

Modeling N₂O emission from grazed grassland

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Report of NOP-project 852078
December 1994

Rapport 24
Haren, 1994

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Introduction

This report is the final result of project 852078, of the Dutch Climate Change Research Programme (NPO-I), on modeling dinitrogen oxide (N_2O) emission from grassland. This project formed part of an integrated study of N_2O fluxes from grassland, within the framework of NOP-I. Participating institutes were, besides AB-DLO, Theoretical Production Ecology (Wageningen Agricultural University), Nutrient Management Institute (NMI), Environmental Sciences (TNO-MW), and Public Health and Environmental Protection (RIVM).

Chapter 1 gives a general introduction of the subject, and places the emission of N_2O from grassland within the wider context of nitrogen losses from dairy cattle farming. It also indicates how to reduce these nitrogen losses, including the emission of N_2O .

Chapter 2 describes the components of an integrated model, which are necessary as a framework to simulate the emission of N_2O from mown and from grazed grassland. Two examples of such more or less complete models from the literature are compared with two modeling approaches, that were followed at AB-DLO.

Chapter 3 describes the simulation model SONICG, that was developed at AB-DLO to describe the emission of N_2O from grassland soils. Details are presented of the modules used in SONICG, followed by results of two preliminary simulation runs for grassland without and with urine application.

Chapter 4 describes results from a simulation model for carbon and nitrogen turnover in mown grassland, developed at AB-DLO by Verberne. This is done because some results from this model are used as input data for the model SONICG.

Chapter 5 describes a recent modification of the model for mown grassland, which makes it suitable to simulate grazed grassland and that discriminates areas unaffected by animal excreta from urine spots.

Instead of a long list of references at the end of the report, we have chosen to inform the reader about the relevant literature sources that we used immediately following each (sub-)chapter of the text.

Contents

Introduction	1
1. Nitrogen losses from grazed grassland, a general introduction	3
2. Modeling N ₂ O emission from (grazed) grassland	9
2.1 Introduction	9
2.2 Two modeling approaches followed at AB-DLO	9
3. Simulation of the nitrogen cycle in (grazed) grassland soil (SONICG)	13
3.1 Introduction	13
3.2 Hydrology	14
3.3 Soil temperature	15
3.4 Soil mineralization immobilization turnover (MIT)	16
3.5 Plant uptake of nutrients	20
3.6 Nitrification	21
3.7 Denitrification	23
3.8 Gas transport	25
3.9 Transport of dissolved substances	26
3.10 Chemical equilibria	27
3.11 Some first simulation results from SONICG	28
3.12 Evaluation, validation and further development of SONICG	29
4. Simulation of carbon and nitrogen turnover in mown grassland	31
4.1 Introduction	31
4.2 Results and discussion	31
5. Simulation of grazed grassland	39
5.1 Introduction	39
5.2 Modifications compared to mown grassland	39
5.3 Modeling example	42

1. Nitrogen losses from grazed grassland, a general introduction

Nitrogen losses from grazed grassland, including N₂O emission, are caused by:

- high N inputs, leading to periods with high concentrations of mineral N in the soil and increasing the chances of N loss via nitrification and denitrification,
- the basically low N efficiency of milk and meat production by cows,
- the limited capacity of grass and soil to act as sinks for mineral N, especially during autumn and winter,
- the concentration of high N inputs in urine and manure spots in the field, with negative effects on grass growth, a reduced N uptake and evapotranspiration, increasing the chances of N loss.

Nitrogen losses from grazed grassland, including N₂O emission, can be reduced:

- at the national scale by reducing feed imports,
- at the farm level by appropriate management, including a reduction of external N inputs and by making optimum use of internal N inputs,
- at the field level by reducing spatial variability of N inputs.

Nitrogen losses from grazed grassland should be considered at three scales:

- the farming system (scale about 50 ha),
- the grassland field (scale about 1 ha),
- urine and feces spots within a field (scale < 1 m²).

The farming system scale

Reduction of nitrogenous emissions to the environment (atmosphere, surface- and groundwater) should be achieved by appropriate management at the farm-system level. A good example of this approach is the research on dairy farming with minimal emissions on the experimental dairy farm "De Marke" (Biewinga et al., 1992). Nitrogen losses from dairy farming are strongly related to the intensity of N turnover as shown by the N-flow schemes for intensive and extensive dairy farms (Fig. 1.1, adapted from Aarts et al., 1992).

Management to minimize N emissions to the environment should consider:

- the number of animals per ha of grassland,
- the feed production on the farm versus imported feed, including the integration of arable farming with grassland utilization,
- a reduction of external inputs, e.g. of mineral fertilizers and of imported animal feed,
- optimal use of internal inputs as animal manure and nitrogen fixation by clover,
- the production capacity of the soil, determined by characteristics as soil type, groundwater level and drainage, water availability for grass production,
- the integration of mowing and grazing,
- continuous grazing versus limited grazing.

A reduction of feed import from other countries will also reduce the input surplus of nutrients on the national nutrient balances.

The grassland field-scale

The potential for grass production and N uptake will strongly depend on the soil characteristics and on the weather conditions in a given year (Verberne, 1992). Grass production will strongly affect C and N turnover in the soil as well as the availability of water by evapotranspiration.

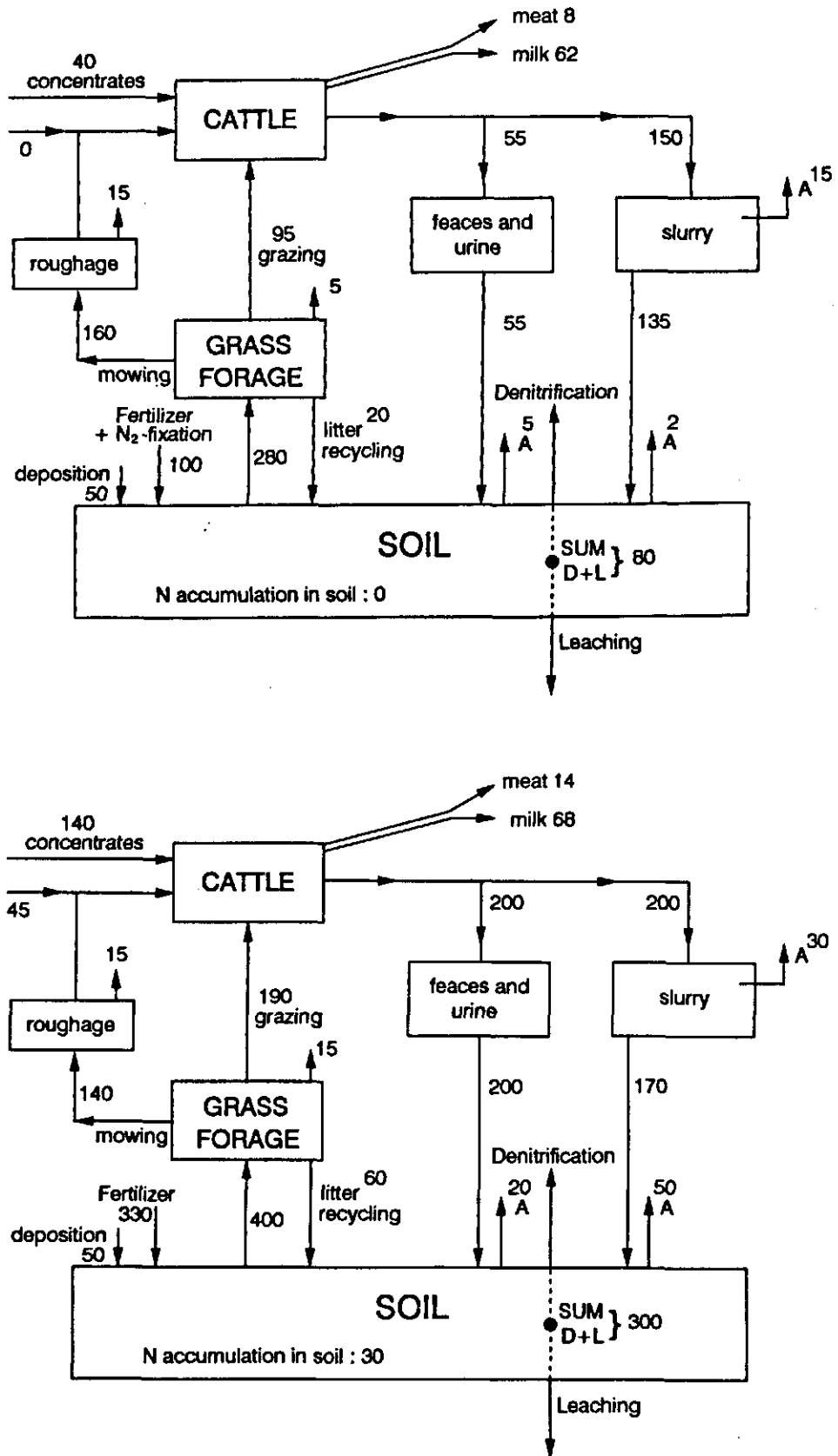


Figure 1.1. Top: Nitrogen flows for the experimental dairy farm with minimal emissions to the environment "De Marke"; from Biewinga et al.(1992). Bottom: Nitrogen flows for specialized dairy farms on sandy soil in the Netherlands, average values for the period 1983-1986; based on data from LEI-DLO.

All values are given in kg ha⁻¹ y⁻¹.

Grass is the main supplier of carbon to the soil by root exudation, dead roots and above-ground litter. N uptake by the grass is a potentially very large sink for soil mineral N. Under optimum conditions for growth, grass can annually take up as much as 800 kg N per ha. Periods with bad conditions for grass growth will lower net production and N uptake and will increase C and N recycling of dead grass litter into the soil.

A shift from arable soil to grassland will lead to an increased level of soil organic matter and to net N immobilization by the build-up of soil organic N. Turning grassland back to arable use will lead to a rapid decrease of soil organic matter and to net N mineralization. Reversal of old grassland to arable land may lead to substantial N losses when the amount of N mineralized from accumulated soil organic matter is much higher than can be taken up by an arable crop.

The apparent N recovery in mown grasslands is high, up to 90%, suggesting that only limited losses to the environment may occur (t Mannelje & Jarvis, 1990). Grazing increases the recycling of C and N in grassland. Of the N taken up by dairy cows about 70-85% is returned to the soil, in feces and urine, and only about 15-30% is removed as milk and meat. The low efficiency of N utilization in grazed grassland explains the high N losses to the environment by NH_3 emission, nitrate leaching and denitrification (van der Meer, 1991). Local deposition of urine and feces can affect grass development, positively as well as negatively, and thus indirectly affect the recycling of C and N. Urine and feces spots are a main source of spatial heterogeneity in the field. Moreover, the deposition of urine and feces is sometimes concentrated on part of the field around a water supply or a milking point. Figure 1.2 shows the nitrogen cycle in grazed grassland and indicates where gaseous N emissions may occur.

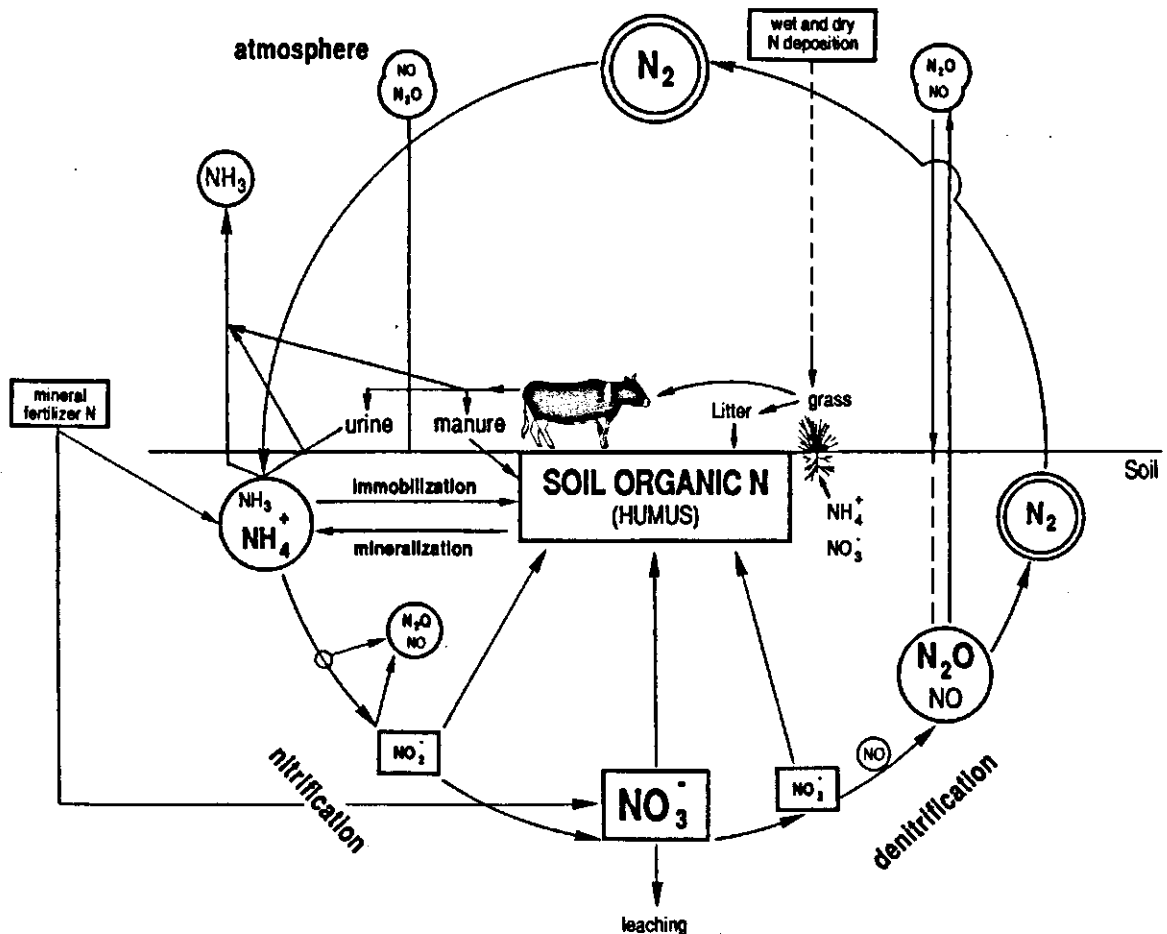


Figure 1.2. The nitrogen cycle in grazed grassland.

