DOCTORAL THESIS

Process-based modelling of N losses from terrestrial ecosystems

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ABSTRACT

Nitrogen (N) loss to atmosphere and ground water can contribute to environmental destruction, by N emission as the greenhouse gas nitrous oxide (N_2O) and by leaching of N to contamination and eutrophication of water. Dynamic models are important keys to increase the knowledge of ecosystems N processes. This thesis studied N fluxes, particularly soil N dynamics, in different ecosystems in relation to interactions between physical and biological processes using a process-based model called the CoupModel.

A sub-model implementation of two important processes contributing to nitrogen oxide (NO), N_2O, and dinitrogen gas (N_2) emissions; nitrification and denitrification, from another process-based model (PnET-N-DNDC) was done. The models were applied on an old spruce forest in Germany and both model outputs of NO and N_2O emissions were compared. After further development of the nitrification and denitrification sub-model, the CoupModel successfully described the general pattern of N dynamics.

The CoupModel was thereafter applied to an organic crop rotation system. The model generated a complete N budget with small uncertainty ranges for simulated N inputs and outputs, but with a trade-off on estimated differences of N storage in the soil; why it could not be conclusively determined whether the system acted as a source or sink for N. As an outcome of the simulation, almost one fifth of the parameters that were calibrated could be identified as being either system- or field-dependent and had a significant impact on the simulation for nitrate leaching and N_2O emission data.

We used the CoupModel to evaluate N_2O emission sensitivity to soil pH on an organic soil in a birch forest. By generating a decrease of the N_2:N_2O ratio in the CoupModel, we successfully described the increased N_2O emission with decreasing soil pH. The simulated dynamic of N_2O emission generated in a time delay compared to measurements, which may be related to uncertainties in the model description of the groundwater dynamics and other processes involved. However, the CoupModel robustly managed to quantify total carbon and nitrogen budgets.

Finally, we applied the CoupModel on data from ten different locations in Sweden with different N deposition and meteorological data. These were investigated for different drainage depth and initial soil N conditions. The soil differences had large impacts on both N mineral leaching and N denitrification. An application of selected parameter sets was tested; revealing that the uncertainty range of parameter values had impact on simulated N budgets, most notable so for the denitrification pool.

LIST OF PAPERS

This thesis is based on the following papers, which are referred to in the text by their Roman numerals:

I. Norman, J., Jansson, P.-E., Farahbakhshazad, N., Butterbach-Bahl, K., Li, C., Klemedtsson, L. Simulation of NO and N_2O emissions from a spruce forest during a freeze/thaw event using an N-flux submodel from the PnET-N-DNDC model integrated to CoupModel. *Ecological Modelling* (2008) 216: 18-30.*

II. Nylinder, J., Stenberg, M., Jansson, P.-E., Kasimir Klemedtsson, Å. Weslien, P. Klemedtsson, L. Uncertainty of simulated nitrate leaching and nitrous oxide emission based on a field experiment with organic crop rotation. *Submitted to Agriculture Ecosystems and Environment*.

III. Klemedtsson, L., Nylinder, J., Weslien, P., Jansson, P.-E., Kasimir Klemedtsson, Å., Rütting, T. Modelling of soil pH on greenhouse gas fluxes from a drained organic forest soil by CoupModel simulations. *Manuscript.*

IV. Nylinder, J., Jansson P.-E., Grip, H., Klemedtsson, L. Simulated N losses from spruce forest in Sweden based on a calibrated ensemble of parameters values. *Manuscript.*

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INTRODUCTION

The nitrogen (N) cycle is of central importance in ecology, particularly when humans are causing changes to the element's cycle both on local and global scales (Galloway *et al.*, 2008). An increase of N deposition and addition of N fertiliser increases plant growth but also increase the potential for N loss (Oenema *et al.*, 2009). The major contributor to N loss from systems is leaching of nitrate (NO_3^-) by water flow and possible to contamination of the ground water (Smith *et al.*, 1999). From the N loss by emission of gases, dinitrogen (N_2) is stabile molecule consisting 75% (Schlesinger, 1997) of the planets atmosphere, nitric oxide (NO) is an unstabile, short-lived molecule contributing to the production of ozone, and nitrous oxide (N_2O), a stabile molecule contributing to the greenhouse gas effect. The later is one of the most important greenhouse gases responsible for 6.2% of the observed anthropogenic radiative forcing (WMO, 2009). The atmospheric concentration of N_2O has increased approximately linear to a rate of 0.8 ppb yr^{-1}, corresponding to 0.25% yr^{-1} over the past few decades to the present concentration of 319 ± 0.12 ppb (IPCC, 2007). With a wide range of uncertainties, agriculture is assumed to contribute with about 60% of total anthropogenic emission of N_2O, mainly associated with the use of N fertilizer and manure applied to soils (IPCC, 2007). For forests the contribution to N_2O emissions is smaller but should not be neglected, and certainly not so for forests growing on organic soils (Ernfors *et al.*, 2007; Maljanen *et al.*, 2003; Weslien *et al.*, 2009), or locations with high N deposition or fertilisation (Butterbach-Bahl *et al.*, 1998).

The NO and N_2O are both produced in anaerobic and aerobic processes; nitrification and denitrification. The concept of forming and emitting NO and N_2O in soils can be illustrated by the "hole-in-the-pipe" model as described by Firestone and Davidson (1989), where the size of the "holes" for NO and N_2O separately, and the pressure (or rate of the process) through the "pipe" of nitrification and denitrification respectively, are governing the amount of each gas emitted. N_2 is only produced under the anaerobic conditions and is the end-product in the denitrification chain.

To interpret N pools and fluxes in various ecosystems, it is important to understand the major abiotic and biotic regulatory processes. In order to identify and quantify the main factors an approach with coupled feedbacks in the system are necessary. Dynamic models are needed as tools to facilitate the understanding of the complexity of the N processes, and to predict effects of future climate change on emissions of greenhouse gases from terrestrial ecosystems.

Many ecosystem models with focus on the soil cycling processes have been developed during the past thirty years. The demand is to construct models mirroring our understanding of greenhouse gas exchange processes for improving utilisation of the large amounts of measured data from various ecosystems. Mechanistic ecosystem models that can handle the temporal and spatial aspects of the flux estimates are restricted regarding their suitability for prediction of greenhouse gas emissions. A great number of models are attuned in water and carbon (C) processes, but diverge in their formulation of nutrient cycling (Tiktak and van Grinsven, 1995). For example, Potter *et al*. (2000) and Parton *et al*. (2001) each developed a full ecosystem model, but with different approaches to describing the emission of gaseous N fluxes from the soils.

Also, lack of capacity to describe the hydrology of soil profiles may cause problems with estimating N gaseous emissions from agriculture land, which was found in a comparison study concluded by Smith *et al*. (2008) of two biogeochemistry-oriented process-models; the DNDC (Li *et al*., 1992) and DAYCENT (Del Grosso *et al*., 2005). The same study showed that models developed for crop-soil interaction was preformed well in predicting water processes in soils, but failed in estimating N gaseous emission. Henault *et al*. (2005) developed a model predicting N_2O emissions by calculations of denitrification and nitrification rates from biological parameters (e.g. maximum potential denitrification rate), water-filled pore space (WFPS), temperature, and mineral N content. Their approach, as well as that in a comparable model developed by Langeveld and Leffelaar (2002), was to simulate N_2O emissions from denitrification for homogeneous soils, and the specific focus was on the random distribution of water and air-filled pores therein. Simulations of N_2O emission from forest ecosystems have also been preformed using the forest version of DNDC (Li *et al*. 2000) and the CoupModel (Paper I and Farahbakhshazad *et al*. in review) using the “hole in the pipe” concept (Firestone and Davidson, 1989) with successful result on WFPS and N gas emissions.

