibration procedure described above utilizes historical assumptions to constrain the future behaviour of the model. While the historical assumptions are just that (assumed, not known), it is often the case that a 'reasonable' estimate of the recent past of an ecosystem can be made. Constraining a model to reproduce this 'reasonable' past as well as to match current observed conditions should result in the simulation of more 'reasonable' and reliable future behaviours of the system.

MATHEMATICAL FORMULATION OF THE MODEL

MERLIN is a dynamic model intended for simulation of temporal changes in nitrogen state variables in response to temporal changes of input forcing functions. Nitrogen state variables in the model include inorganic nitrogen

species (NO_3 and NH_4) and organic nitrogen pools (in the plant and soil compartments). Input forcing functions include: a) time series of atmospheric deposition of inorganic nitrogen (and simulated additions or removals of inorganic nitrogen); b) the temporal pattern of water discharge through the catchment; and c) time series of fluxes and/or pool sizes of organic carbon in the plant and soil compartments. Changes in the nitrogen state variables are regulated by linear and non-linear processes that are themselves functions of the instantaneous values of the nitrogen state variables and the input forcing functions. The inputs, outputs, state variables, equations and parameters are defined and summarized in Tables 1 and 2.

Inorganic nitrogen exists in soil solution and surface waters as NO_3 or NH_4 or both. In the discussion and equations that follow, the generalized notation Nx is used to represent either NO_3 or NH_4 whenever both species participate in a process. Generalized equations and parameters are used in the text. The specific equations and parameters for each nitrogen species are given in Tables 1 and 2.

Catchment input and output fluxes.

Nitrogen inputs to the model ecosystem are time series of inorganic nitrogen fluxes added to the soil solution. The primary inputs are atmospheric deposition of NO_3 and NH_4. Deposition is considered to be a combined function of wet (precipitation) and dry (gaseous and particulate) nitrogen inputs:

$$FNx_{dep} = Q_{ppt} \times (Nx)_{ppt} \times DDF_{Nx} \qquad (1)$$

where FNx_{dep} is the deposition flux of the inorganic nitrogen species (mmol m^{-2} yr^{-1}), Q_{ppt} is the precipitation flux (m yr^{-1}), $(Nx)_{ppt}$ is the concentration of the inorganic nitrogen species in precipitation (mmol m^{-3}), and DDF_{Nx} is the dry deposition factor for the inorganic nitrogen species, a unitless scale factor for expressing total deposition as a function of wet deposition. Separate deposition equations are used for NO_3 and NH_4 in the model (Table 1). Provision is also made in the model for simulation of additional sources of inorganic nitrogen (e.g. fertilization, biological fixation, etc.). Time series of all inorganic nitrogen inputs must be specified *a priori* as forcing functions for the model.

Nitrogen leaching losses from the model ecosystem occur as inorganic nitrogen in soil solution runoff. Losses of inorganic nitrogen by this mechanism are the primary outputs of the model. Leaching fluxes are functions of soil solution concentrations of inorganic nitrogen species and vary during the simulation as these concentrations vary in response to the biotic and abiotic processes: A central objective in developing MERLIN, therefore, was to design explicitly a catchment-scale mass-balance model with the primary function of simulating runoff concentrations of inorganic nitrogen species.

Table 1. Equations in the model.

─────────────────────────────── *Mass Balance* ───────────────────────────────

Organic compartments

$$\frac{d}{dt}C_{plt} = FC_{npp} - FC_{lit} - FC_{wd}$$

$$\frac{d}{dt}N_{plt} = FNH_{4_{upt,plt}} + FNO_{3_{upt,plt}} - FN_{wd}$$

$$\frac{d}{dt}C_{LOM} = FC_{lit} - FC_{dcmp,LOM} - FC_{dcy}$$

$$\frac{d}{dt}N_{LOM} = FN_{lit} + FNH_{4_{upt,LOM}} + FNO_{3_{upt,LOM}} - FN_{dcy}$$

$$\frac{d}{dt}C_{ROM} = FC_{dcy} - FC_{dcmp,ROM} - FC_{exp}$$

$$\frac{d}{dt}N_{ROM} = FN_{dcy} + FNH_{4_{upt,ROM}} + FNO_{3_{upt,ROM}} - FN_{min,ROM} - FN_{exp}$$

Inorganic nitrogen

$$\frac{d}{dt}(NH_4)_{soil} = -\frac{SMS}{SPV} \times \frac{d}{dt}E_{NH_4}$$
$$+ \frac{1}{SPV} \times (FNH_{4_{dep}} + FN_{min,LOM} - FN_{nit} - FNH_{4_{lch}} - FNH_{4_{upt,plt}} - FNH_{4_{upt,LOM}} - FNH_{4_{upt,ROM}})$$

$$\frac{d}{dt}(NO_3)_{soil} = -\frac{SMS}{SPV} \times \frac{d}{dt}E_{NO_3}$$
$$+ \frac{1}{SPV} \times (FNO_{3_{dep}} + FN_{nit} - FNO_{3_{lch}} - FNO_{3_{upt,plt}} - FNO_{3_{upt,LOM}} - FNO_{3_{upt,ROM}} - FN_{den})$$

─────────────────────────── *Catchment inputs and outputs* ───────────────────────────

Deposition of ammonium

$$FNH_{4_{dep}} = Q_{ppt} \times (NH_4)_{ppt} \times DDF_{NH_4}$$

Deposition of nitrate

$$FNO_{3_{dep}} = Q_{ppt} \times (NO_3)_{ppt} \times DDF_{NO_3}$$

Leaching of ammonium

$$FNH_{4_{lch}} = Q_{lch} \times (NH_4)_{soil}$$

Leaching of nitrate

$$FNO_{3_{lch}} = Q_{lch} \times (NO_3)_{soil}$$

─────────────────────────── *Soil Transformations and Definitions* ───────────────────────────

Adsorption of ammonium by soil matrix

$$E_{NH_4} = K_{mx,NH_4,ads} \times \frac{(NH_4)_{soil}}{((K_{hlf,NH_4,ads} + (NH_4)_{soil})}$$

Adsorption of nitrate by soil matrix

$$E_{NO_3} = K_{mx,NO_3,ads} \times \frac{(NO_3)_{soil}}{((K_{hlf,NO_3,ads} + (NO_3)_{soil})}$$

Nitrification

$$FN_{nit} = NIT \times (NH_4)_{soil} \times SPV$$

Soil properties

$$SPV = SDP \times SPO \qquad SMS = SDP \times SBD$$

Table 1. *Continued*

--- *Uptake and Immobilization* ---

Ammonium uptake by plants

$$FNH_{4_{upt,plt}} = K_{mx,NH_4,plt} \times \frac{(NH_4)_{soil}}{\left(K_{hlf,NH_4,plt} + (NH_4)_{soil}\right)}$$

$$K_{mx,NH_4,plt} = FC_{npp} \times M_{NH_4,plt}$$

$$K_{hlf,NH_4,plt} = K_0 \times exp\left(\frac{C:N_{0,plt} - C:N_{plt}}{S_{NH_4,plt}}\right)$$

Nitrate uptake by plants

$$FNO_{3_{upt,plt}} = K_{mx,NO_3,plt} \times \frac{(NO_3)_{soil}}{\left(K_{hlf,NO_3,plt} + (NO_3)_{soil}\right)}$$

$$K_{mx,NO_3,plt} = FC_{npp} \times M_{NO_3,plt}$$

$$K_{hlf,NO_3,plt} = K_0 \times exp\left(\frac{C:N_{0,plt} - C:N_{plt}}{S_{NO_3,plt}}\right)$$

Ammonium immobilization by LOM

$$FNH_{4_{upt,LOM}} = K_{mx,NH_4,LOM} \times \frac{(NH_4)_{soil}}{\left(K_{hlf,NH_4,LOM} + (NH_4)_{soil}\right)}$$

$$K_{mx,NH_4,LOM} = FC_{dcmp,LOM} \times M_{NH_4,LOM}$$

$$K_{hlf,NH_4,LOM} = K_0 \times exp\left(\frac{C:N_{0,LOM} - C:N_{LOM}}{S_{NH_4,LOM}}\right)$$

Nitrate immobilization by LOM

$$FNO_{3_{upt,LOM}} = K_{mx,NO_3,LOM} \times \frac{(NO_3)_{soil}}{\left(K_{hlf,NO_3,LOM} + (NO_3)_{soil}\right)}$$

$$K_{mx,NO_3,LOM} = FC_{dcmp,LOM} \times M_{NO_3,LOM}$$

$$K_{hlf,NO_3,LOM} = K_0 \times exp\left(\frac{C:N_{0,LOM} - C:N_{LOM}}{S_{NO_3,LOM}}\right)$$