Urine and feces spots as active centres for N loss

Nitrogen inputs into the soil of grazed grassland are concentrated in urine spots (about 0.5 m²) and feces spots (about 0.05 m²). Much more nitrogen is deposited there than can be taken up by one grass crop (Deenen & Middelkoop, 1992). Thus a surplus amount of soil mineral N can be present during several months (Afzal et al., 1993) and may lead to N losses (van der Meer & Whitehead, 1990).

Positive as well as negative effects on grass growth can occur (Deenen, 1990; Lantinga et al., 1987), depending on the actual urine concentration and on weather conditions. The nitrogen from urine is rapidly converted into ammonium-N, which may be partly lost by NH₃ volatilization. According to Vertregt & Rutgers (1991) on average about 10% of the urine-N may be lost from urine spots by NH₃ emission. After microbial nitrification of urinary ammonium to nitrate, the latter may partly be lost by leaching and by denitrification. The nitrogen from cow feces mainly consists of organic-N, that is only slowly mineralized, and a fraction of about 10% ammonium-N, that can be lost completely by NH₃ emission (van der Meer, 1991). As shown in figure 1.2, nitrogenous oxides can be produced as a by-product of nitrification (N₂O) or as intermediate products of denitrification (NO, N₂O).

Relevance of emission of N oxides from grassland to atmospheric chemistry

Groffman (1991) discussed the environmental factors that are controlling nitrification and denitrification activity at different scales (Table 1.1). In intensively managed grassland the plant community consists only of one or two productive grass species. According to Groffman, both nitrification and denitrification are likely to occur only in ecosystems with high or excess N availability, as is the case in intensively managed grazed grassland.

In grazed grassland effects of urine and feces on grass growth and senescence affect the field scale controlling factors soil water content, nitrate concentration and carbon supply. Nitrification of large amounts of ammonium in urine spots may take periods of weeks to months. However, as soon as large amounts of nitrate are formed, nitrate concentration is no longer a controlling factor for denitrification, leaving only soil water content and carbon supply as controlling factors. Thus, weeks to months after urine deposition to the soil a period of high rainfall intensity may cause a denitrification peak. The production of N₂O versus its reduction to N₂ will then depend on the carbon availability and the emission of N₂O on the gas diffusion characteristics of the soil and on the depth of the N₂O production/reduction zones. Rainfall during a period of rapid nitrification might also increase N₂O production through nitrifier-denitrification, when oxygen supply through gas diffusion limits complete nitrification (Poth & Focht, 1985).

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Table 1.1 Controlling factors of soil nitrification and denitrification at different scales.

Soil nitrification evaluated at scales relevant to atmospheric chemistry	
Scale of investigation	Controlling factors
Organism	Ammonium, Oxygen
Field	Ammonium supply Soil water
Landscape	Soil type, Plant community
Regional	Geomorphology, Land use
Global	Biome type, Climate

Soil Denitrification evaluated at scales relevant to atmospheric chemistry	
Scale of investigation	Controlling factors
Organism	Nitrate, Oxygen
Field	Nitrate & Carbon supply Soil water
Landscape	Soil type, Plant community
Regional	Geomorphology, Land use
Global	Biome type, Climate

From: P.M. Groffman (1991)

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2. Modeling N₂O emission from (grazed) grassland

2.1 Introduction

In a first literature review several approaches relevant to modeling of N₂O emission from grazed grassland at the field scale, have been discussed (Van Faassen, 1993). Specific attention was directed to modeling of processes in urine patches, as sites where N₂O emission might be largely concentrated.

The emission of N₂O from grazed grassland is the result of the complex interaction of physical, chemical and biological processes. Therefore, to model N₂O emission from grazed grassland we need models that integrate all these processes. This can be done by using submodels (modules), that describe grass development, soil physico-chemical conditions and processes, and soil microbiological carbon and nitrogen cycling.

Integrated models

A large number of integrated models have been published for arable crop-soil ecosystems (Engel et al., 1993; Engel and Baldioli, 1993; Groot et al., 1991). Although many parts of these models are useful for comparative purposes, none of them specifically considers grazed grassland or N₂O emission. Only two extensive models are known to us that specifically simulate the emission of N₂O from soil as part of larger models (Grant, 1994; Li et al., 1992 a,b). Table 2.1 compares these models with the two modeling approaches followed at AB-DLO by Verberne (1992) and by Bril and Van Faassen (this report). A model of nitrogen flows in grassland under grazing or mowing (Thornley & Verberne, 1989) extensively simulated pasture development and effects of grazing by sheep but had only a limited soil submodel.

2.2 Two modeling approaches followed at AB-DLO

Starting from a model for mown grassland

- On the one hand we used the integrated model FSE-GRASS-SOM-WATER (Verberne, 1992), simulating C and N turnover in mown grassland. This model was based on three interacting submodels (Figure 2.1):
 - GRASS simulating C and N turnover of grass,
 - WATNIT simulating transport of water and dissolved mineral N,
 - SOM simulating C and N turnover in soil.

Results from simulation runs with this model, for a sandy soil and a clay soil in years with rather different weather conditions, are given in chapter 4. At the moment we develop a modified version of this model that can be used to simulate grazed grassland.

Development of a detailed model for C and N turnover in grassland soil

- On the other hand, Bril and Faassen (chapter 3) developed the model SONICG for detailed C and for N turnover in soil (Figure 2.2). SONICG includes the B and C modules and module A2 of Table 2.1. Unique is the presence of module B5 on soil chemistry, which calculates equilibrium concentrations of chemical substances in soil solution, adsorbed to the cation exchange complex and in the gas phase. The pH of the soil solution is also calculated and may be used to describe pH effects on soil processes. Physico-chemical equilibria strongly determine the partial pressures of the gases CO₂, NH₃ and N₂O, and thus are essential to modeling gaseous emissions. By using data on grass development as input, the model of Bril can describe N₂O, CO₂ and NH₃ emission from (grazed) grassland. A more detailed description of SONICG is given in chapter 3.

Table 2.1. Modules included, or missing, in integrated simulation models for the nitrogen cycle in soil-(plant)-ecosystems.

References	Modules:	A1	A2	A3	B1	B2	B3	B4	B5	C1	C2	C3
Verberne (1992)		x	-	-x	x	x	x-	-	-	x	-	-
Grant (1991 a/b, 1994); Grant et al. (1993 a/b/c/d, 1994)		x-	-	-	x	x-	x-	x-	-	x	x	x
Li et al. (1992a,b)		x-	-	-	x	x	x-	-	-	x	x-	x
Bril & Van Faassen		in	x	in	x	x	x	x	x	x	x-	x

x = included; - = not included; x- = partly included; in = input needed

Module A: GRASS OR CROP DEVELOPMENT

A1 = carbon (C) and nitrogen (N) turnover (photosynthesis, metabolism, N uptake, litter recycling, removal of C and N with mown grass).

A2 = uptake by the grass of some macroelements (K+Na, Ca+Mg,...).

A3 = effects of grazing and of management (positive and/or negative effects of urine and manure, fertilizer and slurry applications, grass intake, grass regrowth after grazing, different litter recycling under grazing).

Module B: SOIL PHYSICAL CONDITIONS AND PROCESSES

B1 = heat transport (soil temperature profile).

B2 = soil water balance and water transport (water input by rainfall and irrigation; water output by evapotranspiration and leaching).

B3 = transport of substances (nutrients and gases), dissolved in the soil water phase by mass flow and by diffusion.

B4 = transport of gases by gas diffusion through the soil gas phase.

B5 = soil chemical equilibrium calculations of concentrations of substances in the water phase (including pH), in the solid phase (including adsorption to soil CEC) and in the gas phase.

Module C = SOIL MICROBIOLOGICAL TURNOVER PROCESSES

C1 = soil MIT (Mineralization Immobilization Turnover of C and N, including the dynamics of the microbial biomass).

C2 = nitrification, including the dynamics of the nitrifier population.

C3 = denitrification (turnover of organic matter by a part of the microbial biomass included in C1, with the use of nitrate and N₂O as electron acceptors instead of oxygen).

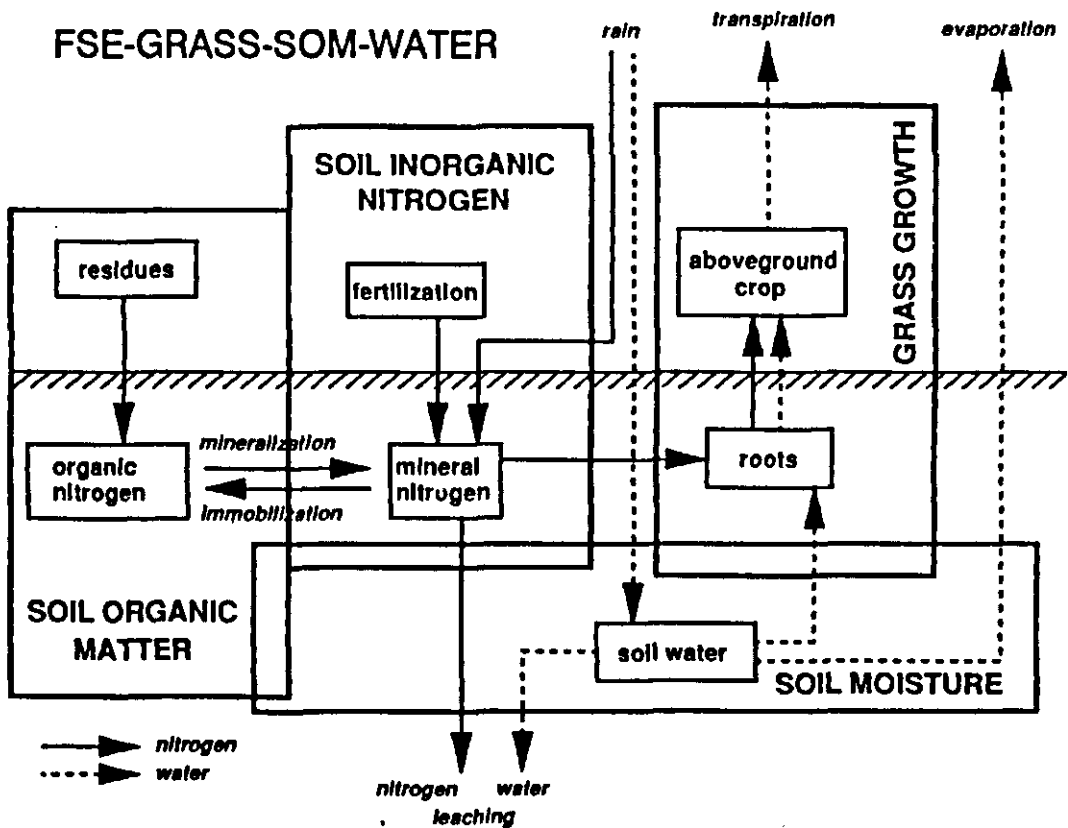


Figure 2.1. Schematic representation of the model structure, which comprises four submodels simulating grass growth and the dynamics of soil moisture, soil organic matter and soil inorganic nitrogen (From Verberne, 1992)

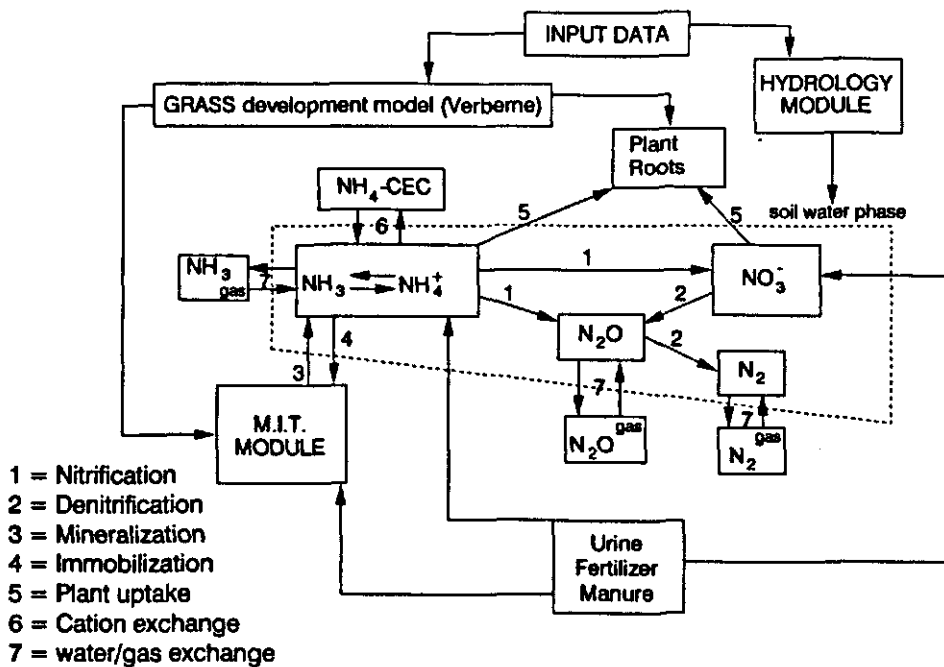


Figure 2.2. Conceptual scheme of N transformations and N exchanges in the model SONICG (Simulation Of the Nitrogen Cycle in Grassland); Brill & Van Faassen

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3. Simulation of the nitrogen cycle in (grazed) grassland soil (SONICG)

3.1 Introduction

As a main part of NOP-project 852078, on modeling N_2O emission from grazed grassland, the simulation model SONICG, on carbon (C) and nitrogen (N) cycling in grassland soil, was developed by Brill and Van Faassen (this chapter). SONICG mechanistically layerwise simulates the relevant soil physical, chemical and biological processes. SONICG uses the model of Verberne (1992, see chapter 4) on grass development and a hydrology module to supply necessary daily input data, and concentrates itself on the nitrogen cycle processes that play a central role in the model SONICG: nitrification and denitrification, including the production and the reduction of N_2O (Figure 2.2).