Objectives

The focus of this thesis is to elucidate knowledge about N processes by coupling functions and coefficients with different terrestrial ecosystem data.
The following objectives are addressed:

- Transfer of an N process module from the PnET-N-DNDC model into the CoupModel to improve its capacity of simulating gaseous losses. Implement the module with needed modifications and validate it using data on WFPS, NO and N_2O emissions from a well-measured spruce forest in southern Germany, Höglwald (Paper I).
- Quantify the uncertainties in the N budgets of two fields in an organic crop rotation, and determine the most important parameters affecting N_2O losses and NO_3^- leaching with the CoupModel as the tool (Paper II).

- Describe the N and C budgets for forested organic soil by using the CoupModel. Demonstrate the calibrated models capacity to simulate how three different soil pHs affects N_2O emissions (Paper III).
- Investigate the influences of parameter applications, ground water depth, initial content of soil organic N and initial C:N ratio in humus by long-term simulations of N losses from spruce forest soils in Sweden. (Paper IV).

BACKGROUND

Nitrogen fluxes from soils

In global N cycling, the microbial processes are important sources and sinks for N_2O. The N decomposition of litter to humus is the first step of the N turnover in soils (as a general reference for below section see Paul (2007)). During mineralisation of humus and litter, organic N decomposes to inorganic N in the form of ammonium (NH_4^+); this step is also called ammonification. The available NH_4^+ will be oxidised to NO_3^- via formation of nitrite (NO_2^-) during nitrification. Some NH_4^+ will also be reformed to organic compounds by immobilization, or as to some extend, be leached from the system, or be subject to plant uptake. Nitrification is an aerobic process, either as oxidation by autotrophic bacteria or as enzymatic oxidation by heterotrophic bacteria and/or fungi (Myrold *et al.*, 1999). During this process NO and N_2O are formed with nitrification rate as one factor controlling the amounts of gases emitted (Firestone and Davidson, 1989). After nitrification, NO_3^- will either undergo assimilatory nitrate reduction resulting in reformation of NH_4^+, being leached from the system, or will be denitrified to NO_2^-, NO, N_2O and N_2. Denitrification is an anaerobic process and high soil water content is crucial for gas formation, and every step in the pathway involves a corresponding enzyme. The first step is an intercellular formation of NO_2^-, which, if C is not availible to the microbe maintenances could not continue to form NO outside the cell. In such case, the high NO_2^- quantities inside the cell are toxic. In all subsequent steps the enzymes are active outside the cell (Spanning, *et al.*, 2007). During the transport through the soil profile, NO, N_2O, and N_2 are available for reactions, but will sooner or later enter into the atmosphere. Even thought nitrification and denitrification, in the way N is transformed above, are the N-gaseous producing processes mostly refer to, other related processes exist, chemical and biological, that contributes to N loss (Paper III).

Atmospheric N_2O and N_2 are possible sources for soil microbes. During N poor conditions in the soil, atmospheric N_2O can be used in the denitrification process forming N_2. Atmospheric N_2 is very important as a soil N input by biological N fixation by bacteria; in free-living forms or symbiotic associated with roots of higher plants.

Major factors regulating the production of NO, N_2O and N_2 are soil temperature, moisture, and pH, but also the amount and quality of organic matter in the soil (SOM), and availability of NH_4^+, and NO_3^- (e.g. Firestone and Davidson, 1989; Schindlbacher *et al*., 2004). The balance between nitrification and denitrification in producing N gases will vary with climate, soil conditions, and soil managements. Generally, high water table, fine soil texture, and high organic C content, promote denitrification, whereas well drained soils and coarse texture promote nitrification (Robertson, 1991). There is also a link between soil temperature and N_2O emission (Smith *et al*., 2003), where, at temperatures between 10 ºC and 35ºC, the N_2O production by organisms increase linear with temperature. However, the emission of N_2O may increase exponentially as an effect of increased volume of oxygen free aggregates in the soil. This condition is created in a combination of soil water content and availability of C for the oxygen consumption, thus affected by temperature (see the anaerobic balloon concept, Paper I). In freeze/thaw cycles there is a high response on N_2O emission produced during denitrification (Öquist *et al*., 2004), where the availability of C is a driving force for the emission (Mørkved *et al*., 2006). Crucial for the denitrification process is also the restricted availability of oxygen in the soil. For optimum production of N_2O the water filled pore space (WFPS) approximately 75%, whereas the optimum for N_2 is total water saturated conditions (Ambus and Zechmeister-Boltenstern, 2007).

Ecosystem models

A number of models have been developed for N processes in soils, many of which are in fact ecosystem models built up by modules calculating different processes in the system, i.e. N flux (review of forest models (Tiktak and van Grinsven, 1995), and of agriculture models (Chen *et al*., 2008)). Mechanistic models are the most widely used models for investigating N_2O emissions from soils and are used to develop mitigation strategies (Chen *et al*., 2008).

In this thesis two models have been used: the PnET-N-DNDC model (Li *et al*., 2000) and the CoupModel (Jansson and Karlberg, 2004). The PnET-N-DNDC model is made up of three parts. The first part is, *PnET*, a photosynthesis–evapotranspiration model, describing photosynthesis, respiration, organic carbon production, and allocation and litter production, for forest ecosystems (Aber and Federer, 1992), the second part is, *N*, a nitrification model, predicting nitrifier growth/death rate, nitrification rate and emissions of NO and N_2O from this process (Stange, 2001), and the third part is, *DNDC*, a denitrification–decomposition model, a biogeochemical model with links between ecological drivers, environmental factors and decomposition, as well as denitrification with emissions of NO and N_2O (Li *et al*., 1992) (Paper I).

The second model used, the CoupModel (Jansson and Karlberg, 2004) represents a flexible coupling between heat and mass transfer for soil–plant–atmosphere systems, where interactions between different components are considered. The model allows for simulation of different spatial and temporal scales, and is well adapted to consider winter conditions with snow and frost. The input data are described either as parameters or by measured variables (Jansson and Karlberg, 2004) (Paper I-IV). The nitrification, denitrification and gas modules in the PnET-N-DNDC model were implemented into the CoupModel in Paper I. In Paper I-IV the CoupModel was used in consideration to increase the knowledge of the N processes in various terrestrial ecosystems, and by development of the model to increase the area of applicability.

MATERIALS AND METHODS

Below is a short description of the sites used in the simulations and the CoupModel used for the research underlying this thesis. For further details, see the respective articles.

Site descriptions

Four ecosystem types were studied using climatic, physical, and biotic data from respective site; Höglwald, Logården, Falköping and Flakaliden (Figure 1, Table 1).

In Paper I the Höglwald site (48 º30’N; 11º11’E) in Germany has been a research site since 1984 (Kreutzer and Weiss, 1998) with, by that time, a 77 year old Norway spruce (*Picea abies* (L.) Karst.) stand. The mean annual air temperature is 7.6 ºC, and the annual mean precipitation is 850 mm (30 years average, 1951-1980). The soil type is loam with an organic top soil layer approximately four cm. Automatically measurements of NO and N_2O flux started in late 1993 (Butterbach-Bahl *et al*., 1997) and is still in progress.