Ammonium immobilization by ROM

$$FNH_{4_{upt,ROM}} = K_{mx,NH_4,ROM} \times \frac{(NH_4)_{soil}}{\left(K_{hlf,NH_4,ROM} + (NH_4)_{soil}\right)}$$

$$K_{mx,NH_4,ROM} = FC_{dcmp,ROM} \times M_{NH_4,ROM}$$

$$K_{hlf,NH_4,ROM} = K_0 \times exp\left(\frac{C:N_{0,ROM} - C:N_{ROM}}{S_{NH_4,ROM}}\right)$$

Nitrate immobilization by ROM

$$FNO_{3_{upt,ROM}} = K_{mx,NO_3,ROM} \times \frac{(NO_3)_{soil}}{\left(K_{hlf,NO_3,ROM} + (NO_3)_{soil}\right)}$$

$$K_{mx,NO_3,ROM} = FC_{dcmp,LOM} \times M_{NO_3,ROM}$$

$$K_{hlf,NO_3,ROM} = K_0 \times exp\left(\frac{C:N_{0,ROM} - C:N_{ROM}}{S_{NO_3,ROM}}\right)$$

--- *Mineralization and Biomass Transfers* ---

Mineralization of LOM

$$FN_{min,LOM} = \frac{FC_{dcmp,LOM}}{C:N_{LOM}}$$

Mineralization of ROM

$$FN_{min,ROM} = \frac{FC_{dcmp,ROM}}{C:N_{ROM}}$$

Nitroget transfer to wood

$$FN_{wd} = \frac{FC_{wd}}{C:N_{wd}}$$

Nitrogen transfer in litter

$$FN_{lit} = \frac{FC_{lit}}{C:N_{plt}}$$

Nitrogen transfer from LOM to ROM

$$FN_{dcy} = \frac{FC_{dcy}}{C:N_{LOM}}$$

Organic nitrogen export

$$FN_{exp} = \frac{FC_{exp}}{C:N_{ROM}}$$

Table 2. Variables and parameters in the model. Items in bold are inputs required by themodel

Description	Variable and Parameter Names	Units
Carbon and Nitrogen Pools		
Organic carbon in biomass compartments	C_{plt} C_{LOM} C_{ROM}	mmol C m^{-2}
Organic nitrogen in biomass compartments	N_{plt} N_{LOM} N_{ROM}	mmol N m^{-2}
Carbon-to-nitrogen ratio of biomass compartments	C:N$_{plt}$ C:N$_{LOM}$ C:N$_{ROM}$	mol C per mol N
Exchangeable NH$_4$ and NO$_3$ on soil matrix	E_{NH_4} E_{NO_3}	mmol N kg^{-1}
Concentrations of NH$_4$ and NO$_3$ in soil solution	$(NH_4)_{soil}$ $(NO_3)_{soil}$	mmol N m^{-3}
International Carbon and Nitrogen Fluxes		
Wood Production	FC_{wd}	mmol C m^{-2} yr^{-1}
Litter Production	FC_{lit}	mmol C m^{-2} yr^{-1}
Decomposition of LOM and ROM	$FC_{demp,LOM}$ $FC_{demp,ROM}$	mmol C m^{-2} yr^{-1}
Organic carbon export	FC_{exp}	mmol C m^{-2} yr^{-1}
Denitrification	FN_{den}	mmol N m^{-2} yr^{-1}
Net primary production of plants	FC_{npp}	mmol C m^{-2} yr^{-1}
Decay (transfer from LOM to ROM)	FC_{dcy}	mmol C m^{-2} yr^{-1}
Biomass transfers of organic nitrogen	FN_{wd} FN_{lit} FN_{dcy} FN_{exp}	mmol N m^{-2} yr^{-1}
Nitrification	FN_{nit}	mmol N m^{-2} yr^{-1}
Mineralization of LOM and ROM	$FN_{min,LOM}$ $FN_{min,ROM}$	mmol N m^{-2} yr^{-1}
Uptake of NH$_4$ and NO$_3$ by plants, LOM and ROM	$FNH4_{upt,plt}$ p$FNH4_{upt,LOM}$ $FNH4_{upt,ROM}$ $FNO3_{upt,plt}$ $FNO3_{upt,LOM}$ $FNO3_{upt,ROM}$	mmol N^{-2} yr^{-1}
Deposition and Discharge Parameters and Fluxes		
Precipitation amount, soil discharge	O_{ppt} Q_{lch}	m yr^{-1}
Concentration of NH$_4$ and NO$_3$ in precipitation	$(NH_4)_{ppt}$ $(NO_3)_{ppt}$	mmol N m^{-3}
Dry deposition factors for NH$_4$ and NO$_3$	DDF$_{NH_4}$ DDF$_{NO_3}$	unitless
Deposition of NH$_4$ and NO$_3$	$FNH4_{dep}$ $FNO3_{dep}$	mmol N m^{-2} yr^{-1}
Leaching of NH$_4$ and NO$_3$	$FNH4_{lch}$ $FNO3_{lch}$	mmol N m^{-2} yr^{-1}
Uptake Parameters		
Target C:N ratio of biomass compartment	C:N$_{0,plt}$ C:N$_{0,LOM}$ C:N$_{0,ROM}$	mol C per mol N
Maximum NH$_4$ or NO$_3$ uptake per unit of carbon production	$M_{NH_4,plt}$ $M_{NH_4,LOM}$ $M_{NH_4,ROM}$ $M_{NO_3,plt}$ $M_{NO_3,LOM}$ $M_{NO_3,ROM}$	mol N per mol C mol N per mol C
Steepness of decline in uptake half-saturation parameter as C:N's of biomass increase	$S_{NH_4,plt}$ $S_{NH_4,LOM}$ $S_{NH_4,ROM}$ $S_{NO_3,plt}$ $S_{NO_3,LOM}$ $S_{NO_3,ROM}$	unitless
Upper limit of uptake half saturation parameter as C:N's of biomass decrease	K_0	mmol m^{-3}

Table 2. *Continued*

Description	Variable and Parameter Names	Units
Maximum rate uptake of NH$_4$ and NO$_3$	$K_{mx,NH_4,plt}$ $K_{mx,NH_4,LOM}$ $K_{mx,NH_4,ROM}$ $K_{mx,NO_3,plt}$ $K_{mx,NO_3,LOM}$ $K_{mx,NO_3,ROM}$	mmol N m^{-3}yr^{-1}
Half-saturation parameter, uptake of NH$_4$ and NO$_3$	$K_{hlf,NH_4,plt}$ $K_{hlf,NH_4,LOM}$ $K_{hlf,NH_4,ROM}$ $K_{hlf,NO_3,plt}$ $K_{hlf,NO_3,LOM}$ $K_{hlf,NO_3,ROM}$	mmol N^{-3}
Soil Parameters		
Depth	SDP	m
Porosity	SDP	unitless
Bulk Density	SBD	kg m^{-3}
Maximum adsorption capacity of NH$_4$ and NO$_3$	$K_{mx,NH_4,ads}$ $K_{mx,NO_3,ads}$	mmol N kg^{-1}
Half saturation constant, NH$_4$ and NO$_3$ adsorption	$K_{hlf,NH_4,ads}$ $K_{hlf,NO_3,ads}$	mmol N m^{-3}
Nitrification rate constant	NIT	yr^{-1}
Pore volume per unit area	SPV	m
Mass per unit area	SMS	kg m^{-2}
Biomass Transfer Parameters		
C:N ratio of wood produced from plants	C:N$_{wd}$	mol C per mol N
C:N ratio of organic matter export from ROM	C:N$_{exp}$	mol C per mol N
C:N ratio or organic matter decomposed by LOM and ROM (optional)	C:N$_{demp,LOM}$ C:N$_{demp,ROM}$	mol C per mol N
C:N ratio of organic matter transferred from	C:N$_{dcy}$	mol C per mol N

$$FNx_{lch} = Q_{lch} \times (Nx)_{soil} \qquad (2)$$

where FNx$_{lch}$ is the leaching flux of the inorganic nitrogen species (mmol m^{-2} yr^{-1}), Q$_{lch}$ is the discharge through the soils (m yr^{-1}), and (Nx)$_{soil}$ is the concentration of the nitrogen species in soil solution (mmol m^{-3}). Provision is made in the model for additional losses of inorganic nitrogen by processes such as denitrification (but not including biotic uptake, for these processes see below). The magnitude and timing of these additional losses may be specified *a priori*, or they may be linked to concentrations of NO$_3$ or NH$_4$ in soil solution using first-order reaction kinetics.

Soil adsorption of inorganic nitrogen.

Both NO$_3$ and NH$_4$ can have adsorbed phases in the model. Adsorption of either inorganic nitrogen species is modelled as a non-linear capacity-limited process using a hyperbolic equation:

$$E_{Nx} = K_{mx,Nx,ads} \times \frac{(Nx)_{soil}}{\left(K_{hlf,Nx,ads} + (Nx)_{soil}\right)} \qquad (3)$$

where E$_{Nx}$ is the amount of exchangeable nitrogen species on the soil matrix (mmol kg^{-1}), (Nx)$_{soil}$ is the concentration of the inorganic nitrogen species in soil solution (mmol m^{-3}), K$_{mx,Nx,ads}$ is the maximum adsorption capacity of the soil for the nitrogen species (mmol kg^{-1}), and K$_{hlf,Nx,ads}$ is the concentration of the nitrogen species in soil solution at which the amount of exchangeable nitrogen equals one-half of the maximum capacity (mmol m^{-3}). Separate equations are used for NO$_3$ and NH$_4$ in the model (Table 1). Adsorption of either NH$_4$ or NO$_3$ can be turned off in the model by setting the maximum capacity for that species to zero.