SONICG simulates processes in homogeneous grassland areas at the field scale. Therefore, separate simulation runs have to be made when large horizontal differences occur within a grassland field, as in the case of grazed grassland (see Chapter 5). The model considers 30 soil layers of 2.5 cm, each with its own properties, but homogeneous properties are used within a layer. The lower border is assumed to be permeable for water but not for gases. Thus gases can only flow out at the bottom of the profile dissolved in water. Above the soil a gas layer of 2.5 cm high is present in the model. Transport of gases through this layer to the atmosphere is assumed to occur only by molecular diffusion, with the rates of diffusion depending on the gas concentration gradients between the atmosphere and the gas phase of the first soil layer.

The model SONICG consist of the following modules:

1. Hydrology
2. Soil temperature
3. Soil organic matter turnover
4. Plant uptake of nutrients
5. Nitrification
6. Denitrification
7. Gas transport
8. Transport of dissolved substances
9. Chemical equilibria

Figure 3.1 shows the flow chart of the model calculations for each timestep of one day. The flow chart shows the order in which the modules are used, where the information needed for each module comes from and where the output of each module goes to. After initialization of the model, input data are READ from the hydrology module as well as other necessary input data. In the following lines a short explanation of each of the modules is given.

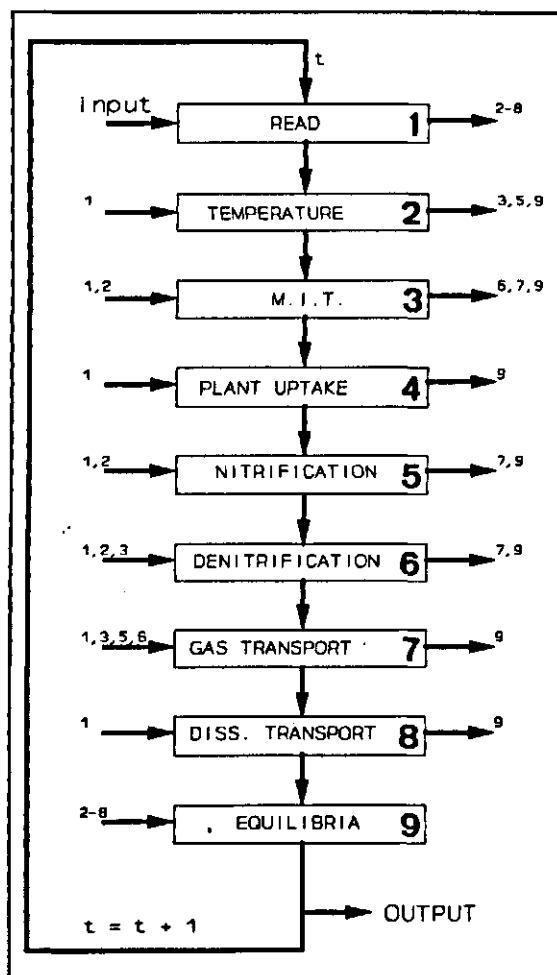


Figure 3.1. Flow chart of the simulation model SONICG, showing the order in which the models are used during each timestep. Input for READ includes data from a separate hydrology model, weather data, C and N input from grass residues into the soil and potential N uptake by the grass. For each module the left arrow indicates from which previous modules input data are used and the right arrow indicates to which following modules output data are going. The output of the chemical equilibria forms the basis for the next timestep of one day.

3.2 Hydrology

In this module the water balance is calculated daily for each soil layer. At day 1 (January 1) calculations start with a wet soil profile. Calculations start at layer 1. Rainfall and surface application of irrigation water, urine and slurry are water inputs for layer 1. Outputs are the physical evaporation of water and water taken up by plant roots and transpired by the grass. Each layer has a maximum and a minimum water holding capacity (WHC). Above the maximum WHC water freely flows to the next lower layer. At the minimum WHC no more water can be evaporated or taken up by plant roots and only inflow from neighbouring layers can occur. Water uptake by the grass is distributed over all the rooted layers, more or less proportional to root area and water availability in each layer. If water content of a layer has increased during a timestep, X% of the increase flows to the next lower layer. If water content has decreased during a timestep, an inflow of Y% of the decrease may occur from the next lower layer, if that layer is wetter. The values of X and Y depend on the physical characteristics of the soil (layer).

After calculations for layer 1, calculations for layer 2 follow and so on till the last layer. Gradients in water content between neighbouring layers are then slightly leveled of.

Physical water evaporation at the soil surface from layer 1 only (mm d⁻¹) is calculated from average daily temperature (T_{air}) and soil water-filled porosity (WFPS) according to equation 1:

$$\text{water evaporation} = 0.1 * T_{air} * [WFPS(1)]^2 \quad (1)$$

Water transpiration by the grass (mm d⁻¹) is calculated by using equation 2, which is a good approximation of the reference water transpiration for grassland according to Makkink (1975). To limit the total yearly water evaporation by the grass to a realistic value, a reduction factor (RF) is added that depends on the water supply capacity of the soil during the growing season.

$$\text{water transpiration} = RF * \{0.65 * \sin[2\pi(\text{day}-30)/365] + 0.16 * T_{air}\} \quad (2)$$

Water transpired by the grass is taken up from all the rooted layers. In case of sandy soil a maximum rooting depth of 45 cm is used. A constant amount of roots is simulated, with a total surface area of 50 m² per m² soil. Root distribution over the rooted layers is calculated according to equation 3:

$$\text{ROOTS}(i) = 50 * \frac{\sum_{i=1}^{i=18} [0.45/\text{depth}(i)]^{2.5}}{\sum [0.45/\text{depth}(i)]^{2.5}} \quad (3)$$

ROOTS(i) is the root surface area in layer i; depth(i) is the average distance of layer i from the soil surface.

The hydrology module uses daily weather data as input: rainfall, minimum and maximum temperature. A weighted daily average temperature T_{air} is calculated from minimum and maximum temperature and day length. In case of urine deposition 5 mm water addition is used as input. A small amount of extra rainfall is given near the end of the year to return to the same amount of water stored in the soil profile as at the start.

References

Makkink, G.F. & H.D.J. van Heemst, 1975. Simulation of the water balance of arable land and pastures. Pudoc, Wageningen, 79 p.

3.3 Soil temperature

Soil temperature is modeled dynamically, using a one-dimensional convection-dispersion equation. First the initial temperature profile on January 1 is calculated from equation 4:

$$T(i) = T_{avg} + \text{Amp} * \sin(2\pi(-121/365) - d(i)/2) * \exp\{-d(i)/2\} \quad (4)$$

T(i) is the temperature of layer i; T_{avg} is the mean annual temperature, taken to be 10 °C; Amp is the amplitude of the yearly temperature variation, also taken as 10 °C; d(i) is the depth of layer i in meters. It is assumed that the damping depth of the temperature wave is 2 meters for sandy soils.

The dynamic calculation of soil temperatures is based on equation 5:

$$\partial T/\partial t = (\lambda/C_w) * \partial^2 T/\partial x^2 \quad (5)$$

Here λC_w is the heat diffusion coefficient, λ is the heat conduction coefficient and C_w is the heat capacity of the soil. The value of λC_w is calculated each timestep for each soil segment. C_w is calculated from the summed heat capacities of water, organic matter and mineral parts in a segment. Specific C_w values of 1000, 600 and 480 kcal m⁻³ °C⁻¹ are used for water, organic matter and minerals, respectively (De Vries, 1963).

$\lambda(i)$ is calculated from the water content of segment i with equation 6:

$$\lambda(i) = 0.04 + 0.35 * [WFPS(i)]^2 / (0.065 + [WFPS(i)]^2) \quad (6)$$

Equation 6 was fitted to the curve of λ for sandy soil, given by Duin (1956). Given the upper and lower boundary conditions as the air temperature and the temperature of the last model segment at the last timestep, a new temperature profile can be calculated.

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3.4 Soil mineralization immobilization turnover (MIT)

Turnover of organic matter by soil microbes is simulated in this module, with inputs from (dead) grass roots, senesced grass litter and organic manure. The MIT module is a variant of a soil organic matter turnover model by Verberne et al. (1990). Figure 3.2 schematically shows the structure of this module, and indicates which products are formed upon degradation of a certain pool of organic matter. Each organic matter pool contains C as well as N with a fixed C:N ratio. Turnover is described in terms of C, and the resulting N turnover is calculated from the C:N ratios of substrates degraded and products formed.

When the products contain less N than the substrates, mineral N is liberated in the form of ammonium (N mineralization). When the products contain more N than the substrates, mineral N becomes immobilized (N immobilization).

All (external) inputs of organic matter to the soil are considered to consist of three fractions: rapidly Decomposable Plant Material (DPM), more slowly decomposable Structural Plant Material (SPM) and rather Resistant Plant Material (RPM). Distribution of inputs over these fractions is based on the overall (C/N)-ratio of the input (C/N). First, the fraction RPM-C is calculated using equation 4:

$$\text{fraction RPM-C} = 0.4 * (C/N)^{1.5} / [200 + (C/N)^{1.5}] \quad (4)$$

Next, the fractions SPM-C and DPM-C can be calculated, using the fixed C/N-ratio's of the three fractions. Figure 3.3 shows the distribution of organic matter input over DPM, RPM and SPM as a function of C/N.

The turnover of these input fractions by soil microbes is separated into turnover by protected (BIOP) and non-protected (BION) microbial biomass. BIOP can be regarded as microbes that are protected against predation by clay particles or because they live in small soil pores, that cannot be entered by their predators. The fraction of the microbial biomass that is protected, f_{prot} , is therefore described as a function of the fraction clay particles by equation 5:

$$f_{prot} = 0.8 * (\text{fraction particles} < 2\mu\text{m})^{0.5} \quad (5)$$

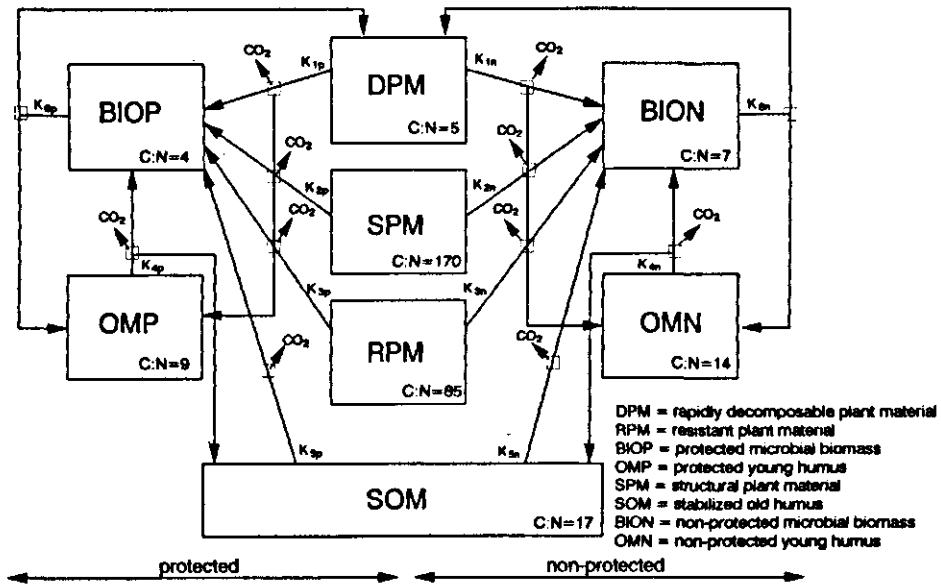


Figure 3.2. Detailed scheme of the MIT module on Mineralization Immobilization Turnover of organic matter in the soil

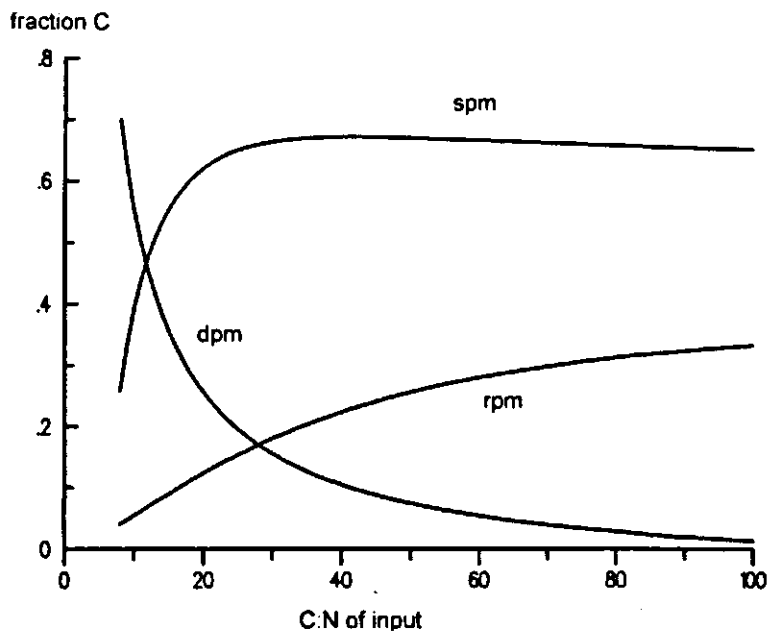


Figure 3.3. Distribution of organic matter input over different pools. SPM = structural plant material, mainly cellulose and hemicellulose; DPM = rapidly decomposable plant material, mainly proteins; RPM = resistant plant material, mainly lignin

The carbon degradation rates of DPM, SPM, and RPM by BIOP and by BION, respectively, are given by equations 6a and 6b:

$$d(C_i)/dt = k_{ip} * f(T)_i * f(WFPS) * C_i * fprot \tag{6a}$$

$$d(C_i)/dt = k_{in} * f(T)_i * f(WFPS) * C_i * (1 - fprot) \quad (6b)$$

were C_i stands for either DPM-C, SPM-C or RPM-C; k_{ip} and k_{in} are the maximum first-order rate constants (d^{-1}) for protected and non-protected fractions; $f(T)_i$ the temperature rate reduction functions and $f(WFPS)$ is the moisture rate reduction function. Thus, the degradation of DPM, SPM and RPM is attributed to BIOP and BION in the ratio $[k_{ip} * fprot] : [k_{in} * (1 - fprot)]$.

Table 3.1 specifies the proportions of products formed, including microbial biomass, the first-order rate constants used for each transformation, and the C/N ratios of the organic matter pools.

Microbial biomass decreases at a death rate that is taken proportional to the size of this pool. Note that the death rate constant of protected microbes is assumed to be less than that of unprotected microbes. This can be explained as a result of the protection against predation, for microbes that live in small pores. Dead microbial biomass C is added in equal amounts to the pools of DPM and OMP or OMN and part of the dead biomass N becomes liberated at the same time.