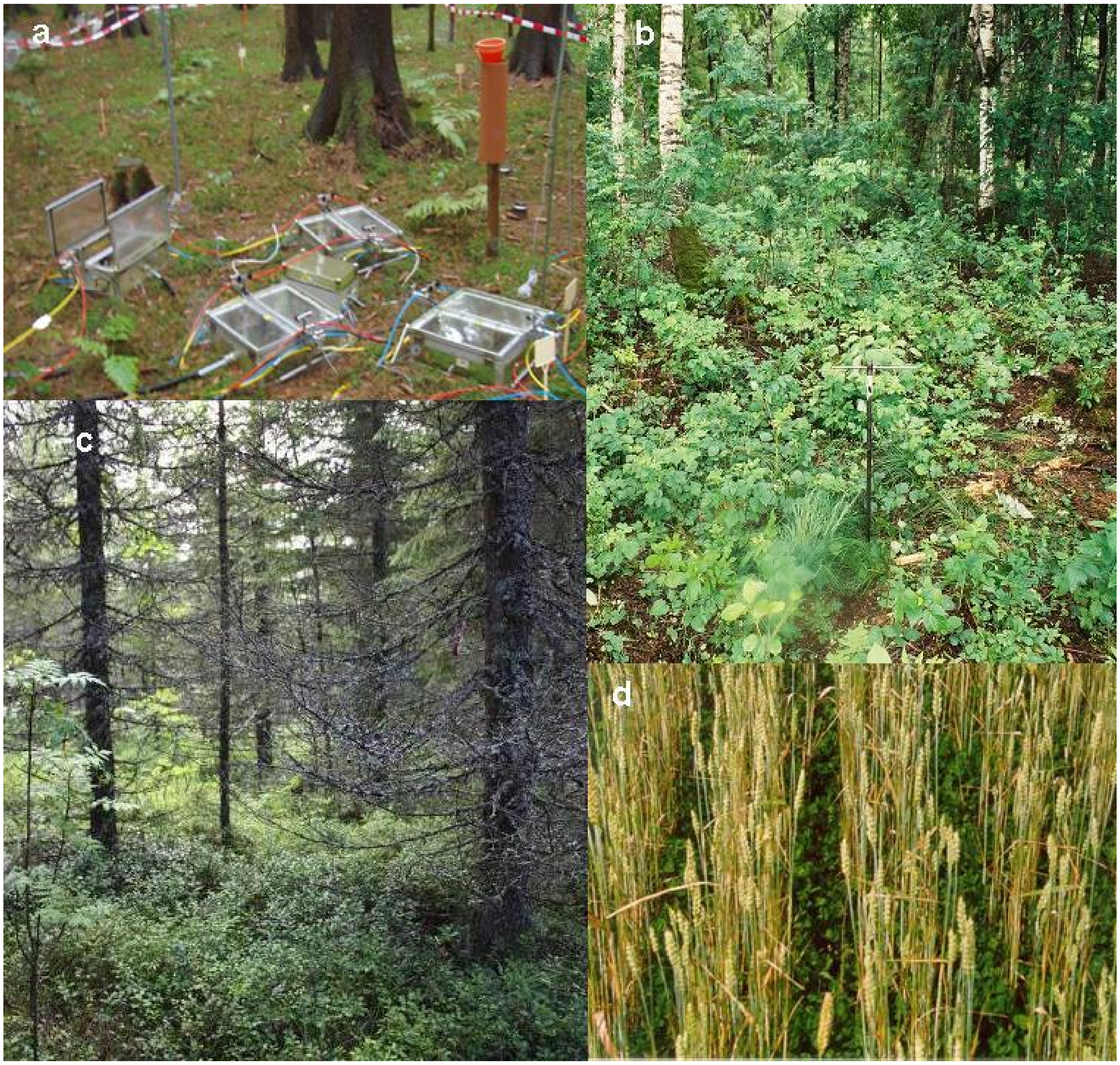

Figure 1. Site view of (a) Höglwald (photo L. Klemedtsson), (b) Falköping (photo P. Weslien), (c) Flakaliden (photo J. Strengbom) and (d) Logården (photo K. Delin).

In Paper II an arable field at the Logården research site (58°20 N: 12°38 E) in south-west of Sweden was investigated. In 1991 the farm was divided into three farming systems, and conventional, organic and integrated farming systems were developed (Helander and Delin, 2004). During the three years of this study (Nov. 2004-Dec. 2007) the crop rotation sequence in the organic and integrated systems was: faba beans (*Vicia faba*) - spring wheat (*Triticum aestivum*) with clover/grass green manure (*Festuca pratensis*, *Trifolium repens* and *Trifolium pratense*) - winter rye (*Secale cereale*). The soil contains 40% clay and soil physical, biological, and chemical variables, were characterized during 2002 and 2003 (Delin, 2003; Roland, 2003; Stenberg *et al.*, 2005). Drainage flow was measured continuously at the well to which the drainage pipe was connected, separate wells for each field. NO_3^- and total N in the sampled drainage water were measured every second week from October 2004. Manual measurements of N_2O fluxes were carried out in five organic and four integrated system plots, with six chambers on each plot to catch the crop sequence. The mean annual temperature is 6.3°C and the annual mean precipitation is 604 mm (30 years average, 1961-1990, SMHI, 2009).

In Paper III a birch (*Betula pendula* Roth) forested organic soil was investigated near by Falköping (58º20'N; 13º30'E). From seven manual chambers, samples of N_2O and carbon dioxide (CO_2) fluxes were collected from August 1994 until October 1997, once a week but more sparsely during winter (Weslien *et al*., 2009). The measurements cover an area with a peat mean depth of 2.2 m and a pH gradient stretching from 3.6 to 5.9 within the site. Soil samples were conducted and characterized in respect to e.g. NH_4^+ and NO_3^- on each flux measurement occasion (Weslien *et al*., 2009). The mean annual temperature is 5°C and the annual mean precipitation is 620 mm (30 year averages, SMHI, 2009).

In Paper IV, the Flakaliden research site (64°07 N, 19°27 E) was used as a reference site for up-scaling of spruce forests in Sweden. The mean annual temperature is 1.9°C, the mean annual precipitation is 587 mm, and the annual N deposition is 2-3 kg (SMHI, 2009). Calibration of parameter values was made in respect to soil water content, soil temperature, snow depth, leaf area index (LAI), stand biomass, soil C and N storage, and soluble organic and inorganic N in the soil water. The Höglwald site, presented above, was used as reference for the parameters.

Table 1. Brief description of sites included in Paper I-IV. R is data used from the reference site.