Nitrification.

Nitrification, microbially mediated transformation of NH_4 to NO_3, is represented in the model by a first-order reaction. The rate of loss of NH_4 (equal to the rate of production of NO_3) is given by the product of a rate constant and the concentration of NH_4 at each time step:

$$FN_{nit} = NIT \times (NH_4)_{soil} \times SPV \qquad (4)$$

where FN_{nit} is the nitrification loss of NH_4 (or gain of NO_3; mmol m^{-2} yr^{-1}), $(NH_4)_{soil}$ is the concentration of NH_4 in soil solution (mmol m^{-3}), NIT is the nitrification rate constant (yr^{-1}), and SPV is the pore volume per unit area of the soils (m).

Uptake of inorganic nitrogen by the plant compartment

Uptake by the plant compartment is modelled as non-linear processes that depend on soil solution concentrations of the inorganic nitrogen species being utilized. The equation is hyperbolic (a typical Michaelis-Menten uptake process):

$$FNx_{upt,plt} = K_{mx,Nx,plt} \times \frac{(Nx)_{soil}}{\left(K_{hlf,Nx,plt} + (Nx)_{soil}\right)} \qquad (5)$$

where $FNx_{upt,plt}$ is the uptake flux of the inorganic nitrogen species by the plant compartment (mmol m^{-2} yr^{-1}), $(Nx)_{soil}$ is the concentration of the inorganic nitrogen species in soil solution (mmol m^{-3}), $K_{mx,Nx,plt}$ is the maximum uptake rate (mmol m^{-2} yr^{-1}), and $K_{hlf,Nx,plt}$ is the half-saturation constant (the concentration of inorganic nitrogen species at which plant uptake proceeds at half of the maximum rate; mmol m^{-3}). Separate equations are included for NH_4 and NO_3 uptake by the plant compartment (Table 1).

The conceptual basis of the model requires that plant uptake be regulated not only by the availability of inorganic nitrogen in soil solution, but also by the productivity of the plant compartment and by the internal nitrogen status of the plant compartment. These additional controls (or feedback) on the uptake process are implemented in the model by making the maximum uptake rate and the half-saturation constant in the above uptake equation into time-varying parameters that are functions of the carbon and nitrogen characteristics of the plant compartment.

The maximum uptake rate of the plants is assumed to be proportional to the carbon productivity of the plants. At zero productivity, there should be no uptake of inorganic nitrogen regardless of the inorganic nitrogen concentrations in soil solution or the internal nitrogen status of the plants. As carbon productivity increases, the maximum uptake rate of inorganic nitrogen should also increase. This relationship is incorporated in the model using a linear equation:

$$K_{mx,Nx,plt} = FC_{npp} \times M_{Nx,plt} \qquad (6)$$

where FC_{npp} is the net carbon primary productivity of the plants (mmol m^{-2} yr^{-1}), and $M_{Nx,plt}$ is a unitless factor determining the maximum number of moles of nitrogen incorporated into plant biomass per mole of carbon incorporated into biomass when plant uptake of nitrogen is not limited by the concentration of inorganic nitrogen in soil solution and the internal nitrogen content of the plant compartment is near zero. Obviously, this factor has no real meaning and cannot be measured directly. It therefore becomes a calibration parameter that must be adjusted empirically when the model is fitted to the data from a given site. The procedure for adjusting the parameter and the effect the parameter has on model functioning is discussed below.

The half-saturation constant of the uptake equation controls the steepness of the uptake curve for a given value of the maximum uptake rate. For small values of $K_{hlf,Nx,plt}$, uptake will proceed at rates near to $K_{mx,Nx,plt}$ even if $(Nx)_{soil}$ is small. As $K_{hlf,Nx,plt}$ increases, the actual uptake rate will decline for the same values of $K_{mx,Nx,plt}$ and $(Nx)_{soil}$. Thus, $K_{hlf,Nx,plt}$ can be thought of as controlling the efficiency of uptake — low $K_{hlf,Nx,plt}$ produces high uptake efficiency while high $K_{hlf,Nx,plt}$ produces low uptake efficiency. The conceptual model assumes that the internal nitrogen status of the plant compartment should control the efficiency of nitrogen uptake—high values of the C:N ratio produce high uptake efficiency, low values of C:N result in decreased uptake efficiency. The mathematical model, therefore, incorporates an inverse relationship between the half-saturation constant of the uptake equation and the C:N ratio of the plant compartment. The relationship is assumed to be exponential (to avoid negative values):

$$K_{hlf,Nx,plt} = K_0 \times \exp\left(\frac{C:N_{0,plt} - C:N_{plt}}{S_{Nx,plt}}\right) \qquad (7)$$

where C:N_{plt} is the simulated C:N ratio of the plant compartment at any time in the simulation, C:$N_{0,plt}$ is the target C:N ratio of the plant compartment, K_0 (mmol m^{-3}) is the value of the half saturation constant when the simulated C:N ratio equals the target C:N ratio, and $S_{Nx,plt}$ is a unitless factor controlling the steepness of the change in $K_{hlf,Nx,plt}$ as C:N_{plt} changes. The target C:N ratio for the plant compartment is specified as an input to the model. The value of K_0 is set to an arbitrarily large number (e.g. 1000 mmol m^{-3}) to produce a low uptake efficiency when C:N_{plt} is equal to C:$N_{0,plt}$. The steepness parameter $S_{Nx,plt}$ is adjusted to control the closeness with which the simulated C:N ratio tracks the target value (assuming inorganic nitrogen is available in solution). Large values of $S_{Nx,plt}$ cause the simulation to track closely. Small values will allow the plant C:N to

depart significantly from the target before significant changes in uptake occur. Separate uptake equations are used for NH₄ and NO₃ in the model (Table 1). If the parameters in the equations for NH₄ and NO₃ are set to different numerical values, preferential uptake of one species of inorganic nitrogen can be simulated.

Immobilization of inorganic nitrogen by soil microorganisms.

Soil microbial processes affect inorganic nitrogen through immobilization of NH_4 and NO_3 and through mineralization of organic matter to produce NH_4 (ammonification). The immobilization equations presented here are for the LOM compartment (Fig. 1). Similar equations are used in the model for the ROM compartment (Table 1). Immobilization is modelled as a non-linear process that depends on the soil solution concentrations of inorganic nitrogen in a manner similar to that used for plant uptake (equation 5):

$$FNx_{upt,LOM} = K_{mx,Nx,LOM} \times \frac{(Nx)_{soil}}{\left(K_{hlf,Nx,LOM} + (NX)_{soil}\right)} \quad (8)$$

where $FNx_{upt,LOM}$ is the uptake of the inorganic nitrogen species by the LOM compartment (mmol m⁻² yr⁻¹), $(Nx)_{soil}$ is the concentration of the inorganic nitrogen species in soil solution (mmol m⁻³), $K_{mx,Nx,LOM}$ is the maximum uptake rate (mmol m⁻² yr⁻¹), and $K_{hlf,Nx,LOM}$ is the concentration of the inorganic nitrogen species at which immobilization proceeds at half of the maximum rate (mmol m⁻³). Separate equations are included for NH_4 and NO_3 uptake by the LOM compartment (Table 1).

Immobilization is assumed to be the result of microbial utilization of inorganic nitrogen from soil solution for growth. This growth depends on energy derived from decomposition of organic matter. Immobilization is assumed, therefore, to be proportional to the secondary productivity of the microbes (as measured by decomposition and assuming a constant microbial substrate use efficiency) in much the same way as plant uptake is proportional to the net primary productivity of the plants. This suggests that $K_{m,Nx,LOM}$ and $K_{s,Nx,LOM}$ in Equation (8) may be parameterized for immobilization in a manner similar to their parameterization for plant uptake.

Specifically, the maximum uptake rate of the LOM compartment is assumed to be proportional to the carbon decomposition of that compartment:

$$K_{mx,Nx,LOM} = FCdcmp,LOM \times MNx,LOM \quad (9)$$

where $FC_{dcmp,LOM}$ is the carbon decomposition of the LOM compartment (mmol m⁻² yr⁻¹), and $M_{Nx,LOM}$ is a unitless factor determining the maximum number of moles of nitrogen incorporated into microbial biomass per mole of carbon decomposed. As with the parameteri-

zation of the plant compartment, $M_{Nx,LOM}$ cannot be measured directly. It becomes, therefore, a calibration parameter that must be adjusted empirically when the model is fitted to the data from a given site. The procedure for adjusting the parameter and the effect the parameter has on model functioning is discussed below.