Table 3.1. Biodegradation reactions of the M.I.T. module (Figure 2), reaction rate constants (d^{-1}) and carbon to nitrogen ratios of organic matter pools.

Biodegradation equations for carbon	Reaction rate constants d^{-1} (*)	
	protected	non-protected
DPM-C → 0.60 CO ₂ -C + 0.35 BIO-C + 0.05 OM-C	$k_{1p} = 0.1$	$k_{1n} = 0.1$
SPM-C → 0.75 CO ₂ -C + 0.20 BIO-C + 0.05 OM-C	$k_{2p} = 0.02$	$k_{2n} = 0.02$
RPM-C → 0.40 CO ₂ -C + 0.05 BIO-C + 0.55 OM-C	$k_{3p} = 0.004$	$k_{3n} = 0.004$
OM-C → 0.80 CO ₂ -C + 0.10 BIO-C + 0.10 SOM-C	$k_{4p} = 0.004$	$k_{4n} = 0.02$
SOM-C → 0.98 CO ₂ -C + 0.02 BIO-C		$k_{5p} = 2 * e^{-5}$ $k_{5n} = 2 * e^{-5}$
BIO-C → 0.50 DPM-C + 0.50 OM-C		$k_{6p} = 0.01$ $k_{6n} = 0.05$

(*) under optimum conditions of temperature and moisture

Carbon to Nitrogen ratios of organic matter pools (C/N)

ORGANIC MATTER POOL	atom ratio	kg C (kg N) ⁻¹
DPM = rapidly Degradable Plant Material	C100 N16	5.4
SPM = Structural Plant Material	C100 N0.5	171.4
RPM = Resistant Plant Material	C100 N1	85.7
OMP = young soil Organic Matter, Protected	C100 N9	9.5
OMN = young soil Org.Matter, Non-protected	C100 N6	14.3
SOM = old Soil Organic Matter	C100 N5	17.1
BIOP= microbial BIOMass, Protected	C100 N20	4.3
BION= microbial BIOMass, Non-protected	C100 N12	7.1

The degradation rates of the protected and unprotected soil organic matter pools OMP, OMN and SOM, by BIOP and by BION, are described by equation 7:

$$d(C_i)/dt = k_i * f(T)_i * f(WFPS) * C_i \quad (7)$$

C_i is the carbon concentration in pool i (OMP, OMN and SOM); k_i , the maximum first-order rate constant, equals k_p for protected pools and k_{in} for non-protected pools.

In contrast to other models, the effect of soil temperature on turnover rates is different for different organic matter pools (Nicolardot et al., 1994).

Three temperature rate reduction functions $f(T)$ are used for materials of different stability (Figure 3.4):

$$f(T)_1 = 0.01095 * T^{1.5} / (1 + 3e-5 * T^3), \text{ for DPM};$$

$$f(T)_2 = 0.00376 * T^{1.75} / (1 + 6e-7 * T^4), \text{ for SPM, RPM, OMN, and OMP.}$$

$$f(T)_3 = 0.001235 * T^2 / (1 + 1e-8 * T^5), \text{ for SOM.}$$

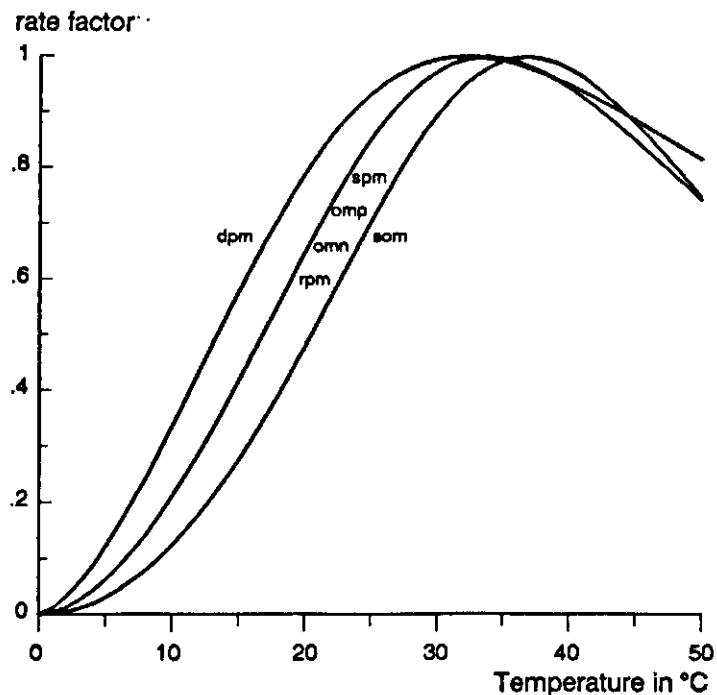


Figure 3.4. Functional dependence of organic matter degradation rates on temperature for different organic matter pools; abbreviations: see Figure 2.

As can be seen from Figure 3.4., the more stable an organic matter pool, the more its relative degradation rate is shifted to higher temperatures. This can be explained by the higher energy of activation necessary to start degradation of more stable organic compounds.

The effect of the fraction soil water-filled pore space (WFPS) on turnover rates is described by one function for all organic matter pools (Figure 3.5):

$$f(WFPS) = 6 * (P_w)^2 / [1 + 9 * (P_w)^4]$$

The function was derived from data of Doran et al. (1990). As shown in Figure 3.5, the biodegradation of organic matter increases with increasing availability of soil water, until oxygen supply becomes rate limiting at $WFPS = \sqrt{1/3}$. From that point onwards denitrification starts to participate in biodegradation and increases with the decreasing oxygen supply by gas diffusion. The exact form of $f(WFPS)$ will still depend on soil type, soil dry bulk density and the aerobic biological activity of the soil, together determining the maximum of WFPS above which oxygen starts to limit oxygen consuming processes (Doran et al., 1990; Neilson & Pepper, 1990).

Thus, $f(\text{WFPS})$ will also depend on soil temperature.

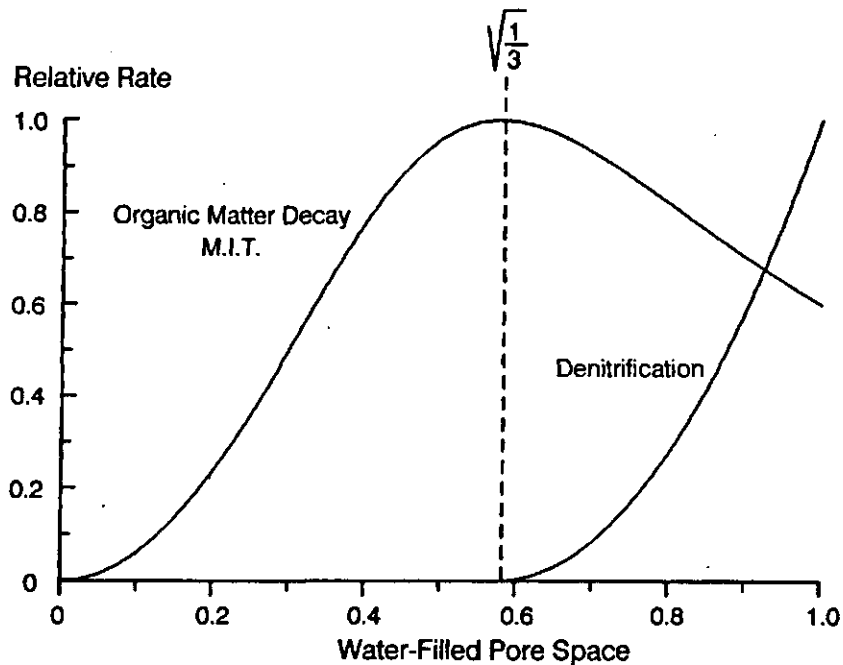


Figure 3.5. Functional dependence of organic matter decay and denitrification rates on soil water-filled pore space

The temperature and moisture rate reduction functions are used independently of each other, thus actual rates are calculated by multiplying the maximum rate constants with both functions.

Daily input data of grass residues were taken from a grass growth model of Verberne (1992), which uses the same daily weather data and the same fertilizer (and urine) N inputs as SONICG.

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3.5 Plant uptake of nutrients

This module describes the grass uptake of mineral N and the concomittant uptake of some macroelements (K+Na, Ca+Mg, ...), based on the given composition of the grass. Input data on potential daily N uptake by the grass were taken from a grass growth model of Verberne (1992), which uses the same daily weather data and fertilizer N inputs as SONICG.

Uptake of dissolved cations and anions by the grass roots is calculated based on a diffusive flux through a water film to the root surface. The average diffusion length is calculated from root surface area and water-filled porosity. The maximum nutrient supply by diffusive flux is limited to 10% of the total amount of a nutrient, present in the water phase plus the solid phase. Uptake of N as ammonium versus nitrate is based on the ratio of their concentrations in the soil solution.

For each rooted layer a potential daily N supply from the diffusive flux is calculated as well as the sum for all rooted layers. The maximum N uptake equals the potential daily uptake when the supply from the diffusive flux is (more than) sufficient. Then the same necessary fraction of the N supply is taken from all contributing layers. Else, the actual N uptake equals the calculated N supply. Nutrients are only taken up from layers where water is taken up. The maximum uptake of other nutrients than N is calculated on the basis of fixed ratios with actual N uptake. If the supply of other nutrients is insufficient to realize the fixed ratio with N uptake, only the actual supply is taken up.

References

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3.6 Nitrification

Nitrification is described, without taking into account the population development of the nitrifying microbes, as a function of soil temperature T , pH of the soil solution, the fraction water-filled pore space, and total (dissolved + adsorbed) ammonium concentration. Nitrate and N_2O were regarded as the only products of nitrification, since sufficient data on nitrite as an intermediate product were lacking. The description includes inhibition of nitrification, at high concentrations of ammonium-N (NH_4-N). The final nitrification function developed is shown by equation 8:

$$dNH_4/dt = f(T) * f(pH) * f(WPFS) * k_1 * [NH_4] / (k_2 + [NH_4]^2) \quad (8)$$

In equation 8, $[NH_4]$ represents the total amount of NH_4-N present in the soil water phase plus the solid phase (in mmol per kg moist soil). Experimental data of Mahli and McGill (1982) were used to develop equation 8. The 'constant' k_1 could as follows be fitted as a function the Cation Exchange Capacity (CEC, in meq per 100 g dry soil) of the soil: $k_1 = 12.3 - 2.9 * \log(CEC)$, for Canadian soils, but for Dutch soils we used: $k_1 = 20.0 - 3.0 * \log(CEC)$, because in Dutch soils larger nitrifier populations and nitrification rates were expected as a result of generally higher ammonium inputs. For k_2 a constant value of $195 \text{ (mmol } NH_4)^2 \text{ (kg wet soil)}^{-2}$ was fitted.

The temperature dependence of nitrification is described by equation 8a:

$$f(T) = 3.15e-3 * T^2 / (1 + 1.0e-7 * T^5) \quad (8a)$$

The optimum temperature for Dutch conditions is taken about $5^\circ C$ higher than for Canadian conditions of Mahli and McGill, because of an expected adaptation of nitrifiers to the different soil temperatures of both countries.

The pH-dependence of nitrification is given by a sigmoidal function, with half the maximum rate at pH 4.7, as given by equation 8b:

$$f(pH) = 1 / (1 + 5 * 10^4 * 10^{-pH}) \quad (8b)$$

Thus $f(\text{pH})$ reflects that nitrification is generally rapid at $\text{pH} > 6$ and slows down as a result of acidification caused by the nitrification process. Since soil solution pH values are calculated in SONICG by the chemical equilibria module, the model can account for pH effects on nitrification.

The dependence of nitrification on WFPS has the same optimum as organic matter decay, but, as oxygen is essential for nitrification, the rate goes to zero at $f(\text{WFPS}) = 1$, as shown in Figure 3.6. $f(\text{WFPS})$ is described by equation 8c:

$$f(\text{WFPS}) = \{\sin(\pi * \text{WFPS}^{1.2})\}^{1.75} \quad (8c)$$

As already mentioned by Mahli and McGill (1982), population development of the nitrifying microbes should be taken into account when a large amount of ammonium is added to the soil at one moment. Table 9 of their paper indeed showed increased average rates of nitrification in such cases. For grazed grassland, the area affected by urine gets such high amounts of ammonium that population development of nitrifiers should be modeled. A second module for nitrification, which includes the population development of ammonium-oxidizers and of nitrite-oxidizers has been made (Van Faassen, unpublished), but has not yet been included in SONICG.

Modeling the development of both nitrifying populations gives insight into conditions that may cause temporary accumulation of nitrite (Belser, 1979), as has been found in experiments where soil was incubated after addition of artificial urine (Monaghan & Barraclough, 1992). Thus, temporary accumulation of nitrite in the soil can be explained from conditions that cause a slower development of nitrite-oxidizing bacteria than of ammonium-oxidizing bacteria. Such inhibitory conditions will often be present in urine spots and should be taken into account when sufficient data are available.

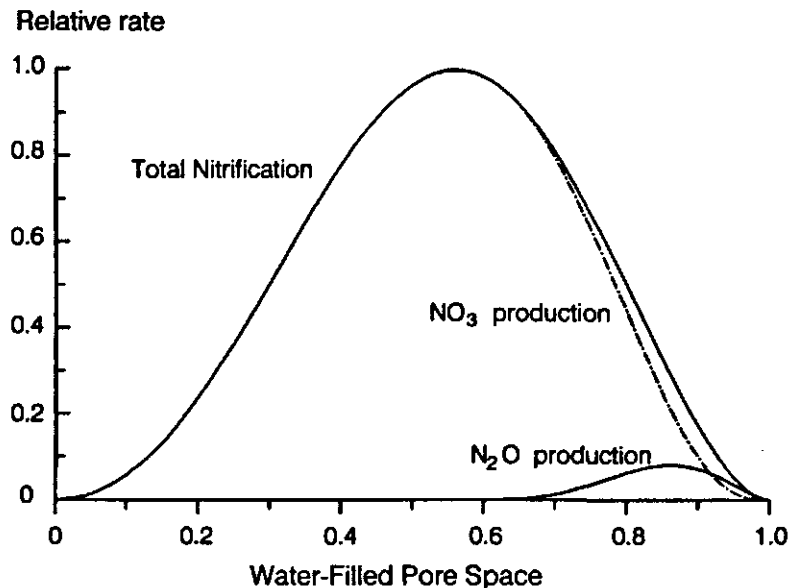


Figure 3.6. Functional dependence of total nitrification, nitrate production and N_2O production rates on soil water-filled pore space.