Site description	Höglwald (I & IV)	Logården (II)	Falköping (III)	Swedish spruce forests (IV)		Flakaliden (IV)
				South[b]	North[a]	
Latitude	48 º30'N	58°20 N	58º20'N	56º26'N	66º05'N	64º07'N
Longitude	11º11'E	12°38 E	13º30'E	15º27'E	17º87'E	19º27'E
Mean annual air temperature (ºC)	7.6	6.3	6.3	-0.1	7.8	1.9
Mean annual precipitation (mm)	850	604	604	666	738	587
N deposition (kg ha^{-1})	30	7	6	1.5	8.1	2-4
Texture	Loam	Clay	Organic	R	R	Sand
pH	3.9 – 4.1	6.1 – 8.1	3.6 – 5.9	R	R	~5-6
Plant type	Spruce	Cereal crops	Birch	Spruce	Spruce	Spruce

[a] Argeplog

[b] Bredåkra

The CoupModel

The CoupModel consists of base processes of heat and water flow in a depth soil profile with atmospheric exchange. The processes in question form a core framework which it is possible to connect modules of interest, and are linked with feedbacks. A module is a set of processes described by empirical functions. Throughout (Papers I-IV), the items to choose for simulations was plant cover, evaporation, ground water flow, snow cover, and C and N fluxes in each system. Climate data and physical properties were used as driving variables or parameters for the simulations.

Water balance in the soil profile is determined by two different soil hydraulic properties, and the model can be parameterized based on measured data. The first soil hydraulic property is the water retention curve, constructed from an expression accounting for macro pores by Brooks and Corey (1964). The second property is the unsaturated conductivity which originates from Mualem (1976), dependent on the saturated matrix conductivity, pore correlation and flow path turtousity, as well as the actual water tension, which are determined by air-entry tension and pore size distribution. The water balance is estimated for each soil layer in the profile. Three soil types (Table 1) were added into the CoupModel database (Papers I-III) during these studies. For Paper IV the reference site, Flakaliden, used for the up-scaling simulations, was already in the database after a prior study (Nordin *et al*. 2009).

Conceptual multiple canopies are added into the model as two plants growing simultaneously with different canopy cover and root depths. In Paper I, III, and IV the two plants simulated were tree and ground vegetation, while in Paper II, main crops with under-sowing of green manure was the two parallel plants during the growth period.

C and N fluxes

Figure 2 shows a schematically view of the C and N flux in the CoupModel. Conceptually, atmospheric CO_2 is the C source for plants, and after uptake via photosynthesis divided in different sizes into leaves, stems, coarse roots and fine roots. In all Papers (I-VI), uptake of C was perceived in a light use efficiency approach, which means that the total plant growth was proportional to the global radiation absorbed by canopy. This process was then limited by unfavourable temperature, N availability, and water conditions. The plant utilise small parts of the assimilated CO_2 to obtain energy for maintenance respiration of leaf, stem, and root. This process is dependent on ambient temperature and a rate coefficient, and will emit CO_2 to the atmosphere through the stomata or via roots to the soil. For survival, the plant also needs N, which by root uptake of NH_4^+ and NO_3^- is

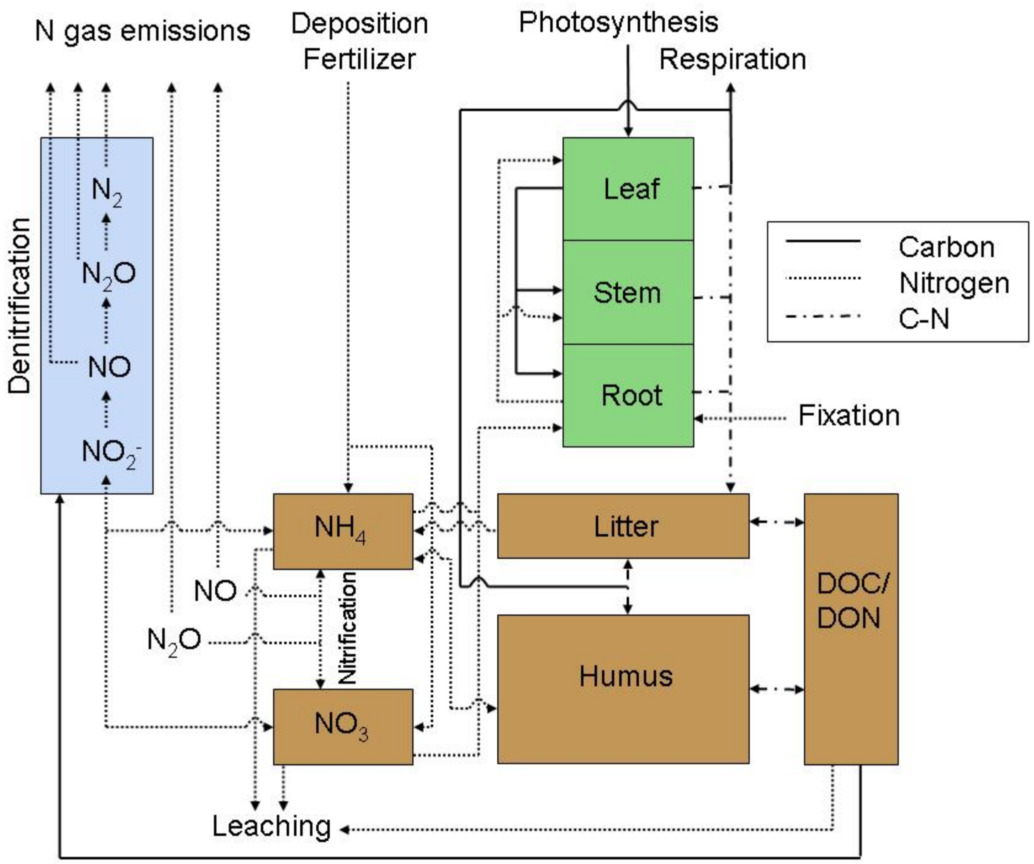

Figure 2. Schematically view of the CoupModel C and N processes and fluxes.

distributed in various amounts to the different plant pools. For plants assimilating N through symbiotic fixation, an extra amount of N will be directly up-taken via roots from the atmospheric N_2.

The plant parts will, at different rates, continually become litter and further form humus, and from both litter and humus will form dissolved organic carbon (DOC), and dissolved organic nitrogen (DON), both being availible for leaching. The C and N contents in different plant parts and organic pools, are determined by the C:N ratio. For plants the allocation of N to a large extent follows the pattern for C. The C:N ratio is therefore governing the N demand in different plant parts, and the N amount in the soil organic pool could estimated by C amount via the C:N ratio.

The approach for litter decomposition will either be where microbes as a pool were not accounted for (Papers II-IV), or where microbes exist as a pool and were substrate dependent (Paper I). CO_2 will be emitted during microbial formation of humus from litter. The DOC will be the C source for growth of the denitrification microbes (Papers II-IV). N will also enter the soil as mineral N in deposition (wet and dry) and if used as fertiliser. Both the N in litter and in humus will continuously form NH_4^+ during the mineralization. Formed NH_4^+ can be immobilised into the humus N pool again, be leached from the system, or go through nitrification forming NO_3^-. During nitrification, which is an aerobic process, NO and N_2O will also be formed. NO_3^- can enter the anaerobic denitrification chain or be immobilized into NH_4^+ again.

Modelling approaches

During the project time the CoupModel was being updated and improved continually. One of the objectives of this thesis was to simulate the N flux with focus on nitrification and denitrification in the soil, and the emissions from these two processes with different questions in focus for Papers I-IV, as addressed below.

In Paper I, parameter values were either measured, or selected after sensitivity analysis by validation. Three CoupModel approaches (option A-C) were compared to fit the measured values of N_2O, NO and soil temperature and water filled pore space (WFPS), at two depths, and compared with an earlier PnET-N-DNDC model simulation by Li *et al.* (2000). Option A directly adopted the anaerobic balloon concept of PnET-N-DNDC, whereas option B differed in parameter setup and modified the exchange rate between the anaerobic and aerobic sites of the soil (Figure 3). Option C was similar to option B, but represented an optional enhanced dry nitrogen deposition rate, to demonstrate the sensitivity of the nitrogen balance of the system to the available inorganic nitrogen in the soil.