The half-saturation constant for immobilization of inorganic nitrogen into the LOM compartment is given by:

$$K_{hlf,Nx,LOM} = K_0 \times \exp\left(\frac{C:N_{0,LOM} - C:N_{LOM}}{S_{Nx,LOM}}\right) \quad (10)$$

where $C:N_{LOM}$ is the carbon to nitrogen ratio of the LOM compartment at any time in the simulation, $C:N_{0,LOM}$ is the target C:N ratio of the LOM compartment, K_0 (mmol m⁻³) is the value of the half saturation constant when the simulated C:N ratio of the LOM compartment equals the target C:N ratio, and $S_{Nx,LOM}$ is a unitless factor controlling the steepness of the change in $K_{hlf,Nx,LOM}$ as $C:N_{LOM}$ changes. These parameters are specified in the model as described for the plant compartment (equation 7). Separate uptake equations are used for NH₄ and NO₃ in the model (Table 1). If the parameters in the equations for NH₄ and NO₃ are set to different numerical values, preferential immobilization of one species of inorganic nitrogen can be simulated.

Mineralization by soil microorganisms.

Mineralization represents the release of inorganic nitrogen from organic matter (Fig. 1). The mineralization product is NH₄ and is produced by both the LOM and ROM compartments. Mineralization is proportional to the carbon decomposition flux and the C:N ratio of the LOM or ROM compartment at the time the decomposition occurs:

$$FN_{min,LOM} = \frac{FC_{dcmp,LOM}}{C:N_{LOM}} \quad (11)$$

where $FN_{min,LOM}$ is the flux of inorganic nitrogen (as ammonium ion) produced by mineralization from the LOM compartment (mmol m⁻² yr⁻¹), $FC_{dcmp,LOM}$ is the carbon decomposition rate of the LOM compartment (mmol m⁻² yr⁻¹), and $C:N_{LOM}$ is the currently simulated C:N ratio of the compartment. The model provides an option for the user to specify a different value $(C:N_{dcmp,LOM})$ of the carbon-to-nitrogen ratio for use in equation 11 in place of the currently simulated value $(C:N_{LOM})$. This option would be invoked if the material being decomposed were assumed to have a significantly different C:N ratio than that of the bulk compartment (for instance, preferential decomposition of substrate with a lower C:N ratio). A similar equation is used in the model for mineralization from the ROM compartment (Table 1).

Biomass transfers of organic nitrogen.

Several translocations of organic nitrogen occur in the model as a result of biomass transfers between compartments. These transfers are storage of organic nitrogen in wood, loss of organic nitrogen through export from ROM, litter (transfer from plants to LOM) and decay (transfer from LOM to ROM). The model is configured to use either of two C:N ratios to calculate the flux of organic nitrogen given the input carbon flux along the pathway (Fig. 1). The two possible C:N ratios are the C:N of the donor compartment or a user specified C:N. Most often the C:N used for wood production and export (losses to long-term storage, Fig. 1) are user specified because the C:N of wood and peat (for instance) are usually very different from the C:N of the donor compartment. While this may also be the case for litter production in some ecosystems, long-term mass balance considerations usually require that the C:N used for litter and decay in the model be those of the donor compartments (to prevent build-up or depletion of nitrogen in the donor compartments). The form of the equations used for these transfers can be illustrated using the wood and litter production functions (all equations are listed in Table 1):

$$FN_{wd} = \frac{FC_{wd}}{C:N_{wd}} \qquad (12)$$

$$FN_{lit} = \frac{FC_{lit}}{C:N_{plt}} \qquad (13)$$

where FN_{wd} and FN_{lit} are the organic nitrogen fluxes in wood and litter production (mmol m^{-2} yr^{-1}), FC_{wd} and FC_{lit} are the carbon fluxes in wood and litter production (mmol m^{-2} yr^{-1}), $C:N_{wd}$ in equation 12 is a user specified C:N ratio that draws nitrogen from the plant compartment for wood production at different (usually much higher) value than that of the bulk plant compartment, and $C:N_{plt}$ in equation 13 is the currently simulated C:N ratio of the plant compartment.

Nitrogen mass balance.

Mass balance is maintained in the model by writing the differential equations for the rate of change of the carbon and nitrogen state variables using the process equations derived above. Mass balances for the organic compartments require that the rates of change of carbon or nitrogen in the compartments be equal to the sources minus the losses for the compartments at any time in the simulation. Using the plant compartment as an example:

$$\frac{d}{dt} C_{plt} = FC_{npp} - FC_{lit} - FC_{wd} \qquad (14)$$

$$\frac{d}{dt} N_{plt} = FNH_{4upt,plt} + FNO_{3upt,plt} - FN_{lit} - FN_{wd} \qquad (15)$$

where C_{plt} and N_{plt} are organic carbon and nitrogen amounts in the plant compartment (mmol m^{-2}), FC_{wd}, FC_{lit}, FN_{wd} and FN_{lit} are fluxes of carbon and nitrogen in wood and litter production (as defined in equations 12 and 13), and FC_{npp}, $FNH_{4upt,plt}$ and $FNO_{3upt,plt}$ are the primary production and inorganic nitrogen uptake fluxes of the plant compartment (as defined in equations 5, 6 and 7). Equations for all organic compartments are given in Table 1.

Mass balances for the inorganic nitrogen species require that the rate of change of ammonium or nitrate in the soils of the ecosystem be equal to the sources minus the losses at any time in the simulation. The situation is complicated somewhat by the fact that both species have a potential adsorbed phase. For example, the total ammonium ion present in the soils is written as:

$$NH_{4tot} = SPV \times (NH_4)_{soil} + SMS \times E_{NH_4} \qquad (16)$$

where NH_{4tot} is the total ammonium in the soils (mmol m^{-2}), $(NH_4)_{soil}$ is the concentration of ammonium in soil solution (mmol m^{-3}), SPV is the pore volume per unit area of the soils (m), E_{NH_4} is the amount of exchangeable ammonium on the soil matrix (mmol kg^{-1}; see equation 3), and SMS is the mass of soil per unit area (kg m^{-2}). The rate of change of total ammonium in the soil solution is equal to the sum of all input fluxes of ammonium (deposition and mineralization) minus the output fluxes of ammonium (nitrification, uptake and leaching). Differentiating equation 16 with respect to time, rearranging, and identifying the appropriate ammonium source and loss fluxes yields the NH$_4$ mass balance equation:

$$\frac{d}{dt}(NH_4)_{soil} = -\frac{SML}{SPV} \times \frac{d}{dt} E_{NH_4} + \sum Sources - \sum Losses \qquad (17)$$

where

$$\sum Sources = FNH_{4dep} + FN_{min,LOM} + FN_{min,ROM}$$

$$\sum Losses = FN_{nit} + FNH_{4lch} + FNH_{4upt,LOM} + FNH_{4upt,ROM}$$

and FN has been defined in equations 1, 2, 4, 5, 8 and 11. A similar approach yields the mass balance equation for NO$_3$ (Table 1).

MODEL IMPLEMENTATION AND CALIBRATION

The model is designed for annual or seasonal resolution and a simulation period of 50 to 150 years. The state variables in the model are, of course, time variable. Some of the parameters (such as the maximum uptake rates for inorganic nitrogen) are also time variable due to the nature of their definition as functions of state variables.

Other parameters, such as the target C:N ratios of the compartments, will usually be true constants. Provision has been made, however, for these 'constant' parameters to be changed during the course of a simulation if the assumptions of the simulation require a change (for instance, land use changes involving introduction of a new species of plant may require a new target C:N value for the plant compartment). In general, the inputs required for the model are: 1) temporal sequences of carbon fluxes and pools; hydrological discharge through the soils, and external sources of inorganic nitrogen; 2) initial conditions (amounts of carbon and nitrogen) for each compartment including the soil solution; and 3) a number of constants to specify the nitrogen dynamics of the organic compartments and the characteristics of the soils. Outputs from the model include: 1) concentrations and fluxes of NO_3 and NH_4 in soil water and runoff; 2) total nitrogen contents of the organic and inorganic compartments; 3) C:N ratios of the aggregated plant and soil compartments; and 4) magnitudes of important processes in the nitrogen cycle of the simulated system (i.e., uptake, gross and net mineralization, and immobilization). The inputs, state variables and constants are summarized in Tables 1 and 2.

The model is implemented by solving the mass balance equations in Table 1. The equations are in many cases non-linear, however, so a numerical (rather than explicit) solution scheme has been adopted that depends on frequent re-linearization. That is, many parameters affecting state variables depend on the current values of those same state variables. Therefore, even if the model is providing annual or seasonal resolution, the time steps used in the simulation are much smaller than yearly or monthly. At the end of each step, the parameters depending on state variables are 'updated' with the current value of the state variables. The updated parameters are then used to simulate new values of the state variables for the next update in an iterative procedure.