Production of N_2O during nitrification

A production of N_2O by "nitrifier-denitrification" has been shown to occur even at atmospheric oxygen pressure ($p\text{O}_2$), and to increase with decreasing $p\text{O}_2$ (Blackmer et al., 1980; Goreau et al.,

1980; Klemedtsson et al., 1988; Poth & Focht, 1985). On the field-scale pO_2 is a function of WFPS and to simulate the mentioned literature data at the field-scale we described the fraction of ammonium-N transformed into N_2O in layer i , $\alpha(i)$, by equation 9:

$$\alpha(i) = 0.005 + 0.4 * [(WFPS(i) - 0.6) / 0.4]^3 \quad (9)$$

Equation 9 is used when $WFPS(i) > 0.6$ and when $WFPS(i) < 0.6$, $\alpha(i)$ is given a constant value of 0.005. The relative production rates of N_2O -N and nitrate-N by nitrification as a function of WFPS are shown in Figure 3.6.

As mentioned for aerobic organic matter degradation, the exact form of $f(WFPS)$ for nitrification and N_2O production will still depend on a number of variables as soil type, soil dry bulk density and the rate of oxygen consuming processes. In case of a high input of NH_4 -N, the oxygen need for high nitrification rates may contribute considerably to total oxygen consumption of the soil.

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3.7 Denitrification

Starting point in modeling denitrification is the assumption that the aerobic biodegradation of organic matter is partly taken over by denitrification with decreasing pO_2 in soil. Thus, at the field-scale both soil respiration and denitrification can be described as functions of WFPS (Figure 3.5). As shown in Figure 2.2, N_2O is taken as the only and obligatory intermediate product in the denitrification of nitrate to N_2 . When nitrate is fully reduced to N_2 , the nitrate disappearance rate can be described as a fraction of organic carbon degradation rate, dC/dt , as shown in equation 10, derived from experimental data of Mahli et al. (1990):

$$-5 * d(NO_3^-)/dt = 10 * d(N_2)/dt = NO_3^- / (k_{d1} + NO_3^-) * f(WFPS) * 4 * dC/dt \quad (10)$$

Thus denitrification follows Michaelis-Menten kinetics, with k_{d1} the amount of nitrate at which half the maximum rate is reached at optimal water content, when $f(WFPS) = 1$. The value of dC/dt is calculated in the MIT module.

The dependence of denitrification rates on WFPS, above optimum WFPS for aerobic degradation, as used in SONICG is shown in Figure 3.5. The form of $f(\text{WFPS})$ is related to the decrease of the oxygen supply rate by gas diffusion, which is a function of gas-filled pore space, GFPS ($= 1 - \text{WFPS}$). As already mentioned for aerobic degradation, the exact form of $f(\text{WFPS})$ for denitrification can also depend on soil type and on soil water hysteresis effects (Sexstone et al., 1988; Groffman and Tiedje, 1988).

The use of nitrate and of N_2O , as electron-acceptors competing with O_2 , is calculated on the basis of electronequivalents (Cho, 1982). The factors 5, 10 and 4 in equation 10 are conversion factors from moles to electron-equivalents. When N_2O as well as N_2 are produced the left-hand side of equation 10 becomes:

$$-4 \cdot d(\text{NO}_3)/dt + 2 \cdot d(\text{N}_2)/dt \quad (10a)$$

The maximum amount of nitrate that can be denitrified per day is limited in the model to 25% of the amount present.

The ratio of N_2O production to N_2 production

The ratio $\text{N}_2\text{O}/\text{N}_2$ depends on the fractions of electrons accepted by nitrate and by N_2O , respectively, and is known to increase with decreasing pH. The production rates of N_2O from nitrate and of N_2 from N_2O , in terms of electron equivalents, can be described by the first-order rate equations 11a and 11b:

$$r_1 = -d(\text{NO}_3)/dt = k_a \cdot [\text{NO}_3] \cdot 4 \quad (11a)$$

$$r_2 = d(\text{N}_2)/dt = k_b \cdot f(\text{pH}) \cdot [\text{N}_2\text{O}] \cdot 2 \quad (11b)$$

Thus, the reduction rate of nitrate is assumed to be independent of pH, whereas the reduction rate of N_2O is known to depend on pH (Blackmer & Bremner, 1978). The fraction of electrons going to N_2O , $\text{frel}(\text{N}_2\text{O})$, is equal to $r_2/(r_2+r_1)$ and by substituting r_1 and r_2 from equations 11a and 11b we get:

$$\text{frel}(\text{N}_2\text{O}) = f(\text{pH}) \cdot [\text{N}_2\text{O}] / (f(\text{pH}) \cdot [\text{N}_2\text{O}] + (k_a/k_b) \cdot 2 \cdot [\text{NO}_3]) \quad (11c)$$

When the total denitrification rate is known from equation 10, multiplication with $\text{frel}(\text{N}_2\text{O})$ from equation 11c gives the amount of N_2O that is reduced to N_2 , after conversion from electron equivalents to moles. Subtraction of N_2O reduction from total denitrification gives nitrate reduced to N_2O .

From data of Blackmer & Bremner (1978) we derived that $f(\text{pH})$ can be described by equation 11a:

$$f(\text{pH}) = 10^{(\text{pH} - 6.5)/3} \quad (11d)$$

N_2O in the gas phase is considered to be as available as dissolved N_2O to accept electrons, because the exchange of N_2O between gas and water phase is assumed to be very rapid. Thus, the total amount of N_2O in a layer is used to calculate the N_2O concentration in equation 11c.

An alternative way is to describe the ratio of the firstorder rate constants for N_2O and nitrate reduction, respectively, as can be derived from equations 11a and 11b and is shown in equation 11d:

$$2 \cdot r_2 / [\text{N}_2\text{O}] = (k_a/k_b) \cdot f(\text{pH}) \cdot r_1 / [\text{NO}_3] \quad (11e)$$

Again, the absolute amounts of nitrate and of N_2O reduced during denitrification can be calculated from equations 10 and 11e.

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3.8 Gas transport

Gas diffusion in the soil is calculated with a one-dimensional, fully implicit transport model using zero- and first-order reaction terms. Equilibrium with the water phase is simulated with Henry constants, which are used as first-order withdrawal terms, whereas the amount in solution at $t-1$ is a zero-order input term. Equation 12 generally describes the change in concentration of a gas during a timestep for each soil layer:

$$\partial C_g / \partial t = D_{eff} * \partial^2 C_g / \partial z^2 - V_{adv} * \partial C_g / \partial z + R_o - R_1 * C_g \quad (12)$$

The right-hand side of equation 12 consists of a diffusion term, an advection term, a zero-order production term and a first-order withdrawal term. Gas transport is calculated for the gases CO_2 , NH_3 and N_2O . For CO_2 , the production term dC/dt from the decay of organic matter, as calculated by the MIT module, is included as a zero-order input into each layer. For N_2O , the production from nitrification plus denitrification is included as zero-order input to each layer, whereas the consumption of N_2O by denitrification to N_2 is included as a first-order withdrawal from each layer.

The effective gas diffusion coefficient, D_{eff} ($m^2 d^{-1}$), for each interface in the soil column is calculated from equation 13:

$$D_{eff} = a * D_{air} * (GFPS_{avg})^b \quad (13)$$

where D_{air} is the binary diffusion coefficient for the gas in free air and $GFPS_{avg}$ is the average gas-filled porosity of the two layers that border the interface. The constants a and b depend on the soil type (Washington et al., 1994; Bruckler et al., 1989; Campbell, 1985).

Bakker et al. (1987) summarize a lot of gas diffusion measurements on different Dutch soils. Variations in the total porosity of a soil can occur as a result of compaction. The effect of total porosity is included in constant a . The constant b reflects the continuity of pores. Blockage of pores by water has been shown to depend on the way of moistening. Ball (1981) found higher D_{eff} values in a silt loam at pF 3.7 when soil of pF 4 was moistened than when saturated soil was dried to pF 3.7. This hysteresis effect can be important in denitrification.

Often, pores in the soil are not homogeneously distributed and pore systems of different order may exist together. This can be the case in aggregated soils, where large inter-aggregate pores and small intra-aggregate pores can be present. The same type of differences can be found in

rooted versus unrooted soils or between soils with and without worm holes. Soils that form cracks upon drying may allow gas transport already at low overall GFPS.

In SONICG equation 13 was used for D_{eff} of a sandy soil, taking $a = 1$ and $b = 2$, as a best fit to measurements of Bruckler et al. (1989). The soil column is assumed to be closed for gas transport at the bottom. However, gases dissolved in water can leave the soil column at the bottom with drainwater. The model includes a gas layer of 2.5 cm on top of the soil column, which is used only as a "buffer" for gas transport between the soil and the atmosphere. This gas layer more or less simulates the gas layer in the field situation, where the horizontal component of the windspeed is very low. Thus, effects of windspeed and of atmospheric pressure variations are not considered.

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3.9 Transport of dissolved substances

Water flow between the segments of the schematization is provided by the hydrological model. Since the dissolved concentrations of all components at $t-1$ are known (from the last performed equilibrium calculation), the mass transported between segments i and $i+1$ is, when the flow is from segment i to segment $i+1$ (downward flow):

$$M_{\text{trans}(i,i+1)} = \text{flow}_{i,i+1} * C_{i,t-1} \quad (\text{explicit transport})$$

When the flow is upwards, then

$$M_{\text{trans}(i+1,i)} = \text{flow}_{i+1,i} * C_{i+1,t-1}$$

However, this approach is only valid when the flow in the timestep is small compared to the volume of water in the source segment. This is generally true for upward flow, but not for downward flow. When this is not the case, then an implicit transport scheme is adopted:

$$M_{\text{trans}(i,i+1)} = \text{flow}_{i,i+1} * C_{i,t} \quad (\text{implicit transport})$$

$C_{i,t}$ is calculated assuming conservative mixing behavior for all dissolved components with a numerical onedimensional transport model.

For each segment the mass balance for each component is (downward flow):

$$M_{i,t} = M_{i,t-1} + M_{\text{trans}(i-1,i)} - M_{\text{trans}(i,i+1)}$$

Since the transport scheme is numerical, numerical dispersion is introduced. The size of the

numerical dispersion depends on the segment size, and the flow rate. The calculation assumes the numerical dispersion to account for diffusion/dispersion in the soil solution, so no diffusion/dispersion term is included in the transport equation.

3.10 Chemical equilibria

Each layer of the physical schematization is considered to be an equilibrium system, where cation exchange, complexation in solution, precipitation/dissolution of calcite and the exchange of gases between the soil porewater and the soil atmosphere is in chemical equilibrium each timestep. The chemical equilibrium system distinguishes components (building blocks of matter), species (the existing substances) and phases (chemically homogeneous, physically distinguishable parts of an equilibrium system). The components of the equilibrium system which are used in SONICG are: H₂O, H⁺, Ca⁺⁺, K⁺, NH₄⁺, NO₃⁻, N₂O, CO₃⁻, Cl⁻, CEC (cation exchange capacity) and IG (inert gas, i.e. all gasses except the explicitly modeled gasses: CO₂, NH₃ and N₂O). Species in the water phase are: H₂O, H⁺, OH⁻, NH₃, NH₄⁺, N₂O, CO₂, Cl⁻, HCO₃⁻, CO₃⁻, NO₃⁻, K⁺, Ca⁺⁺, CaHCO₃⁺, CaCO₃⁰.

Cation exchange is calculated with 4 cations: H⁺, K⁺, Ca⁺⁺ and NH₄⁺. Cation exchange is modeled according to the so-called Gapon convention. For the reaction of replacing sorbed calcium with potassium the equilibrium relation is:



The Gapon exchange constant for this reaction is taken as 5.7 l⁵.mol⁻⁵. The same reaction with ammonium instead of potassium has an exchange constant of 2.1 l⁵.mol⁻⁵. For H⁺ the constant is 3000 l⁵.mol⁻⁵.

The solubility product of calcium carbonate is taken as 10^{-8.05} mol².l⁻² (T = 25 °C, 1 atm, at ionic strength I = 0), which makes calcium carbonate more soluble than the theoretical solubility (K_{sp} = 10^{-8.35}). It is our experience that calculations with this increased solubility give more realistic results.

The Henry equilibrium constants used for the gasses are: for CO₂: K_H = 10^{-1.48} l.mol⁻¹, for NH₃: K_H = 10^{1.76} l.mol⁻¹, and for N₂O: K_H = 10^{-1.615} l.mol⁻¹.

Temperature corrections for equilibrium constants are performed using the van 't Hoff relation:

$$\ln K_T - \ln K_0 = - (1/T - 1/T_0) * \Delta H/R$$

Here T = temperature in °K, T₀ = 298.15 °K, ΔH = the enthalpy of the reaction (J.mol⁻¹) and R the universal gas constant (8.3144 J. °K⁻¹.mol⁻¹).

Ionic strength effects are calculated with the extended Debye-Hückel equation:

$$\log \gamma = - A * z^2 * \sqrt{I} / (1 + B * \hat{a} * \sqrt{I})$$

where γ is the activity coefficient of an ionic species, z is the charge of that ionic species, I is the ionic strength of the solution, A and B are temperature-dependent constants for water (at 25 °C, A = 0.509, B = 0.328), and \hat{a} is an ion-specific constant, describing the effective hydrated ionic radius in Ångstrom (e.g. Ca⁺⁺ = 6). Activities a_i of chemical species are used in all the equilibrium calculations, with a_i = γ_i * C_i.

3.11 Some first simulation results from SONICG

Input of the model

Daily C and N inputs with grass residues as well as potential daily N uptake by the grass have been taken from the model for mown grassland of Verberne (see Chapter 4). The simulations have been run for a sandy soil and the same daily weather conditions ("Wageningen, 1989") were used as in the model of Verberne.

Two preliminary simulation runs

Since the programming of SONICG was completed only recently (November '94), we were not yet able to test the model extensively. A first impression that the model functioned rather well was obtained from two simulations that are discussed in the following.