The development of the exchange between anaerobic and aerobic sites (the change from A to B) was done to provide an opportunity for the system to emit gases from the anaerobic site even when the soil was fully occupied by the anaerobic fraction. This was used to account for heterogeneity within the soil in a broader perspective, which can be set to explicitly account for the gas transport within completely saturated soils. The gas diffusion exchange function, $f(O_2)$, was before development (option A, Figure 3) described by:

$$f(O_2) = f_A(1 - f_A)O_r o_d \qquad (1)$$

where f_A is the volumetric anaerobic fraction, O_r is the oxygen diffusion rate and o_d is the oxygen diffusion reduction parameter. After sensitivity analyses, the gas diffusion exchange function, $f(O_2)$ was developed to (option B, Figure 3):

$$f(O_2) = o_b + f_A(1 - f_A)O_r o_d \qquad (2)$$

where o_b is the parameter describing the base level of oxygen diffusion function.

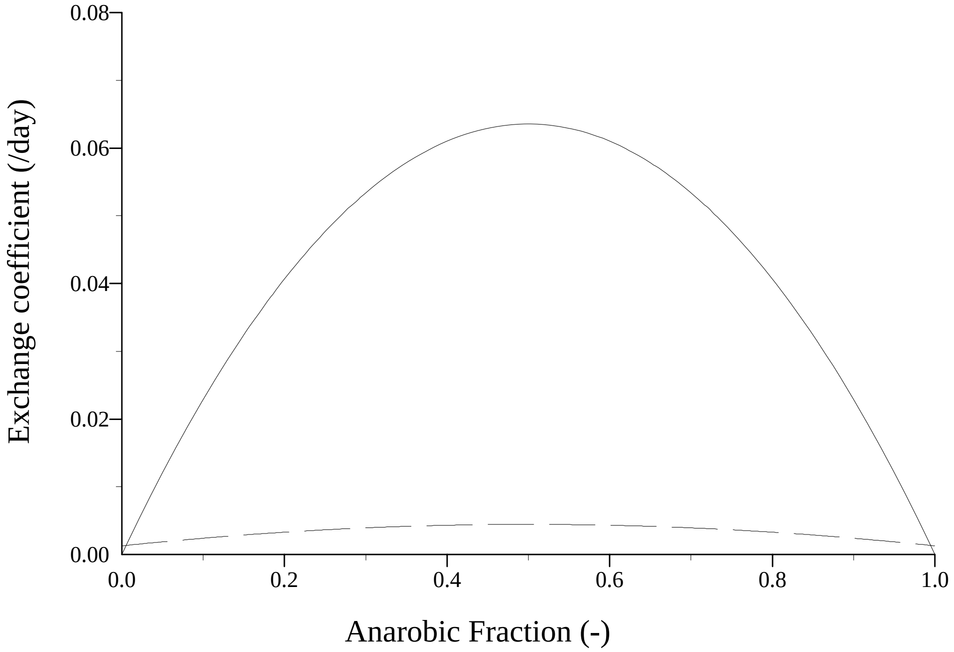

Figure 3. Oxygen diffusion exchange coefficient as a function of anaerobic volumetric fraction for option A (dashed line) and B (solid line).

In Paper II, the new nitrification, denitrification, and gas sub-model with the developed gas diffusion exchange function from Paper I, was used in the investigation of two fields of organic crop rotations. The approach was to quantify uncertainties in the N budgets based on measurements of N_2O emission and NO_3^- leaching. Measured data used for the selection of the runs was also soil NH_4^+ and NO_3^- content, N grain, N fixation, N harvested, water discharge, and soil temperature.

In Paper III the aim was, among other things, to investigate the soil pH in relation to N_2O emission, which, according to measurements, increased with decreasing soil pH. To mimic this response, the value of the parameter, $d_{growthN2O}$, which governs microbial growth of denitrifiers producing N_2 was applied with lower value at lower pHs. This responded in decreased N_2:N_2O ratio and increased the N_2O emission from denitrification. The loss of N_2O from the anaerobic pool due to microbial growth is calculated as:

$$N_{N_2O \rightarrow micrDN} = d_{growthN2O} f(N_{N2OConc}) f(N_{NO_3Concinhib}) M_{activity} N_{micrDN} \qquad (3)$$

where $f(N_{N2OConc})$ is a response function for N concentration in the anaerobic pool of N_2O, $f(N_{NO3Concinhib})$ is an inhibition response function controlled by soil NO_3^- content, and N_{micrDN} is the total biomass of the microbes. For pH 7 the parameter value of $d_{growthN2O}$ was set to 40 day^{-1}, for pH 6, $d_{growthN2O}$ was 5.05 day^{-1}, and for pH 5, $d_{growthN2O}$ was 2.0 day^{-1}.

In Paper IV, the description of dying denitrification microbes was developed to always keep a microbial population alive. The denitrifiers are in general heterotrophic, growing on soil C, and respiring oxygen during aerobic condition, while during anaerobic conditions using N compounds as electron acceptors. Thus, with this concept, the population will not die in conditions where there is a lack of N. The change was done to mimic the dormancy of denitrifiers during N limited conditions and allow them to grow immediately when C and N were available. The previous death rate is calculated as:

$$M_{DNdeath} = d_{denitdie} M_{activity} N_{DNmic} \tag{4}$$

where $d_{denitdie}$ is the death rate coefficient, $M_{activity}$ is the microbial activity and N_{DNmic} is the total biomass of the denitrifiers. With further development the death rate is calculated as:

$$M_{DNdeath} = d_{denitdie} \cdot \max(N_{DNmic} - N_{threshold}, 0) + d_{denitdorm} N_{DNmic} \tag{5}$$

where $N_{threshold}$ is the parameter for threshold of the microbial biomass and $d_{denitdorm}$ is the death rate coefficient when the microbes are dormant.

Paper I is distinguished according to how the nitrification is described. In this case the nitrification is assumed to only be by heterotrophic respiration based on site information. In paper II-IV, both heterotrophic and autotrophic respiration are accounted for in the model, which is accepted in these ecosystems (Paul, 2007)

Calibration method

Many different methods have been suggested within the field of ecological modelling for estimating uncertainties within availible data to evaluate the performance of a model, and carry out inverse estimation of model parameter values. Van Oijen *et al*. (2005) stated that parameters from a dynamic model should be obtained from systematic calibration procedure to get a more reliable output compared to measurements i.e. outputs with uncertainty ranges. The Generalized Likelihood Uncertainty Estimation (GLUE) (Beven and Binley, 1992) methodology is proposed when many parameter sets within the model could give similar model responses due to the complex interactions of parameters. The GLUE method aims at quantifying the uncertainties associated with the model predictions within predefined limits for the parameters. The likelihoods estimated by GLUE are used to characterise a desirable quality in the relationship between model output and corresponding data observed. The calibration of parameters has two motives in the studies; first find runs generating good predictions of included data, and second, find sensitivity parameters for this particular selection.