A number of the parameters in the model cannot be measured directly (either as a result of the level of aggregation or because of difficulty in making the measurements). These parameters have been designated as calibration parameters for the model. Their values are selected to provide a good fit to current observations on the system of interest (as described in the conceptual description of the model). In particular, the parameters used in the uptake equations ($M_{Nx,plt}$, equation 6 and $S_{Nx,plt}$, equation 7) are used to control the relative effectiveness of any organic compartment in obtaining inorganic nitrogen from the soil solution. To illustrate, consider the mass balance equation for ammonium (equation 17) and, to simplify, consider that the only source is constant deposition (no mineralization), that the only losses are leaching and plant uptake (no immobilization by LOM or ROM), and that there is no adsorption by the soils. Under these assumptions equation 17 combined with equations 2 and 5 becomes:

$$\frac{d}{dt}(NH_4)_{soil} = FNH_{4_{dep}} - (NH_4)_{soil} \times$$
$$\left(\frac{Q_{lch}}{SPV} + \frac{K_{mx,NH_4,plt}}{\left(SPV \times (K_{hlf,NH_4,plt} + (NH_4)_{soil})\right)} \right) \quad (18)$$

The two terms in the brackets on the right hand side of equation 18 each have units of yr^{-1} and can be considered the rate constants of hydrological leaching and plant uptake respectively. It can be shown that, in the numerical solution to the equation, the term having the larger rate constant (smaller turnover time) will become the dominant flux for ammonium ion. The larger the difference, the larger the NH_4 flux in the preferred pathway. This suggests a direct dynamic 'competition' between biotic and abiotic processes and is a unique feature of the MERLIN model.

Equation 18 can also be used to illustrate the calibration procedure for the model. Given values of SPV and Q_{lch}, adjusting the value of K_{mx,NH_4},plt can make the plants better or worse 'competitors' for NH_4. If the maximum rate is too large, the plants become too rich in nitrogen and the soil leachate concentration will be too low. If the maximum rate is too low, the plants will become impoverished with respect to nitrogen and the soil leachate concentration will be too large. For a given carbon flux, the maximum rate is a function of the calibration parameter $M_{Nx,plt}$ (see equation 6) and adjustments of $M_{Nx,plt}$ during calibration have the effects described above. Note that $(NH_4)_{soil}$, a state variable, also appears in the term for the plant uptake rate constant. This is one of the non-linearities inherent in the model and is accounted for by re-linearizing the equations frequently during solution. The presence of the state variable in the term can affect the calibration sensitivity, however, and cause it to vary during the simulation. Additional terms, (and rate constants) will appear in equation 18 as nitrification, immobilization by LOM and by ROM and soil adsorption are added. Each new process will 'compete' for NH_4 and will have a calibration parameter that can be adjusted to achieve simultaneous fits to all nitrogen pools and the soil leachate concentration. Similar calibration adjustments can be made using the parameters affecting uptake, immobilization and adsorption of nitrate.

Simulation examples

The functioning of the model can best be demonstrated in a series of speculative simulation exercises. These exercises are hypothetical in that the values of parameters and variables used in the model are not observed on a real system. The values are chosen to be approximately those of forested systems in northern Europe, but the dynamics of the system are simplified in order to isolate

and demonstrate the effects of individual variables in the model. Two types of simulation are presented: 1) simulations using constant carbon dynamics (i.e., steady state ecosystems); and 2) simulations using time varying carbon dynamics (i.e., land use changes). Each of these types of simulations was driven by three inorganic nitrogen input sequences. The resultant six simulations demonstrate the sensitivity of the model to carbon and nitrogen inputs. An application of the model to a forested site in Wales where the nitrogen inputs were manipulated is described in Emmett et al. (in press) which also provides a calibration/validation exercise using observed data.

The same soil parameters were used for all simulations described below (depth 1.0 m; porosity 0.5; bulk density 1000 kg m^{-3}; adsorption of NH$_4$—maximum capacity 50 mmol kg^{-1}, half-saturation constant 50 mmol m^{-3}; no adsorption of NO$_3$; nitrification rate constant 1000 yr^{-1}; discharge 1.0 m yr^{-1}). All simulations used the C:N ratio of the donor compartment for calculating biomass transfers and decomposition. None of the simulations included wood production; organic matter export from ROM or denitrification. All simulations used the same values of the uptake and immobilization parameters (see Table 2; target C:N ratios—plant = 56, LOM = 24, ROM = 15; maximum NH$_4$ or NO$_3$ uptake per unit carbon- plant = .02, LOM = .04, ROM = .04; steepness factor—plant, LOM and ROM = 0.5; upper limit of half-saturation parameter—plant, LOM and ROM = 1000). Initial nitrogen contents of the compartments were calculated to give the same initial C:N ratio in a given

compartment for each simulation (plant = 60; LOM = 28; ROM = 18). Carbon pools and fluxes and inorganic nitrogen inputs were varied among the simulations and are described below.

SIMULATIONS USING CONSTANT CARBON DYNAMICS (DEPOSITION EFFECTS)

Three simulations were performed in which the pools and fluxes of carbon were held constant throughout the simulations and inputs of inorganic nitrogen were varied to examine the responses to different deposition regimes. The constant carbon pools and fluxes for these simulations were: plant compartment biomass 100 mol m^{-2}; LOM compartment biomass 150 mol m^{-2}; ROM compartment biomass 1000 mol m^{-2}; litter production 15 mol m^{-2} yr^{-1}; LOM decomposition 7.5 mol m^{-2} yr^{-1}; and ROM decomposition 7.5 mol m^{-2} yr^{-1}; Simulations were run for 60 years. The first 10 years were steady state with respect to all inputs and variables. Starting at year 11 in the simulation, inorganic nitrogen was added in three patterns to the system (Fig. 2A): 1) a pulse input—a large increase lasting only one year; 2) a step input—a moderate increase in year 11 followed by constant input at the new level for the remaining 50 years; and 3) a ramp input—a linear increase starting in year 11 and continuing at the same rate of increase for the remaining 50 years of the simulation. The integral under each input sequence (the total inorganic nitrogen added) was the same in all three simulations (5000 mmol m^{-2}). The nitrogen was added as equal amounts of nitrate and
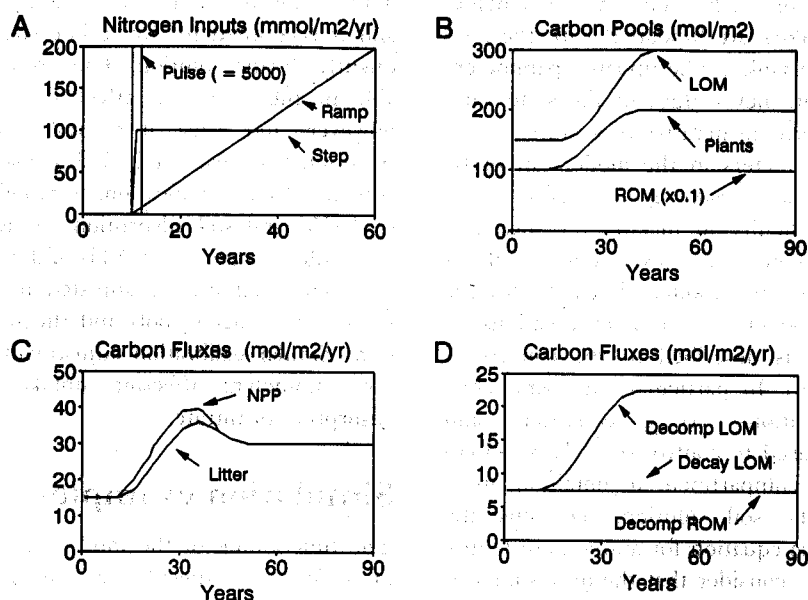

Fig. 2 *Carbon and nitrogen sequences used for the simulations described in the text: A) the nitrogen input sequences for the simulations with constant carbon dynamics; B) the sequences of carbon standing crop for the land use change simulations—the ROM value is scaled to fit on the plot; the actual value is 1000 mol m^{-2}; C) the net production and litter fluxes for the land use change simulations; and D) the decomposition and decay fluxes for the land use change simulations.*

ammonium ions (2500 mmol m^{-2} each). The outputs are presented as *changes* in state variables and fluxes from the initial steady state conditions as a result of the modified deposition (value in reference year minus value in year 1).

Results for input/output fluxes and nitrogen pools (deposition effects)

The pulse input produced an immediate response in nitrogen leaching with about 30% of the nitrogen input lost in the following year (Fig. 3A). This high nitrogen leaching was, however, short lived and the output flux rapidly declined such that within about 10 years the system output reverted to its steady state level. The important controlling mechanism on nitrogen leaching was initially the ability of the soil to adsorb NH$_4$ (Fig. 3B). As the adsorbed nitrogen was released, other processes increased in importance. Plant uptake and immobilization by soil microbial processes resulted in a re-partitioning of the added nitrogen over the next 30 years into the LOM and ROM compartments. The plant compartment did

not act as a long-term store of nitrogen, but behaved as a small pool with a rapid turnover. The ultimate storage location for the bulk of the nitrogen retained in the system was the ROM compartment. This behaviour is qualitatively consistent with observations of nitrogen leaching following forest fertilization (Harriman 1978) and of nitrogen partitioning following fertilizer application using ^{15}N as a tracer (Heilman *et al.* 1982, Nambiar and Bowen 1986, Hulm and Killham 1990, Preston and Mead 1994).