One simulation run was made for mown grassland, fertilized at a rate of 480 kg N per ha. A second simulation run was made where, in addition to mineral N applications, urine N was applied to mown grassland on day 140 at a rate of 420 kg per ha. The second run should simulate a urine spot in grazed grassland. However, effects of grazing on grass development (Chapter 5) were not yet included. These simulation runs were used to test the overall performance of SONICG and more specifically some of the modules, as discussed under model output.

Output of the model

The model simulation output has two possibilities:

- some parameters of interest can be followed on a daily basis on the PC screen during the simulation run for a year. Thus, the variation of some key parameters is made visible;
- pool sizes can be given at the end of a simulation run, or even on a daily basis, and yearly flows can be calculated as well as balances for water, carbon, nitrogen and other elements.

The following parameters have been selected for dynamic representation on the PC screen:

- pH of the soil solution for each layer. This parameter is a sensitive element for the performance of the soil chemistry module. The limited pH-buffering capacity of the soil solution led to pH-oscillations when urine spots were simulated. The emission of CO₂ led to rapid increase of pH, which promoted rapid NH₃ emission, the latter causing a rapid pH decrease. To limit these oscillations, the percentage of a gas that could leave the water phase during a timestep was limited to 60%;
- water-filled soil porosity for each layer was chosen because it affects the relative activities of aerobic degradation, nitrification and denitrification via the rate-reduction functions f(WFPS). The maximum water holding capacity of the upper three soil layers had to be decreased to limit denitrification for a sandy soil to realistic values;
- nitrate concentration in the soil solution for each layer was chosen because it is a prerequisite for N₂O production via denitrification;
- the total amount of N₂O for each layer was chosen because it forms the driving force for the emission of N₂O.

The day-to-day variation of these four parameters for each soil layer gives a rapid and informative view of "what is going on" during a simulation year.

Emission of N₂O

The main parameter of interest, the daily emission rate of N₂O from the soil to the atmosphere is shown on the screen in a fifth graph. In this case the daily values are plotted as a continuous graph that develops on the screen during the simulation. Thus, at the end of a simulation run

this graph on the screen shows the pattern of N_2O emission during the year. Figure 3.7 gives an example of two simulation runs for grassland without and with application of urine at day 140. As shown in Figure 3.7, a much larger N_2O emission results from urine treated grassland than from the control grassland with mineral N fertilizer only.

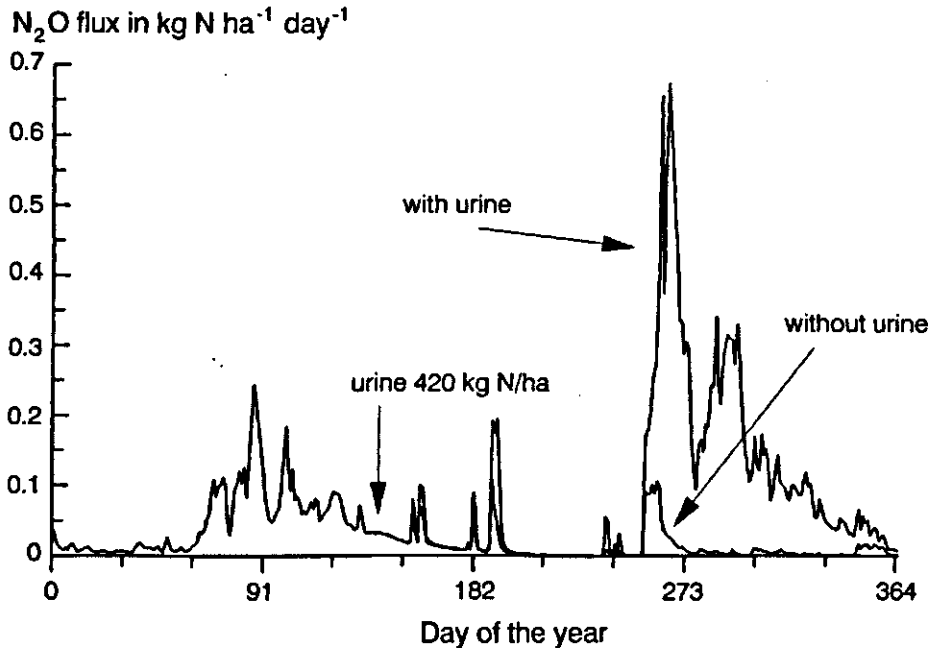


Figure 3.7. Daily fluxes of N_2O -N from grassland unaffected by urine and from urine spots, as simulated by SONICG for a sandy soil and weather conditions of Wageningen 1989. Urine was applied on day 140, at a dosage rate corresponding to 420 kg of N per ha of urine-affected area.

Figure 3.7 shows that the large peaks in N_2O emission appeared more than 100 days after urine application. This can be explained from the fact that complete nitrification of NH_4 -N from urine takes considerable time. In autumn high nitrate concentrations will thus be present in the soil, leading to N_2O production when rainfall makes soil conditions conducive to denitrification. The smaller peaks in N_2O emission in spring are related to the application of mineral fertilizer N, and are partly the result of N_2O production by nitrification. The model may calculate how much nitrification and denitrification each contributed to the production of N_2O . The model may also calculate how much of this N_2O is reduced to N_2 and how much is leached with water at the bottom of the modeled profile.

It must be stressed that the result shown in Figure 3.7 is just a first preliminary result of SONICG, without possible adjustments of model parameters. However, the characteristic peaks that were found in the field are also shown in these first results.

The model can even produce a screen graph of both N_2O and NH_3 emission. The emission of CO_2 can also be presented on the screen, but because of the different scale cannot be combined with the graphs of the N emissions.

3.12 Evaluation, validation and further development of SONICG

The SONICG model will be used to simulate the emission of N_2O from the grassland locations where extensive measurements have been made by Velthof (NOP project 852073). By using the local input data and weather conditions gathered by Velthof, several simulation outputs of

SONICG will be compared with the actual values, for instance of N₂O emission rates, soil water contents and N uptake by the grass. The evaluation, validation and further development of SONICG will be made as part of the DLO Research Programme on Climate Change 1995-1999.

4. Simulation of carbon and nitrogen turnover in mown grassland

4.1 Introduction

A mechanistic simulation model for carbon and nitrogen turnover in mown grassland, developed by Verberne (1992), was run for three different years and for two soil types, a sandy soil and a clay soil. The model made use of daily weather data from a weather station near Wageningen for three different years: a dry year (1982), an average year (1989) and a wet year (1965). The results of these six simulation runs showed that conditions favouring good grass production led to low N losses to the environment, whereas conditions unfavourable to or limiting grass production led to large accumulations of mineral N in the soil, with the risk of large N losses by nitrate leaching and/or denitrification. However, the model considered nitrate leaching as the only nitrogen loss to the environment and showed it to vary potentially from 0-250 kg ha⁻¹, depending on the interaction of weather conditions, grass development and C and N turnover in the system.

4.2 Results and discussion

Yearly N balances and N flows

Total N input to grassland (Table 4.1) differed mainly because of differences in fertilizer application, based on the number of grass harvests. Only two or three harvests were possible in the dry year 1982, compared to eight harvests for both soils in the wet year 1965 (Table 4.2).

The availability of water was a main limiting factor for grass production in these simulations, especially for the clay soil. The modeled soil profiles had a storage/water supply capacity of about 120 mm for the clay soil and 220 mm for the sandy soil.

Except for clay soil in 1982, N uptake by the grass was (much) higher than the total N input (Table 4.3). This showed that under favourable conditions for grass growth this crop could represent a large sink for mineral N. Even the amount of N removed with harvested grass was higher than the total N input in two cases (Table 4.2).

Leaching of nitrate below 100 cm (Table 4.2) was relatively low at the end of each year, because the main part of nitrate leaching should occur in the period January till May of the next year.

The potential for further N losses, either by leaching or by denitrification, was indicated by the increased storage of mineral N in the soil profile at the end of 1982 for both soils and at the end of 1989 for the clay soil (Table 4.2). Unfavorable conditions for grass growth, especially prolonged drought periods, increased senescence of the grass and the recycling of dead grass litter in 1982 for clay soil and in 1982 for both soils (Table 4.3).

Net mineralization of N from soil organic matter pools (microbial biomass and humus) was always larger in the clay soil than in the sandy soil (Table 4.3). This can be explained from a much higher amount of soil organic nitrogen in the clay soil than in the sandy soil: about 7000 and 4000 kg ha⁻¹, respectively. The highest net N mineralization for the clay soil in 1989 might be explained by the higher average temperature and by the larger input of grass residues, the latter leading to more (N mineralization from) microbial biomass and young humus (Table 4.3).

The first step in turnover of grass litter in the soil always caused some net immobilization of mineral N in the clay soil, but only once (1989) in the sandy soil (Table 4.3). This difference between soil types had to do with the lower average C/N ratio of the soil microbial biomass, growing on grass litter, in the clay soil than in the sandy soil. A difference in C/N ratio of grass residues also played some role: under unfavorable conditions for grass growth less N from senescent litter could be reused by growing plant parts and then litter with a lower C/N ratio was recycled into the soil, and increased the chance of net N mineralization.

Table 4.1. Rainfall (RAIN), average daily air temperature (TEMP) and N input (kg ha⁻¹) with mineral fertilizer (FERT-N) and with rainfall (RAIN-N).

SOIL TYPE	SAND	SAND	SAND	CLAY	CLAY	CLAY
YEAR	1982	1989	1965	1982	1989	1965
RAIN (mm)	566	697	989	566	697	989
TEMP (°C)	9.7	10.3	8.6	9.7	10.3	8.6
N-INPUT						
FERT-N	400	480	480	320	400	480
RAIN-N	28	35	49	28	35	49
TOTAL-N	428	515	529	348	435	529

Table 4.2. N output with grass harvests (HARV-N) and nitrate leaching (LEACH-N), and changes in storage of N in grass (GRASS-N), N in soil organic matter (SOILORGN) and in soil mineral N (SOILNMIN) in (kg ha⁻¹).

HARVESTS	3	6	8	2	4	8
HARV-N	261	487	584	134	339	602
LEACH-N	20	7	30	25	20	12
GRASS-N	+32	+34	-1	+26	+19	0
SOILORGN	+24	-13	-84	-70	-39	-91
SOILNMIN	+92	-5	-4	+233	+96	+1
TOTAL-N	428	515	529	348	435	529

Table 4.3. Internal N flows (kg ha^{-1}): N uptake by the grass (N-UPTAKE), N recycled in the form of above-ground litter (aLITT-N), below-ground litter (bLITT-N), net mineralization from soil organic matter (MINER-N), and nett immobilization as a result of crop residu turnover (IMMOB-N).

N-UPTAKE	477	713	707	298	587	731
aLITT-N	170	180	114	121	216	120
bLITT-N	15	13	9	17	14	9
MINER-N	160	206	236	236	291	263
IMMOB-N	0	0	28	29	22	42

Distribution of mineral N fertilizer applications in the simulations: 120 - 100 - 100 - (80) - (80) kg ha^{-1} . The first application was when the sum of average daily temperature was more than 280 °C. The other applications were after each harvest of about 2000 $\text{kg grass dry matter per ha}$.

Nitrogen turnover in mown grassland: summary of results from six simulation runs with the model FSE-GRASS-SOM-WATER (Verberne, 1992)

Dynamics of carbon and nitrogen within a year (some examples)

The conditions for grass growth were very favorable during the wet year 1965, as shown by the almost linear increase of the cumulative amount of carbon assimilated by the grass (Figure 4.1, top). Very unfavorable growth conditions however, around week 30 in the dry year 1982, almost stopped gross C assimilation by the grass and resulted in a very limited grass production (Figure 4.1, bottom). The amounts of assimilated C lost by respiration and by senescence, the net amount of C resulting in the grass, the amount of grass-C harvested and the amount of grass-C present in the standing crop are also indicated in Figures 4.1a and 4.1b.

The (cumulative) N uptake by the grass on the clay soil in 1965 and 1982, respectively, showed the same trends as the (cumulative) gross C-assimilation (Figures 4.2, top and 4.2, bottom compared to 4.1, top and 4.1, bottom). Thus, under favorable conditions for grass growth, as in 1965, almost all the available mineral N is taken up by the grass, leaving very low concentrations of mineral N in the soil from week 35 onwards. Grass growth being impaired by drought in 1982, on the other hand, led to very limited N uptake and mineral N concentrations in soil increased almost continuously. Such high concentrations of soil mineral N, in spite of limited N fertilization in 1982, make large N losses very likely when later on conditions become favorable for denitrification or leaching of nitrate.