In Paper II-III the GLUE approach was applied for parameter calibrations. In all cases the investigations of uncertainties were focusing on the N budgets and the sensitivity of calibrated parameters by using measured data. In Paper IV, GLUE calibration was done as a pre-preparation to the study and parameters were selected from that.

RESULT AND DISCUSSION

Model estimates of N losses

According to this thesis the CoupModel description of N processes is applicable in three types of ecosystem. The parameter linking the papers included was the emission of N_2O, which, in the model, have been generated properly in different degrees as compared to measurements.

Application of the imported nitrification and denitrification processes into the CoupModel (Paper I) resulted in well described NO and N_2O emission rates compared to the measured data from Höglwald (N_2O emission is described in Figure 4).

The two different approaches to describing the exchange of gases from the anaerobic to aerobic sites (option A and B) in the CoupModel, resulted in a very different dynamic for the N_2O emission. Option A, which is the unchanged adoption of the exchange equation (1) from PnET-N-DNDC, resulted in two very high and narrow time peaks. This was because the CoupModel generated in not fully applicable exchange description when the soil was close to saturation. When the heterogeneity of the soil close to saturation was taken into account by adding a base parameter, the simulation manages to properly describe N_2O emission rates (option B). Options A and B generated almost the same dynamics for NO emission rate. This can be interpreted as low influences in the changes in the emission description from denitrification, and that the majority of the NO emits during the nitrification.

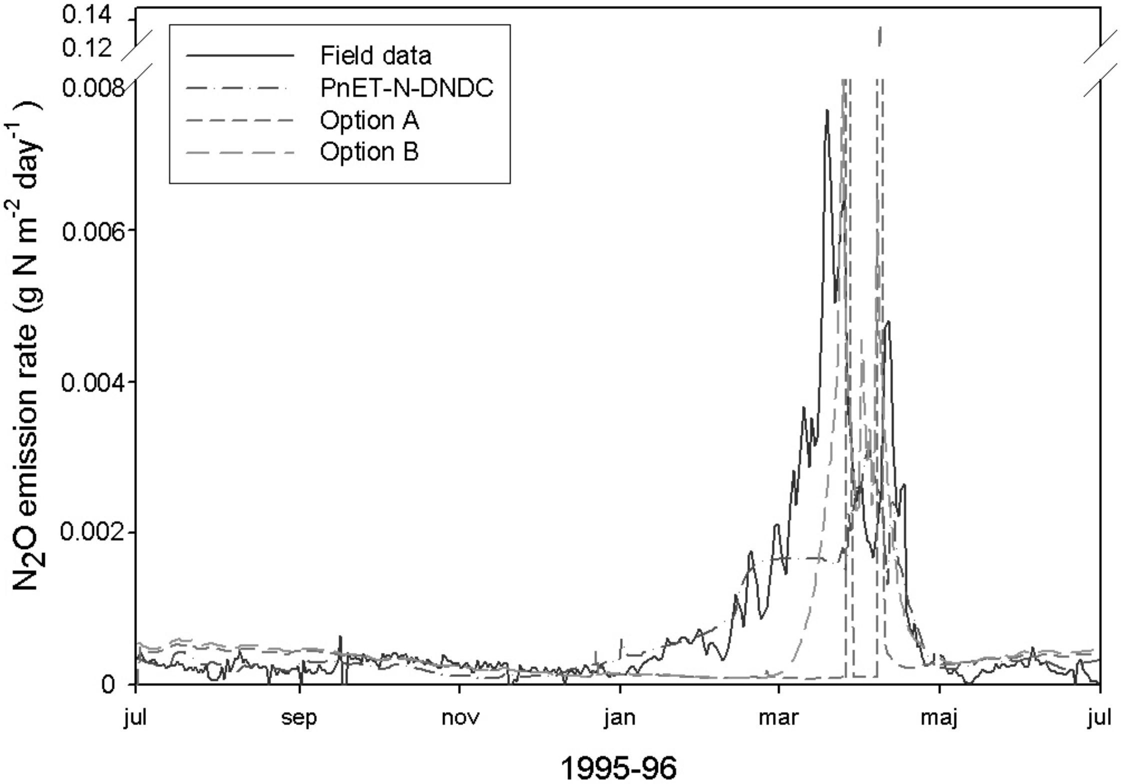

Figure 4. (a) NO emission rate and (b) N_2O emission rate for PnET-N-DNDC, options A and B, and measured data.

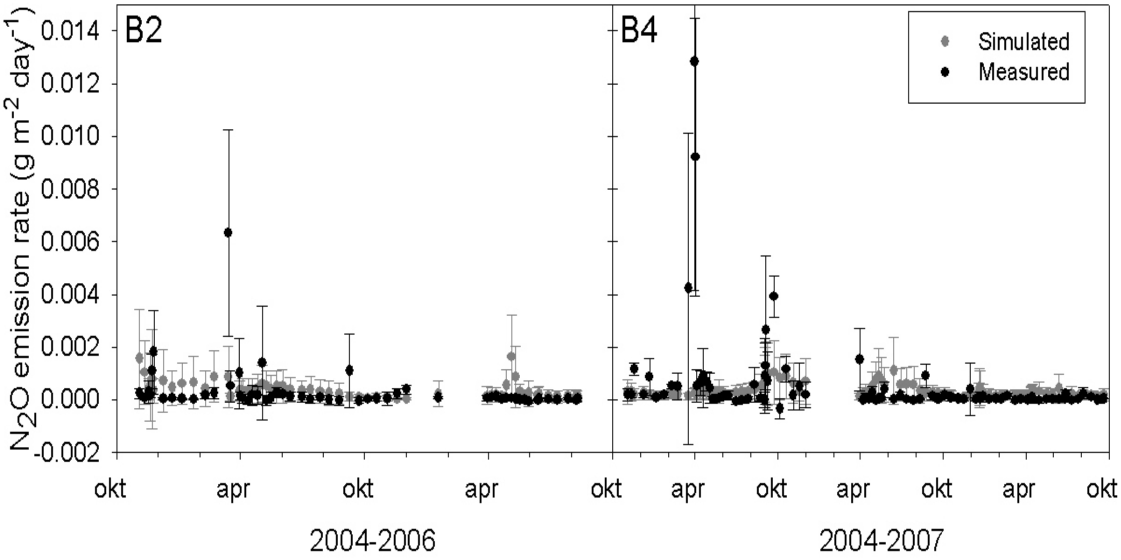

Figure 5. N_2O emission rates from the two fields B2 and B4 as indicated by measured (black circles) and simulated (gray circles) with standard deviations.

In Paper II, the simulated dynamics revealed none of the peaks in N_2O emission rate measured in 2005, but did provide a satisfying description of the low baseline of measured N_2O emission (Figure 5). The underestimation, due to the missing peaks in the simulated N_2O emissions at beginning of the period, led to higher accumulated values for the measured (0.032 and 0.055 g N m^{-2}), than for the simulated (0.020 and 0.037 g N m^{-2}), for both B2 and B4 respectively. If we expanded the accumulated mean by summing up diurnal values for the simulation, it resulted in estimated values of 0.47 and 0.67 g N m^{-2}, and for the integrated measurement in 0.25 and 0.98 g N m^{-2}, for B2 and B4 respectively. The accumulated measured value for B4 indicates how measured high peaks could influence these kinds of estimations. The simulation values for NO_3^- leaching indicated higher levels from B4 than from B2, while the difference in measured NO_3^- leaching between the fields was slightly lower. Better performance of the B2 than B4 simulation compared to measured NO_3^- leaching was observed. This was related to overestimated values in B4 during the first half of the three year period followed by a subsequent underestimation during the second half.