In response to a step change in nitrogen input, nitrogen leaching increased immediately and then levelled off in the long term (Fig. 3C). Both the adsorbed phase and the LOM compartment were important in sequestering nitrogen in this simulation and showed a qualitatively similar shape of response (Fig. 3D).. The ultimate sink for the added nitrogen, however, was again the ROM compartment and this pool increased rapidly and steadily. Step changes in nitrogen inputs have been initiated at several sites in Europe as part of the NITREX project (Wright and van Breemen 1995) in an attempt to
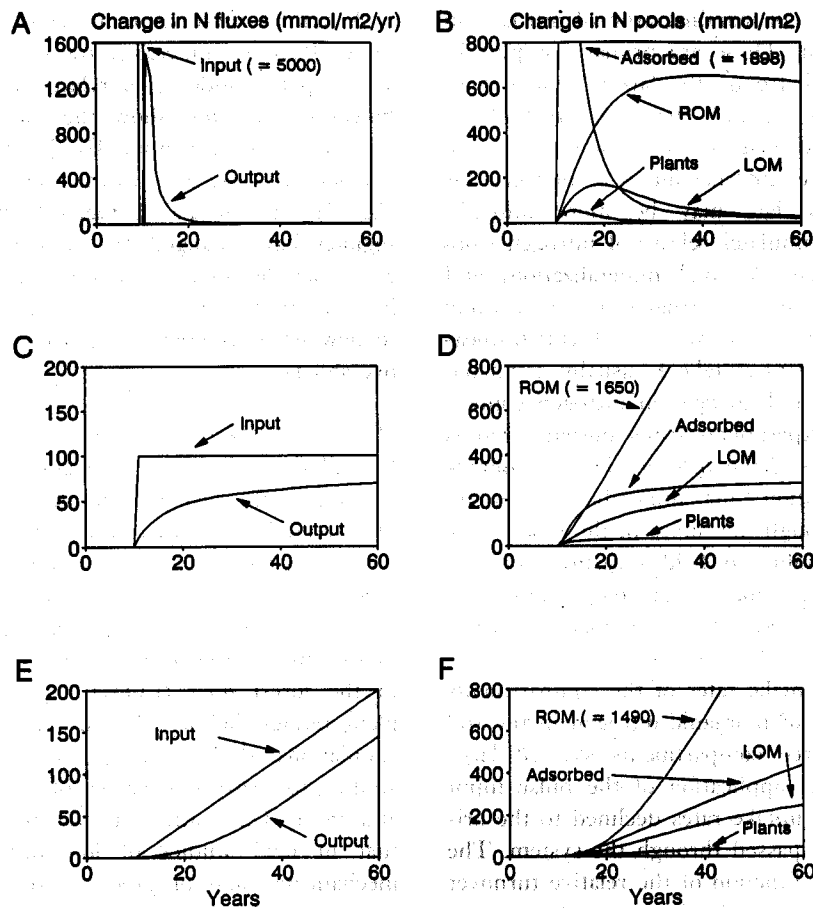

Fig. 3 *Changes in the simulated values of the nitrogen input/output fluxes (A, C and E) and the nitrogen contents of the organic compartments (B, D and F) in response to three scenarios of inorganic nitrogen inputs: A and B) pulse addition; C and D) step change; E and F) ramp increase. Changes are relative to the initial steady state conditions (first ten years of the simulations). The integral of the input (total nitrogen added) is the same in all three cases.*

determine the ecosystem controls on nitrogen leaching. Both the output response and internal nitrogen dynamics simulated by the model during the first years following the step input are at least qualitatively consistent with observations from these manipulation experiments (Wright *et al.* 1995, Tietema *et al.* 1996).

The simulated response to a ramp increase in nitrogen input closely followed that of the step response in that output flux, adsorbed phase, LOM and ROM pools increased rapidly (Figs. 3E and 3F). Under this scenario, however, output flux and internal N pools continued to increase throughout the simulation. The short time lag before the output flux began to increase is consistent with observed relatively rapid catchment responses to increased nitrogen deposition (Kahl *et al.* 1993, Moldan *et al.* 1995). The model output indicated a close relationship between nitrogen input and nitrogen leaching once leaching began and this behaviour is supported by survey data from forested systems in Europe (Dise and Wright 1995).

Results for internal nitrogen fluxes (deposition effects)

The preceding discussion focuses on the input/output fluxes and the pool sizes or standing crop of nitrogen in the simulated ecosystem. These are primary outputs of the model and there are frequently data to which these model outputs can be compared (the aggregation of the model was conceived with such comparisons in mind). The model also simulates internal fluxes of nitrogen for which comparisons to data may be more difficult. Specifically the model simulates release of nitrogen from the organic compartments ('gross' mineralization) and uptake (or immobilization) of nitrogen by the organic compartments. These internal fluxes are difficult to measure on real systems. Plant uptake is usually estimated from biomass increases and changes in nitrogen content of tissues. Incubation experiments using buried columns or bags provide estimates of the *difference* between immobilization and mineralization ('net' mineralization) of soil compartments. Even though the fluxes in the model may not be directly comparable to field measurements (or perhaps *because* they are not comparable), there is a heuristic utility in examining these simulated internal fluxes.

The changes in the uptake rates of the compartments reflected the availability of inorganic nitrogen in the soil solution in that all three compartments showed large increases in uptake after application of the pulse input (Fig. 4A). The elevated uptake rates declined to the original levels as the pulse passed through the system. The pattern of decline was a function of the relative turnover times of the compartments with plants (rapid turnover) re-establishing the steady state uptake rates before the LOM compartment, and the LOM compartment before the ROM compartment. The pulse input increased mineralization of the LOM compartment (Fig. 4B) initially

but, as the nitrogen pulse passed through the system, this effect also declined. ROM mineralization increased but the effect was slower and more prolonged, reflecting the delay in nitrogen reaching the ROM compartment and its longer residence time there.

A step increase of nitrogen input to the simulated system resulted in persistent changes in the nitrogen uptake and release fluxes of the model compartments (Figs. 4C and D). Mineralization of both LOM and ROM again increased with added inorganic nitrogen but with some delay as the nitrogen was incorporated into the organic matter in each compartment. Uptake increases were more immediate and declined somewhat by year 60. The initial steep rise in uptake was a direct result of the dependence of the uptake equations on soil solution inorganic nitrogen concentrations. The decline after the initial rise was a result of the feedback in the equation based on the C:N ratios within the compartments. Increased uptake lowered the C:N, increasing mineralization and also lowering the uptake demand. These simulations would have settled eventually to a steady state condition with both uptake and mineralization constant at higher values if the period of simulation had been longer.

A ramped increase of nitrogen inputs has almost the same effect on mineralization as the step addition (Fig. 4F). Uptake under this relatively slow input increase, however, does not show the pronounced initial surge caused by the step input. By the time the ramped input reaches the same level as the step input (i.e., year 60 in Fig. 4), the internal nitrogen fluxes under both input regimes have changed by the same amount. This suggests that the internal nitrogen fluxes were closely tracking the input availability of nitrogen, and that adaptation to new levels is relatively quick without large delays or overshoots.