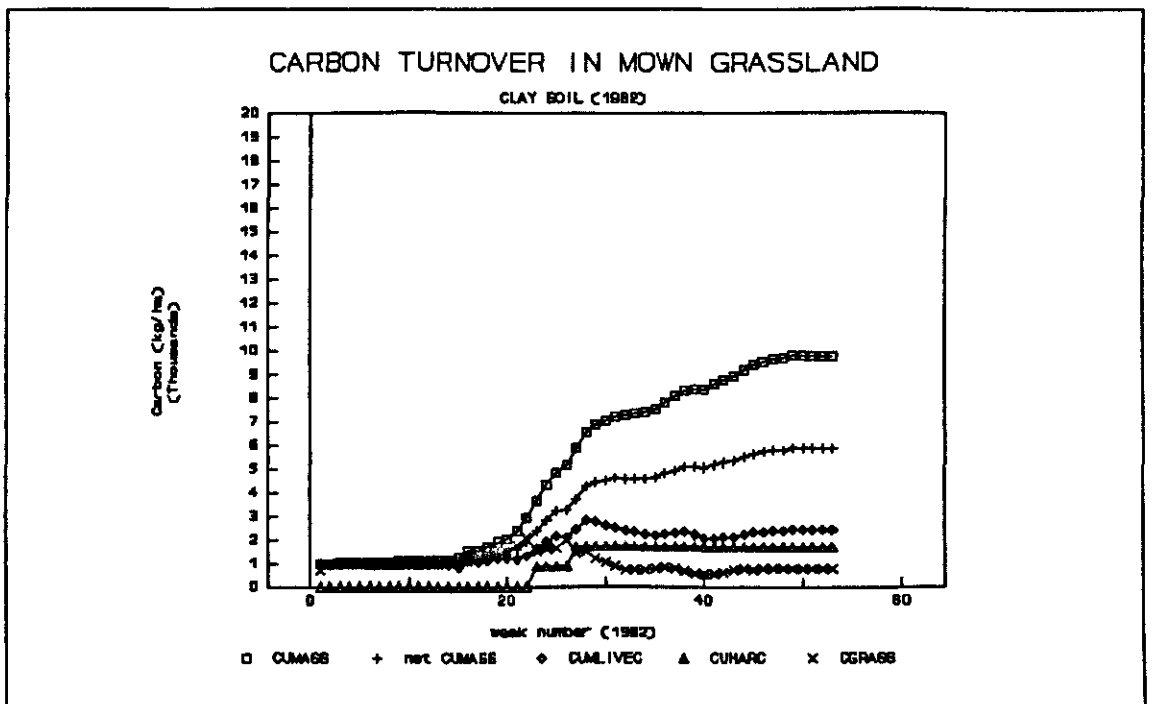
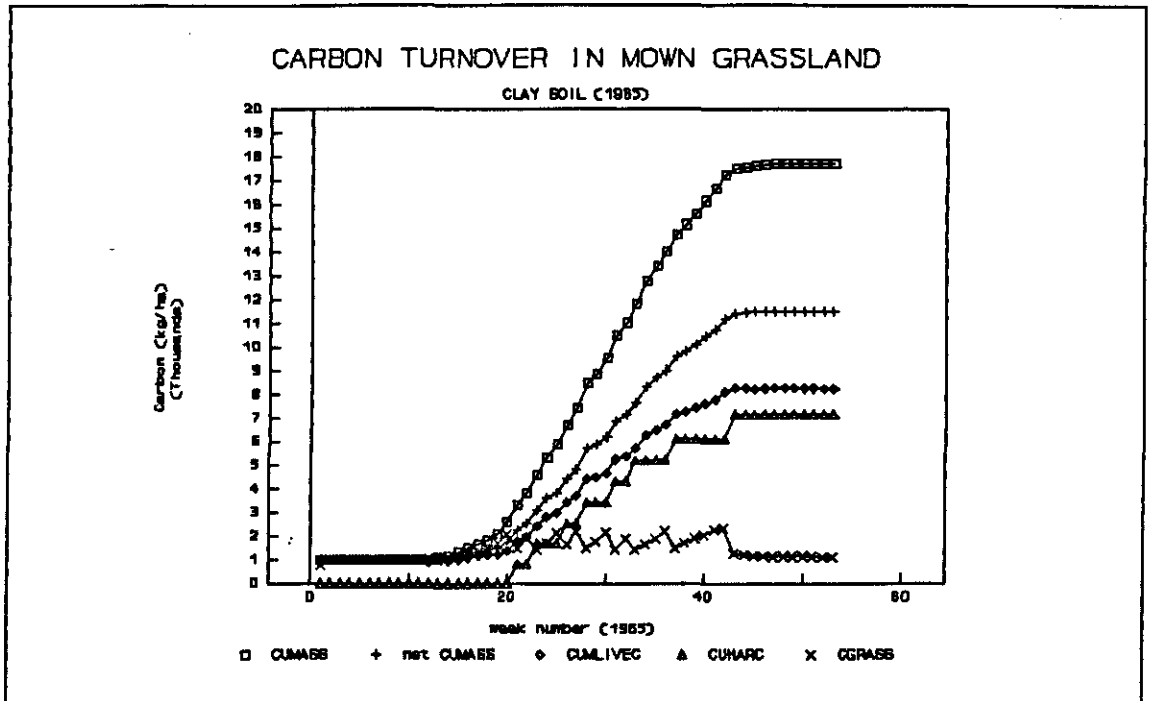


Figure 4.1. Simulated carbon turnover by grass in mown grassland, in a favorable (1965, top) and in an unfavorable year (1982, bottom) for grass production.

CUMASS = grass-C (at t = 0) + cumulative gross C assimilation
net CUMASS = CUMASS - (respired C)
CUMLIVEC = net CUMASS - (grass-C recycled as dead litter)
CUHARC = cumulative harvested grass-C
CGRASS = carbon in the standing grass crop

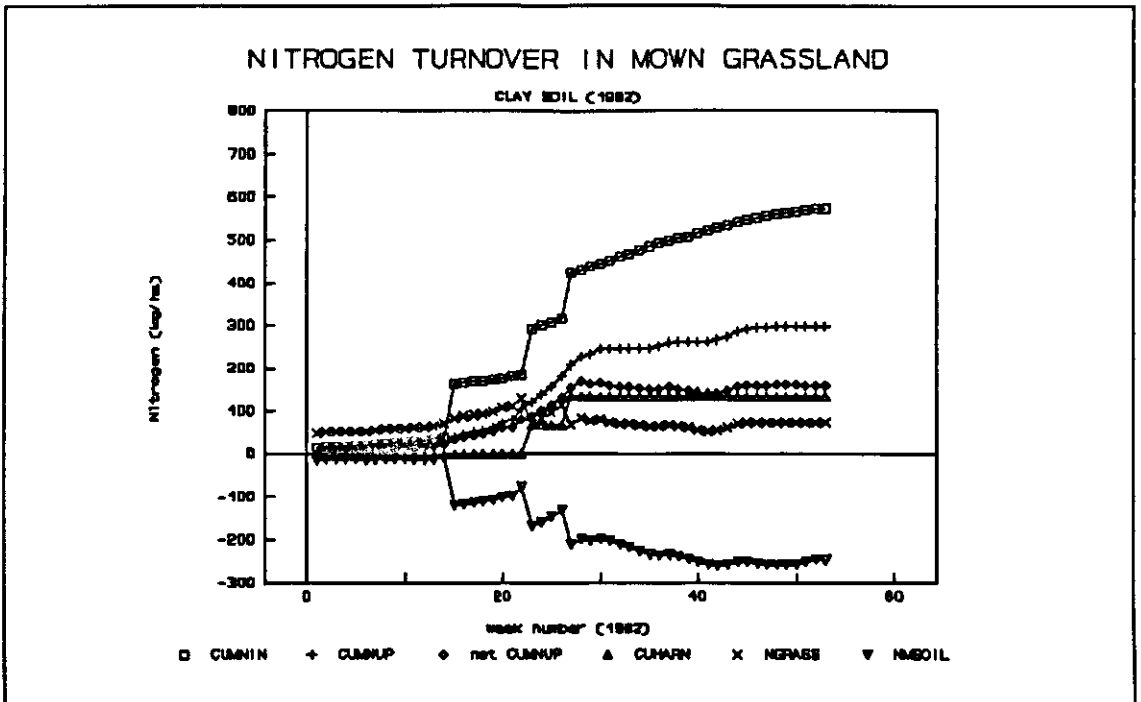
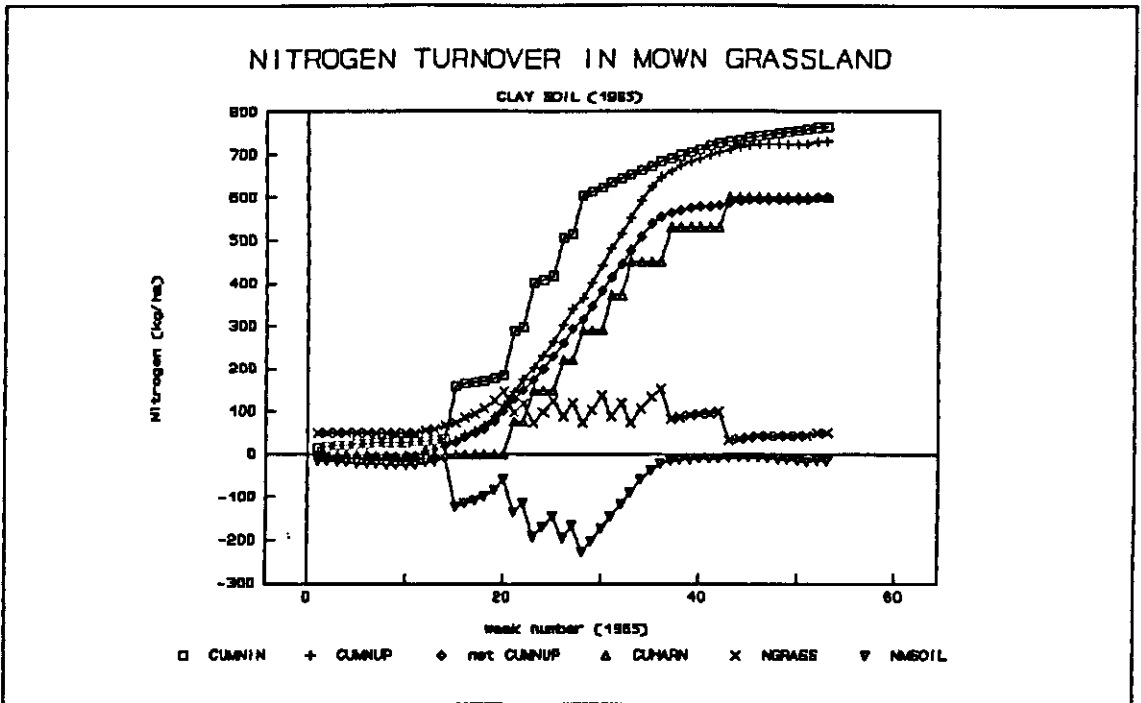


Figure 4.2. Simulated nitrogen turnover by grass in mown grassland, in a favorable (1965, top) and an unfavorable year (1982, bottom) for grass production.

- CUMNIN = mineral N (at t = 0) + fertilizer N + net N mineralization + N deposition with rainfall;
- CUMNUP = cumulative N uptake by the grass;
- net CUMNUP = CUMNUP - (grass-N recycled as dead litter);
- CUHARN = cumulative grass-N removed by mowing;
- NGRASS = N in the standing grass crop;
- NMSOIL = mineral N in the 0-100 cm layer of the soil.

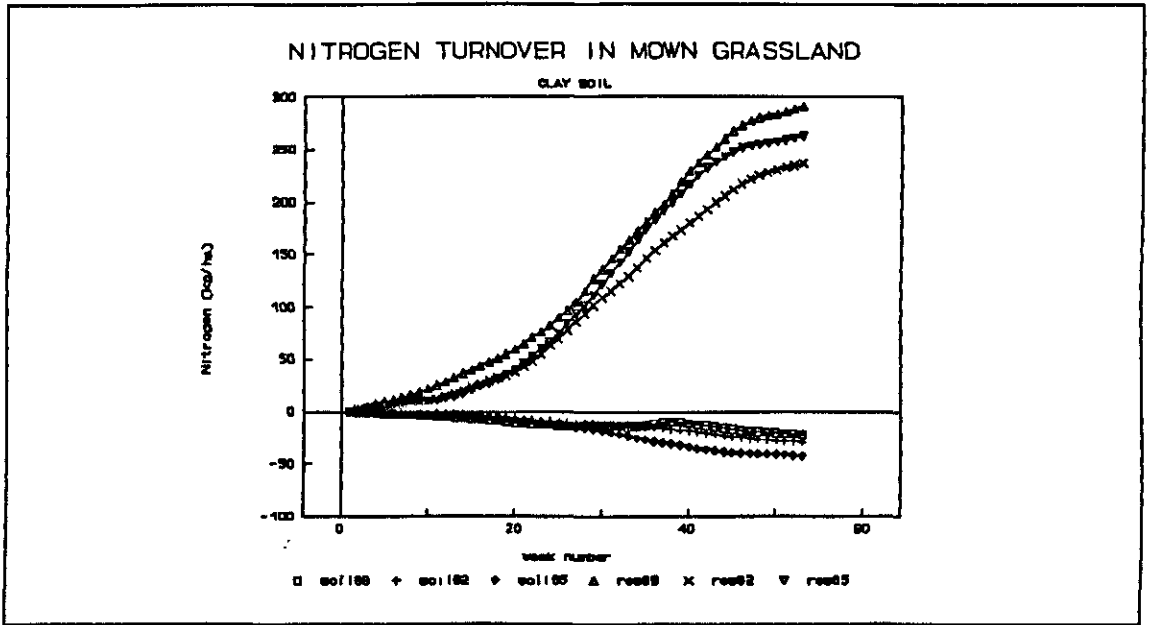


Figure 4.3. Simulated (cumulative) net N mineralization from soil organic matter and from grass residues, in three years with quite different weather conditions: 1989 ('average'), 1982('dry') and 1965('wet'); negative values indicate net N immobilization.

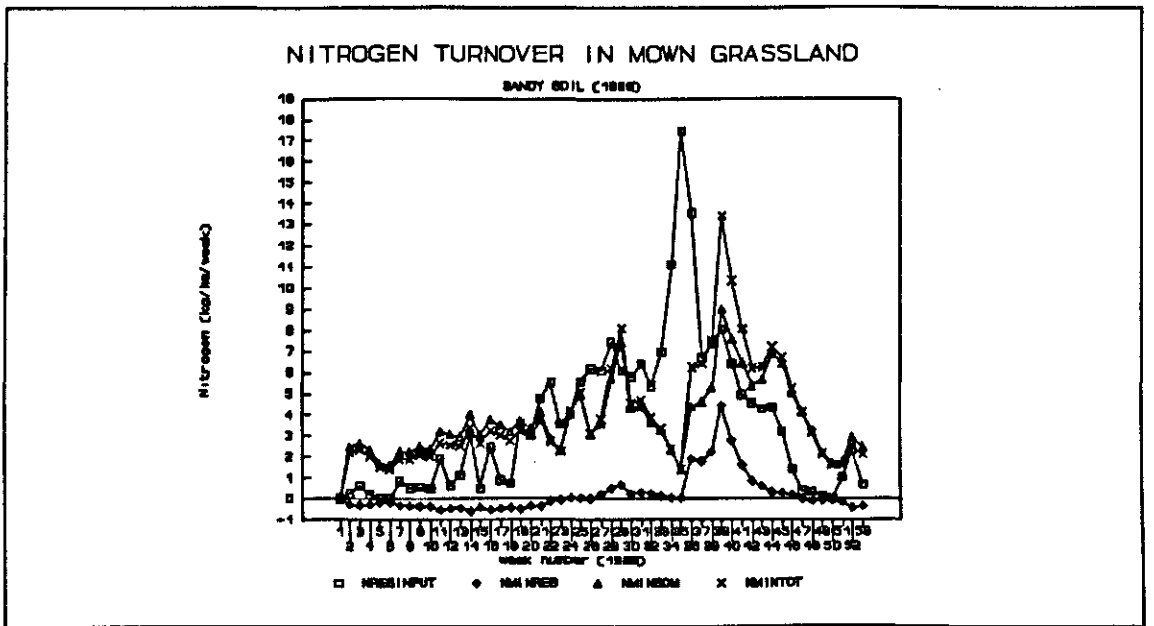


Figure 4.4. Simulated rates of N turnover in a sandy grassland soil: input of N from grass residues (NRESINPUT), N mineralization from grass residues (NMINRES) and from soil organic matter (NMINRESOM) and total N mineralization in the soil (NMINTOT).