In Paper III, both the *ensemble parameter value representation* (**EPR**) simulations (Figure 6) as well as the *single parameter value representation* (**SPR**) resulted in time delay for the dynamic of N_2O emissions according to measurements. The **EPR** simulation generated in dynamic uncertainties within the range of the measured N_2O emissions (Figure 6). By **SPR** simulations, we generated N_2O emission for three different pHs i.e. 4, 5 and 6 (see Figure 11 in Paper III). In the three simulations, as well as for measured N_2O emissions at mentioned pHs, the N_2O emission increased with decreasing pH. According to our approach the different emission rates were only a result of the parameter governing microbial growth of denitrifier producing N_2, and not as clarified by Li *et al*. (2000) and Stange (2001) a combination of N_2 inhibition and a decreasing rate of the denitrification with decreasing pH. But, based on Simek and Cooper (2002), we assumed that denitrification rate did not change with pH, due to the high soil organic content at Falköping and to that the pH gradient has most likely lasted for centuries, allowing for adaptation of the organisms to the prevailing pH.

The time delay observed for NO emissions from Höglwald (Paper I), could in this case be due to limited availability of NH_4^+ for the nitrification process. According to Dinnes *et al*. (2002), and Zhang *et al*. (2002), a possible explanation is that during this period the competition for NH_4^+ and NO_3^- between plants and microbes is at its peak. But the N_2O emission from Falköping (Paper III), which also had a time delay, was possible not caused by high levels of soil NH_4^+. Rather, this is a sign of production of N_2O via other pathways than nitrification and denitrification or by a too high simulated groundwater level (Paper III).

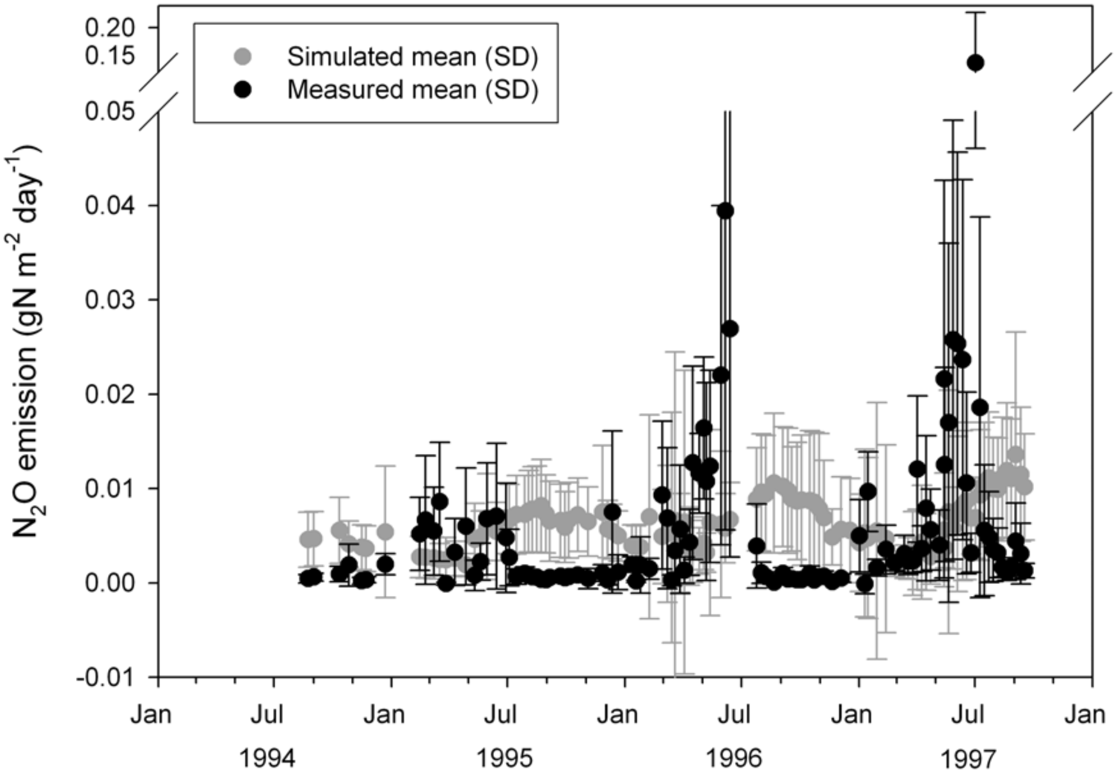

Figure 6. N_2O emission rates from Falköping as indicated by measured (black circles) and simulated (gray circles) with standard deviation (SD).

N_2O emissions are temporally dynamic and responses of biotic and abiotic properties are not easy to completely describe in models. According to the mentioned results poses modelling N_2O fluxes on a yearly basis a great challenge. This has been shown in a study by Henault *et al.* (2005), where an overestimation of simulated flux by approximately 50% for three out of five sites was found for N_2O emissions from agriculture, whereas an underestimation of N_2O flux was simulated in a study by Parton *et al.* (2001) for a grassland site on a sandy loam. However, the winter 1995-96, included in the Höglwald simulation in Paper I and IV, was noteworthy with high fluxes of N_2O occurring during an extended period of frost, with several intermediate periods of surface thawing (Papen and Butterbach-Bahl, 1999). High peaks of N_2O emission related to freeze/thaw events are also found from Logården in April 2005 (Figure 5) and from Falköping in Marsh 1996 and January 1997 (Figure 6). These gas peaks are linked to increased organic C availability from dead plant material (Koponen *et al.*, 2006; Mørkved *et al.*, 2006), and found to be a product of increased denitrification (Koponen and Martikainen, 2004; Öquist *et al.*, 2004). But to construct better models for this kind of N_2O emission hotspots Groffman *et al.* (2009) suggest that more field measurements are needed.

Model estimates of N budgets

Total N budget analyses were presented for Logården (Paper II), Falköping (Paper III), and for ten spruce stands in Sweden with different assumptions for soil properties (Paper IV) respectively (Table 2). The Höglwald simulation, (Paper I), in Table 2 was distinguished by the extremely high N deposition, which seems to contribute to the simulated high NO_3^- leaching. However, the measured and simulated high amounts of N_2O and NO were, according to the simulation, not exclusively produced during denitrification, even though high peaks of N_2O emissions were simulated.

The largest simulated deviant pool in the dataset (Table 2) was the high denitrification for Falköping (Paper III). This complies with that the N difference in the system had the largest negative number compared to the other systems (Table 2).

Table 2. Annual mean for the simulations in Paper I-IV.

Budget N	Högl-	Logården		Fal-	Swedish spruce forests			
(g m^{-2})	wald[a]	B2	B4	köping	G	S	SN	NN
Deposition	10.7	0.73	0.71	0.56	0.75	0.53	0.27	0.17
Fixation	0	8.81[b]	4.54[b]	0	0.05	0.06	0.06	0.08
Fertilisation	0	0	2.18	0	0	0	0	0
Harvest	0	7.98	6.24	0	1.19[c]	0.92[c]	0.53[c]	0.36[c]
Mineral N leaching	5.1	1.65	2.05	1.18	0.07	0.07	0.04	0.04
Dissolved N leaching	1.9	0.17	0.06	1.09	0.09	0.12	0.13	0.19
Denitrification	0.5	0.70	0.68	32.82	0.11	0.11	0.07	0.08
Total system difference	-6.3	-1.63	-2.68	-18.3	-0.65	-0.64	-0.43	-0.41

[a] Simulation with the implemented PnET-N-DNDC module and the new exchange parameter from the anaerobic balloon.