Discussion of deposition effects

For all three deposition scenarios (with constant carbon dynamics), the responses of the compartments in terms of increased long-term storage of deposited nitrogen was ROM > adsorbed > LOM > plants. The bulk organic and inorganic storage components were more important than the LOM and plant compartments in retaining long-term or large nitrogen inputs. In addition, storage in the forest floor (LOM) was greater than in active plant tissues. While these are the results of speculative simulations, they are based on mass balance principles applied to reasonable values of carbon pools and fluxes and tissue C:N ratios. It may be suggested, therefore, that in field studies of long-term nitrogen retention mechanisms (and of processes disrupting these mechanisms), a major part of the field effort should be focused on the processes occurring in soil organic matter. The simulations also suggest that while the changes in the ROM, LOM and adsorbed pools may be the most important, these changes may be hard to detect in the
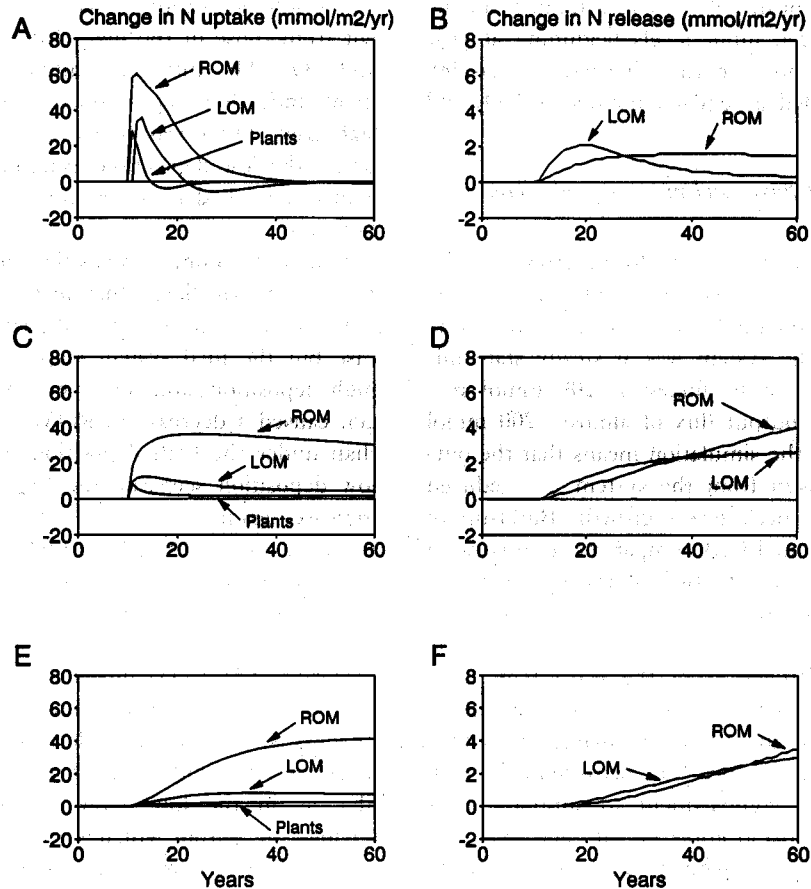
Fig. 4 *Changes in simulated internal nitrogen fluxes (mineralization—A,C,E; uptake—B,D,F) in response to three scenarios of inorganic nitrogen inputs: A and B) pulse addition; C and D) step change; E and F) ramp increase. Changes are relative to the initial steady state fluxes (first ten years of the simulations).*

field for at least two reasons. First, the changes occur relatively slowly over periods of several years, and second the changes (while large in absolute terms) are small relative to the existing pool sizes.

SIMULATIONS USING VARIABLE CARBON DYNAMICS (LAND USE CHANGE EFFECTS)

Three simulations were performed in which the pools and fluxes of carbon were changed during the course of the simulation to examine land-use effects on nitrogen dynamics (afforestation for instance). The carbon pools and fluxes and sequences of changes in carbon storage and fluxes were selected to be consistent with observed and estimated values for biomass production (Miller *et al.* 1980a and b), wood production (Hamilton and Christie 1971), litter production (Miller and Miller 1987, Stevens *et al.* 1992) and forest floor accumulation (Emmett *et al.* 1993) in a newly planted forest. The dynamics were calculated to be comparable with forest growth of a Yield Class 16 crop (i.e. a crop that exhibits

a mean annual increment maximum of approximately 16 $m^3 ha^{-1}$).

Simulations were run for 90 years. The first 10 years were steady state with respect to all inputs and variables. Starting at year 11 the forest growth sequence was initiated. Forest growth was simulated by doubling the carbon pools and litter flux, such that the plant compartment increased from 100–200 mol $C m^{-2}$, the LOM compartment increased from 150 to 300 mol C m^{-2}, and the litter flux increased from 15 to 30 mol C $m^{-2} yr^{-1}$ (Figs. 2B and 2C). Net primary productivity necessarily increased rapidly in the early stages of forest growth (NPP in Fig. 2C). To reach pool size stability at the higher levels following forest growth, a three-fold increase in decomposition of the LOM compartment was needed to balance the increased flux of litter (Fig. 2D). The pool size and the decomposition rate of the ROM compartment were both held constant (Figs. 2B and 2D).

This pattern of land-use change was simulated under three regimes of inorganic nitrogen input: 1) constant high nitrogen input (200 mmol $m^{-2} yr^{-1}$); 2) constant low

nitrogen input (10 mmol m^{-2} yr^{-1}); and a ramp from the low to the high nitrogen input levels beginning at year 11 in the simulation and increasing linearly to year 90. The nitrogen was added as equal amounts of NO$_3$ and NH$_4$ ions.

Results for input/output fluxes and nitrogen pools (land use change effects)

The simulated nitrogen response to forest growth under high deposition was a decrease in output flux as the nitrogen requirements for the biomass increases were met (Fig. 5A). Note that the system was at steady state initially with input and output fluxes of 200 mmol m^{-2} yr^{-1}, so the change in output flux of almost −200 mmol m^{-2} yr^{-1} by year 30 of the simulation means that the output of inorganic nitrogen from the system was reduced almost to zero during peak forest growth. Build-up of nitrogen in the plant and LOM compartments was rapid (Fig. 5B). In spite of the retention of the nitrogen that had been leached before forest growth began, the biomass increases of the plant and LOM compartments required additional nitrogen from the ecosystem. This additional nitrogen was derived from the ROM compartment as evidenced by the negative changes in ROM nitrogen (Fig. 5B). In essence the ecosystem 'mined' nitrogen from the soil compartment to support forest growth. This internal reallocation of nitrogen occurred even in the presence of a relatively high deposition of nitrogen. After canopy closure and stabilization of the carbon pools (year 40 in the simulation), ROM nitrogen began to recover to its original level. This re-storage of nitrogen in the bulk soil organic matter delayed the recovery of output flux so that by the end of the simulation outputs had not completely recovered to pre-afforestation levels. The output flux did begin to increase, however, as the new forest stabilized, and outputs continued to increase as the forest aged.

Under low constant nitrogen deposition (Figs. 5C and 5D), the decline in output fluxes was less than that for high deposition. The steady state system before planting, however, only had an output of 10 mmol m^{-2} yr^{-1} and this was reduced to zero very early in the forest sequence and remained at zero throughout the simulation. Unlike the forest planted at high deposition (Fig. 5A), the forest planted at low deposition (Fig. 5C) did not show a pattern of increased leaching losses with age after canopy closure. In this system there was much less nitrogen available from external sources for forest growth, so the 'mining' of nitrogen from the ROM compartment was much larger (Fig. 5D). The plant compartment in both the high and low deposition situations achieved the same nitrogen pool size at about the same time. The LOM compartment in the simulation under low deposition was, however, considerably nitrogen deficient compared to the high deposition situation.

The behaviour of the bulk soil nitrogen compartments

in the low deposition scenario were also markedly different from those of the high deposition scenario (Figs. 5B and 5D). The nitrogen content of the ROM compartment under low deposition did not recover as the forest stabilized. There was also a net loss of adsorbed nitrogen under the low deposition scenario as opposed to the net gain in adsorbed nitrogen simulated for the high deposition case.

Under a ramped deposition increase (Figs. 5E and 5F), an intermediate situation was simulated. The beginning of forest growth was similar to the low deposition case but the final system responses resembled more the high deposition situation. The 'mining' of organic nitrogen caused a decrease in ROM nitrogen to a lower level than under the high deposition scenario, but, unlike the low deposition scenario, the ROM nitrogen content did increase again after forest maturation. These changes reflected the enhanced availability of nitrogen as deposition increased through time and forest development slowed. Plant compartment nitrogen content again reached the same levels at the same time as in the other scenarios. The LOM nitrogen response was intermediate between those of the low and high situations. Adsorbed nitrogen showed an initial loss but increased above initial levels near the end of the simulation. Output fluxes (Fig. 5E), as in the low deposition scenario went to zero (change in output equal to −10 mmol m^{-2} yr^{-1}) and remained at zero until very late in the simulation when leaching finally began (at about year 80).

These simulation results are in broad agreement with observed and hypothesized behaviour of nitrogen dynamics in growing forests although time series of data describing the dynamics of all ecosystem compartments at a site are not available. The onset of nitrogen leaching simulated by the model resulted from increased or prolonged nitrogen deposition and decreased plant requirement for nitrogen with age. These patterns are at least qualitatively consistent with observations and experimental data (Wright et al. 1995, Stoddard 1994). The quantitative correctness of the model is examined by Emmett et al. (in press) in a further paper.