[a] Biological N fixation was active every year.

[b] Harvested at a stand age of 100 years.

Further, the N fixation at Logården (Paper II) was higher than for the forest systems, which was justified from that the fields were under organic farming and the major input of N was an undergrowth of green manure crop. In these simulations, both fields acted as N sources and sinks, reflecting internal turnover uncertainties.

The pools for the spruce forest ecosystems (Paper IV) were comparatively low compared to the other system presented in Table 2. A gradient from high N deposition in the south, to low in the northern parts of Sweden was distinguished when N harvest follows the same pattern. The dissolved organic and mineral N leaching had opposite patterns from south to north, where dissolved organic N leaching increased, and mineral N leaching decreased. This could be due to differences in N uptake by roots, which is less in the northern parts according to e.g. shorter annual growing period.

Parameters sensitivity

In Paper I we show that the new construction of the model was robust with the same assumptions on parameters involved in the nitrification and denitrification processes. But, the addition of an exchange base parameter, provide proof for the sensitivity in description of the denitrification process in the CoupModel. The simulation with this new parameter, explained by heterogeneity in soils, generated a better agreement between measured and simulated N_2O.

Using the GLUE method (Paper II-IV) for uncertainty and sensitivity analyses of the systems, we managed to find parameter sensitive related to N processes. For the two fields at Logården (Paper II) we distinguish how less than 20% of the accepted parameters could be considered to be sensitive within the system. The parameters distinguished were sensitive either according to N_2O emission and/or NO_3^- leaching for either one or both of the fields.

In Paper III, a sensitivity analysis of soil pH was done with respect to N_2O emission. This showed the sensitivity in the inhibition of producing the last step in the denitrification chain, N_2, and how the changes in N_2:N_2O ratio affect the N_2O emission.

In Paper IV, where 13 parameters in 16 parameter sets were selected for the investigation, the uncertainty range of parameter values showed impacts on the simulated N budget, mainly for the N losses and for sites with high N deposition. One, out of two categories of parameters, was identified to create substantially larger denitrification losses, especially for wet N reach soil. Less uncertainty was found on the simulated N leaching. The parameter governing the NO_3^- flux in the denitrification due to microbial growth had great influence in governing the division of NO_3^- for different pathways; as plant uptake, leaching and denitrification.

CONCLUDING REMARKS

The implementation of the PnET-N-DNDC sub-model enhanced the capacity of CoupModel in predicting N_2O emissions, while providing a foundation for robust simulations in the sub-sequent papers of this thesis. However, one major adjustment of the anaerobic balloon description, namely the exchange between anaerobic and aerobic sites, was necessary to obtain reasonable results.

Simulations of the organic crop rotation system and the birch forested organic soil, demonstrated model robustness for N budgets and processes. The simulated inputs and outputs of N, following GLUE calibration, showed relatively small uncertainty ranges for both systems, despite the N denitrification being distinguished by higher uncertainty ranges for the birch forest. Large variability for differences in N storage reflects the internal uncertainties in both cases.

The study on crop rotation also generated parameter uncertainties providing knowledge about the N loss processes, and will hopefully facilitate model designs of other systems. For this system, less than 20% of the calibrated parameters turned out to be sensitive, either indicating the model could be simplified, or that the measurements have to be done with higher precision and covering more events of different characteristics.

The up-scaling for spruce forest stands in Sweden shows how selected parameter sets from one site can be successfully applied to another site, promising predictability beyond the limitations in sites chosen for this study. Further were drainage level, initial content of N in humus, and initial C:N ratio in humus, demonstrated to have large impacts on both N mineral leaching and N denitrification. The uncertainty range of parameter values showed impacts on the simulated N budget, certainly N losses, and especially for sites with high N deposition.

The concept in this thesis, based on quantifying the role and functionality of a number of crucial processes, by merging model structures with experimental data has been successful in various ways. It demonstrated how data could be used to reduce the uncertainty and also how data could be used to identify gaps in our understanding. The current knowledge was also extended to make suggestion outside the investigated domain.

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SAMMANFATTNING

Lustgas N_2O är en växthusgas som har en halveringstid på 11 år vilket medför stor fördröjning om en minskning av växthusgasen skulle ske. Enligt IPCC *Intergovernmental Panel of Climate Change* har N_2O dock ökat linjärt de senaste tiotal åren. Människans påverkan i detta avseende rör framförallt jordbruket eftersom N_2O är starkt kopplad till kvävegödsling, men även gödsling och dränering av skogsmark ökar produktionen av N_2O i marken starkt. N_2O produceras i en aerob process som kallas nitrifikation och en anaerob process som kallas denitrifikation. I nitrifikationen produceras även kvävemonoxid NO medan det i dentrifikationen, förutom N_2O och NO även produceras kvävgas N_2.

Projektet syfte i stort var att genom matematisk modellering utveckla och analysera kväveprocesser i olika typer av marker. Jag har använt en processorienterad ekosystemmodell som heter *CoupModel*. Den kopplar marken, växterna och atmosfären med grunden baserad på värme- och vattenprocesser i en markprofil uppdelad i lager. Vidare är dessa processer sedan kopplade med kol- och kväveflöden mellan och inom mark, växt och atmosfär.

Den första uppgiften var att integrera en nirtifikations- och denitrificationsdel (modul) från en annan processorienterad modell *PnET-N-DNDC* baserat på bl.a. väderdata, vatteninnehåll i marken, N_2O- och NO-emission från marken från en granskog i södra Tyskland. Modulen var inte helt kompatibel med CoupModellen. Vi utvecklade därför processen för utbytet mellan de anaeroba och de aeroba delarna i marken av de gaser som producerades under denitrifikationen. Resultatet var nu bra med avseende på de uppmätta N_2O och NO emissionerna.

Uppföljningen var att applicera den ”nya” modellen på jordbruksmark och skogsmark i Sverige. Två typer av system valdes: fält ekologiskt odling på Logården, försöksgård i västra Götaland och en björkskog i närheten av Falköping odlad på gammal bördig torvmark. Som drivdata för modellen användes uppmätt väderdata och markfysikaliska egenskaper från respektive plats. Bl.a. markinnehåll av ammonium NH_4^+ och nitrat NO_3^- samt utlakning av NO_3^- och N_2O emission från Logården och N_2O- och CO_2-emissioner från Falköping jämfördes med modellens beräkningar på respektive system. De av modellen beräknade och de uppmätta värdena resulterade i god överensstämmelse från båda platserna. Modellberäkningarna var kopplade med en osäkerhetsanalys för att utröna känsligheten i viktiga processer i systemet. Känslighetsanalysen för Logården visade att vissa parametrar var viktiga för hela systemet och andra för bara ett av fälten, en del för N_2O emissionerna och en del för NO_3^--urlakningen.

Avslutningsvis gjordes en simulering av granskogar i en gradient över Sverige beroende på N deposition. Det visade sig att förutom att innehållet av kväve i träden ökade från norr till söder ökade också kväve som denitrifieras. Kväve som urlakas minskar däremot från norr till söder.