Results for internal nitrogen fluxes (land-use change effects)

The increases in nitrogen uptake were much larger for the land-use change simulations (Figs. 6A and 6C) than for the deposition effects simulations (Figs. 4A, 4C and 4E). This was to be expected in that the simulated forest growth required a large sequestration of nitrogen. The large change in nitrogen release from the LOM compartment (Figs. 6B and 6C) was also expected because of the increased decomposition of the LOM compartment as the simulated forest matured. What was not necessarily to be expected was the decline in uptake by the ROM compartment (Figs. 6A and 6C). This decline occurred because the plant and LOM compartments had a higher demand for nitrogen during the simulated growth phase
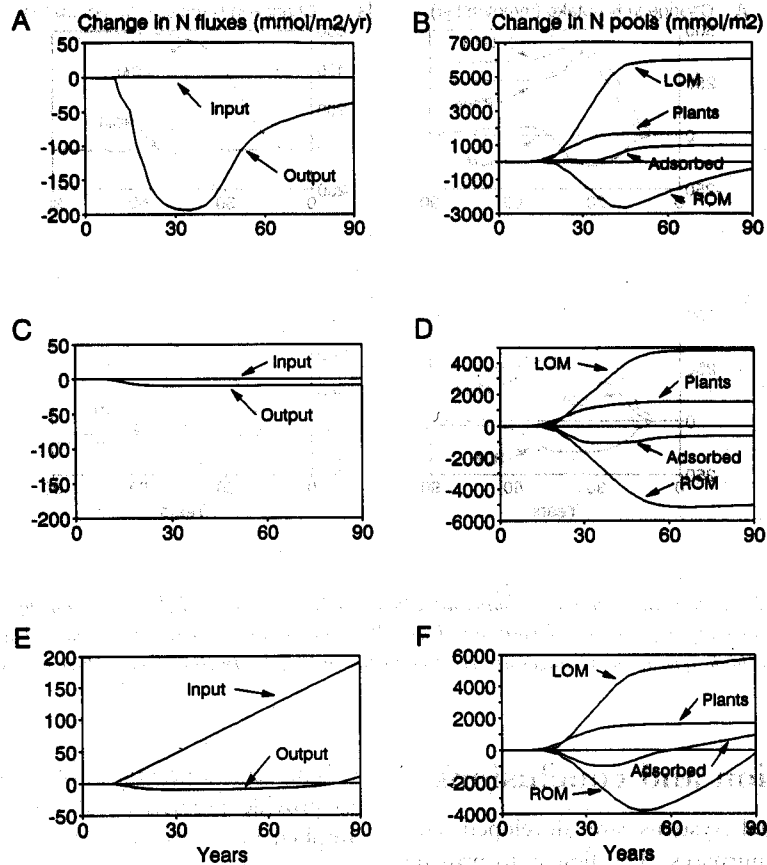
Fig. 5 *Changes in the simulated responses of the nitrogen input/output fluxes (A, C and E) and the nitrogen contents of the organic compartments (B, D and F) in response to a land use change implemented under three scenarios of inorganic nitrogen deposition: A and B) high constant deposition; C and D) low constant deposition; E and F) ramp increase from low to high deposition. Changes are relative to the initial steady state conditions (first ten years of the simulations).*

of the forest and 'out-competed' the ROM compartment for the available nitrogen (a demonstration of the dynamic competition for nitrogen inherent in the structure of the model).

There was not much difference in the changes of internal fluxes, however, between the two levels of deposition when only the land-use change scenarios are considered. Changes in uptake and release at high deposition (Figs. 6A and 6B) are slightly larger than for the low deposition case (Figs. 6C and 6D), largely due to the increased nitrogen availability under high deposition. The results for the ramp deposition scenario are not shown because they are intermediate between the two very similar situations already displayed.

Discussion of land-use change effects

For all three land-use change simulations, forest growth promoted net nitrogen mineralization in the ROM compartment and net nitrogen immobilization in the LOM compartment during forest growth. This re-allocation of

internal nitrogen stores was necessary even under relatively high deposition conditions. In all cases, the plant compartment took up nitrogen to the same degree. Note, however, that under the simplified conditions of these simulations there was no attempt to reduce plant carbon productivity in the low deposition scenario. While this may be a questionable assumption, the magnitudes of the changes in the other compartments were so large relative to the changes in the plant compartment, that it is not likely that changes in plant productivity of 20% or 30% as a result of nitrogen limitation would have changed the overall patterns simulated here. Those patterns are: 1) that forest growth, even under high deposition, requires reallocation of internally stored nitrogen; 2) that leaching of nitrogen from afforested sites will be reduced or even prevented during the active growing phase regardless of deposition level; and 3) that leaching from mature forests may be delayed or accelerated depending on the deposition history to the site and the degree to which the forest used internal nitrogen sources during the growth phase.
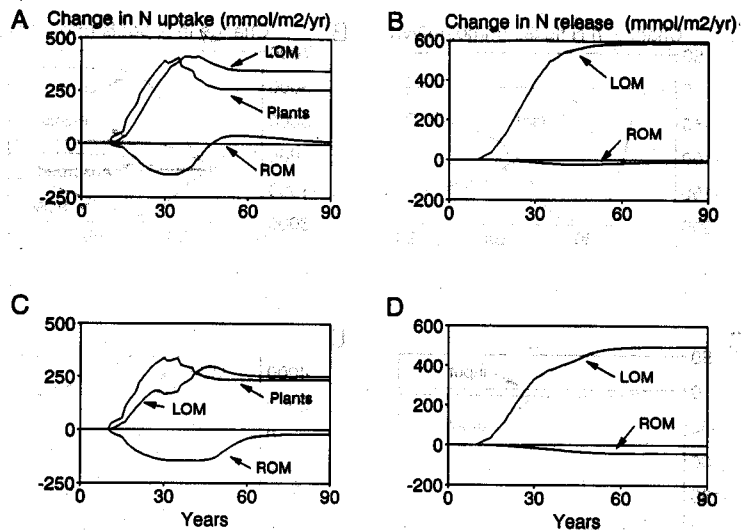
Fig. 6 *Changes in simulated internal nitrogen fluxes (mineralization—A,C,E; uptake—B,D,F) in response to a land use change imple-mented under three scenarios of inorganic nitrogen deposition: A and B) high constant deposition; C and D) low constant deposition; E and F) ramp increase from low to high deposition. Changes are relative to the initial steady state fluxes (first ten years of the simulations).*

General discussion and conclusions.

Models of environmental systems are developed and applied for two general purposes. The first is to provide aid or direction in solving a problem or understanding a complex system. Models developed for these heuristic purposes (and the assumptions embodied within the models) may often be unjustified or even incapable of justification. These models are useful primarily as exploratory problem solving tools. The construction of these models and their subsequent use for speculative simulation is a self-education process. These models are tools to express and test hypotheses about the function-ing of simple or complex systems. The outputs of such models do not need to be quantitative to be useful or to provide tests of the model. Often it is the case that reli-able or extensive quantitative observations from the sys-tem being modelled are not available, so evaluation of these models must often be based on qualitative behaviours. The fact that such models cannot be verified quantitatively, however, does not diminish the utility of these models in advancing knowledge from a perceptual understanding of a problem (an intuitive or empirical cognition based on observation) to a conceptual expres-sion of the problem (a complex, symbolic product of abstract or reflective reasoning). The models, once con-structed, often guide the collection of data for further model testing and refinement of ideas by highlighting the inevitable consequences of the assumptions and the cur-rent understanding of system functioning that has been incorporated in the model structure.

The second general purpose for constructing models is to provide predictions of future behaviour of a system. Implicit in the use of models for this purpose is the need or desire to take some management action based on the outcome of the model predictions. The costs of such management actions are often large. As a result, models used for predictive purposes are subject to different stan-dards of testing and acceptance than are models used for heuristic purposes. It is not enough that the models pro-vide insight into the system processes. Predictive models must be shown to function correctly and consistently to establish confidence in the use of their predictions. Pre-dictive models do not necessarily have to be quantitative to be useful. Models that simply predict whether or not some event occurs (a qualitative response) can be valu-able in making policy decisions. Most often however, predictive models are used in quantitative analyses. In either case, measures of the reliability of the models are needed to establish confidence in their use. Model relia-bility is most often assessed through validation or verification exercises. The models are used to predict system responses in given situations and the model pre-dictions are compared to observation of real system response. The paradigm for such tests requires that the data used in the test were not used in constructing or calibrating the model. As an increasing number of such tests are performed and the model functions reliably in each case, confidence in the model's predictive capabili-ties grows.

It is often the case that the same model will be (or must be) used for both heuristic and predictive purposes,

particularly in the analysis of environmental systems. This is the case for the model presented here. Construction of MERLIN was guided as much by a need to understand the influences of linked biotic and abiotic processes on nitrogen dynamics in ecosystems as by a need to provide a (preliminary) tool to predict future ecosystem response to atmospheric nitrogen deposition. This paper demonstrates the heuristic utility of the modelling procedure: the perception of the problem (nitrogen leaching), the conceptualization of the processes involved (the model structure) and the examination of the implications of current assumptions and understanding of nitrogen dynamics incorporated in the model structure (the speculative simulations). Based on the analyses presented here, MERLIN appears to be a useful tool for examining the retention and loss of nitrogen at the plot or catchment scale in response to changes in nitrogen deposition and/or land-use changes. The structure of the model is process-based, the aggregation of components is consonant with those field measurements most frequently available, the dynamic responses of the model are consistent with many current observations on nitrogen dynamics in natural and manipulated systems, and the model can be used to focus and guide future field experiments and data collection efforts.

Acknowledgements

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