The cumulative mineralization of N from soil organic matter and immobilization of N resulting from litter (dead grass residues) turnover in the clay soil is shown in Figure 4.3. Differences between the years are the overall result of differences in soil temperature and moisture and in the amounts and composition of grass litter inputs. For the sandy soil in 1989 the weekly(!) rates of N input with grass litter, of N mineralization from soil organic matter and of N immobilization/mineralization from grass litter is shown in Figure 4.4. A large N input with grass litter around week 34 indicates a period where considerable senescence of the grass occurred, leading to a peak in N mineralization from these residues around week 39. Till week 26 turnover of grass litter only led to N immobilization. Compared with a maximum daily(!) N uptake by the grass of about 6 kg ha^{-1} in the simulations, it can be seen from Figure 4.4 that optimum grass growth also needs an external N supply in addition to N supply from the soil.

Conclusion

The results of six simulation runs for carbon and nitrogen turnover in mown grassland showed strong interactions between C and N turnover, by the grass and in the soil, with weather conditions that influenced the moisture status of the soil and the water availability to the grass. Therefore, only models that consider all these interacting factors together can give reliable estimates of N losses to the environment as a function of N input and other management factors.

Reference

Verberne, E., 1992. Simulation of the nitrogen and water balance in a system of grassland and soil. Nota 258, 56 p. + appendices. IB-DLO, Haren.

5. Simulation of grazed grassland

5.1 Introduction

The effects of nitrogen fertilizer application on grassland has been subject of study for many years now. Because of the complexity of the highly interacting systems, it is hard to study these effects through direct empirical research. Mechanistic models can be used to understand the behavior of the system under any given combination of management strategies.

The objective of this chapter is to give a description of the grazing submodel which is used as an addition to the mechanistic grass growth model as proposed by Verberne (1992). The main difference between grazing and mowing is the fact that in case of grazing nitrogen is partly returned to the pasture in urine and feces spots. In these spots the N input is very high: about 40-200 g m⁻² (Lantinga et al., 1987). Because most of the excreted N is present in urine, and urine spots cover an about 10 times larger area than feces spots, the latter are neglected in the model. Another difference is a higher loss of litter in case of grazing then in case of mowing. Figure 5.1. shows the structure of the submodel, including the links with the existing submodels (Verberne, 1992).

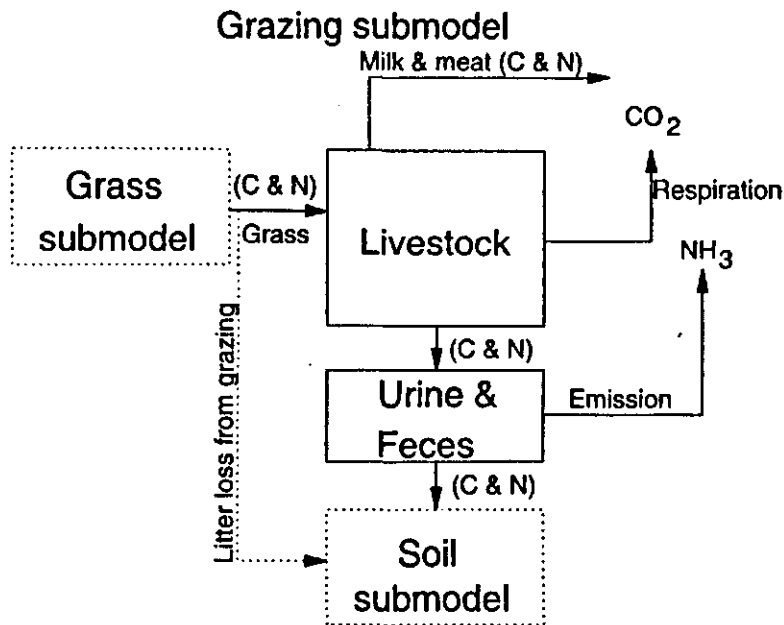


Figure 5.1. Schematic presentation of the grazing submodel with its links to other submodels.

5.2 Modifications compared to mown grassland

Fertilization

The fertilization of the soil takes place one day after a harvest, or one day after a grazing period. The fertilization scheme, as recommended by Verberne (1992), is used to determine the amount of nitrogen fertilizer application. To simulate the effect of urine two model runs are necessary. The first run determines the grazing scheme (number of grazing periods and total

cow grazing days). During this first run the soil is not affected by urine depositions. The same grazing scheme is then forced on the second model run. The urine depositions are simulated in this second run by an N application of 420 g m⁻² one day after the second grazing period.

Grazing by dairy cows

When the option switch 'GRAZE' is set to one, the animal intake will begin when more than 3500 kg DM ha⁻¹ is available. The duration of the grazing period equals the number of days it takes to reduce the standing crop to less than 3500 kg DM ha⁻¹, increased with a variable number of days which is the minimum grazing period (parameter 'DUGR').

The stocking density is calculated using equation 1:

$$n = \frac{(WSHBT - 2000)}{(DUGR * G_{max})} \quad (1)$$

Where G_{max} is the maximum daily animal intake (kg DM animal⁻¹ day⁻¹) and WSHBT is the standing crop (kg DM ha⁻¹).

The actual animal intake, G (kg DM animal⁻¹ day⁻¹), is assumed to be determined by the maximum daily intake, G_{max} and the leaf area index, L (Thornley & Verberne, 1989):

$$G = G_{max} * \frac{\left(\frac{L}{K_g}\right)^q}{1 + \left(\frac{L}{K_g}\right)^q} \quad (2)$$

K_g determines the half-maximum response (if $L = K_g$, G equals $G_{max}/2$), and q determines the sigmoidicity of the response.

It is assumed that the material removed by the livestock (nG) is taken from the four age categories of the shoot material only. Let $G_{dm,i}$ denote the dry matter intake due to grazing of the age categories i (kg DM ha⁻¹ day⁻¹):

$$nG = \sum_{i=1}^4 G_{dm,i} \quad (3)$$

The dry matter intake from age category i ($G_{dm,i}$) depends on the leaf area index of age category i (L_i), and on a affinity-index (a_i) allowing different removal due to selectivity or availability:

$$G_{dm,i} = \frac{a_i * L_i}{\sum_{i=1}^4 a_i * L_i} * nG \quad (4)$$

Carbon and nitrogen intake

The total carbon and nitrogen concentrations (C_{plant} and N_{plant}) in the lamina, sheath and stem of the plant are determined by the total substrate carbon and substrate nitrogen content (W_C and W_N respectively), the total structural dry matter (W_G) and the total dry matter of shoot parts of the plant (W_T ; consisting of shoot and substrates):

$$C_{plant} = \frac{W_C + f_C * W_G}{W_T} \quad N_{plant} = \frac{W_N + f_N * W_G}{W_T} \quad (5)$$

f_C and f_N are fractional C and N contents of shoot parts of the plants structural dry matter.

The animal intake of nitrogen and carbon per day is (using equations 3 and 5):

$$I_C = C_{plant} * nG \quad I_N = N_{plant} * nG \quad (6)$$

The fraction of the N intake retained by the animal ($f_{N,ret}$) has a constant low value and can be used to calculate the retained N and C:

$$F_{N,ret} = f_{N,ret} * I_N \quad F_{C,ret} = \lambda_{CN,ret} * F_{N,ret} \quad (7)$$

The parameter $\lambda_{CN,ret}$ is the C/N ratio of the retained biomass; the value of $\lambda_{CN,ret}$ is constant and reflects the C/N ratio of proteins, the main component of meat and milk.

The yield coefficient Y_{animal} (kg C in product [kg C assimilated]⁻¹) is introduced to reflect the loss of C due to animal respiration. The respiration rate (R_{animal} kg C ha⁻¹ day⁻¹) can now be calculated:

$$R_{animal} = F_{C,ret} * \frac{(1 - Y_{animal})}{Y_{animal}} \quad (8)$$

Excretions

The total excreted N flux, $F_{N,exc}$ is defined as the difference between the nitrogen intake (I_N) and the retained N:

$$F_{N,exc} = I_N - F_{N,ret} \quad (9)$$

The amount of N excreted in urine is calculated with the use of a regression curve (Valk, 1991; Lantinga et al., 1987). With the $f_{N,urine}$ known, the expressions for the fluxes of C and N to urine and feces (kg C or N ha⁻¹ day⁻¹) can easily be defined (Thornley & Verberne, 1989):

$$F_{N,urine} = f_{N,urine} * F_{N,exc} \quad (10)$$

$$F_{C,urine} = \left(\frac{12}{28}\right) * F_{N,urine} \quad (11)$$

$$F_{C,faeces} = I_C - F_{C,ret} - R_{animal} - F_{C,urine} \quad (12)$$

$$F_{N,faeces} = (1 - f_{N,urine}) * F_{N,exc} \quad (13)$$

The C and N in urine are assumed to be present in the form of urea only and thus C in urine can be calculated (eq. 11) when urine N is known (eq. 10).

Ammonia volatilization

The volatilization of ammonia is modelled after Bussink (1994). The relationship between the total NH_3 volatilization (V , $\text{kg N ha}^{-1} \text{ yr}^{-1}$) and the total N excreted over a year ($F_{N \text{ tot,exc}}$) can adequately be described by a power function of the type $V = x * F_{N \text{ tot,exc}}^y$. To determine the values of the parameters x and y datasets from 1987, 1988 and 1990 were used (Bussink, 1994):

$$V = 7.70 * 10^{-6} * (F_{N \text{ tot,exc}})^{2.491} \quad (14)$$

5.3 Modeling example

To run the model an extended set of input parameters is necessary. The parameter set can roughly be divided into: pasture data, hydrology parameters, grazing parameters, organic matter parameters and weather parameters. The model itself also requires a couple of control parameters which contain the names of in- and output files, the size of the integration step, the simulated year, the soil type (clay or sand) etc. All parameters (except the parameters necessary for the simulation of grazing) are listed by Verberne (1992).

During the model's run, the output, in the form of numerical values of variables, is produced. This output can be made graphical by using other software. The output variables can be selected by adjusting the model and re-compiling it. After linking the newly compiled version, a new set of output data can be calculated.

In this example different parameter sets were used to calculate the difference in the nitrogen balance between grazed and a mown grassland. In the first simulation run no grazing took place, just harvesting. The fertilization scheme according to Verberne (1992) was used to determine the inorganic nitrogen input. The first fertilization is when the temperature sum equals 280°C . The next fertilizer applications take place after each harvest, but only if the precipitation equals 5 mm or more. The grass is harvested when more than $4000 \text{ kg DM ha}^{-1}$ (shoot material) is available. After harvesting the shoot material is reduced to $2000 \text{ kg DM ha}^{-1}$.

The nitrogen balance of a mown grassland field in 1989 is schematically shown in Figure 5.2. Each numerical value has the dimension $\text{kg N ha}^{-1} \text{ year}^{-1}$, and the fertilization scheme is put between parentheses.

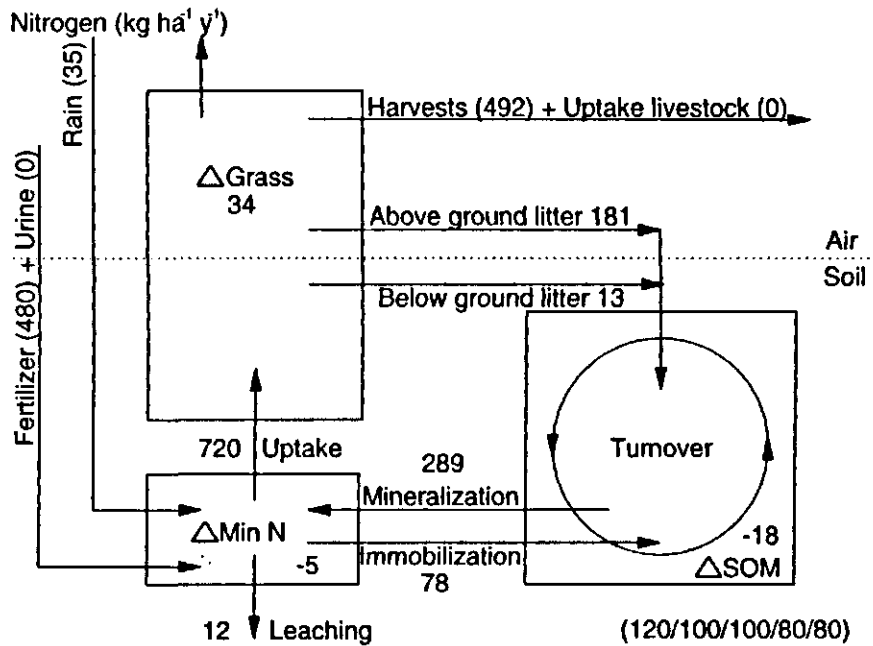


Figure 5.2. Schematic presentation of the nitrogen balance of a mown pasture.

When the option 'GRAZE' is set to one, animals will begin with the intake of grass when more than 3500 kg DM ha⁻¹ is available. The urine and feces produced by the animals can optionally be returned to the pasture, but in this example the excreta are not fed back directly. Instead, the urine spots were simulated by an extra N input of 420 kg N ha⁻¹.

Figure 5.3 shows the N balance of a urine spot in grazed pasture and Figure 5.4 shows the N balance for the area that was unaffected by urine. Effects of feces were not yet taken into account, but are presumed to be small. From the number of cow grazing days the area affected by urine spots can be calculated, when we assume that one cow affects 6.8 m² of pasture daily by urine (Lantinga et al., 1987). Next, the N balance for a grazed pasture can be calculated by summation of N balances for urine spots and area unaffected by urine, on an area basis. For this example about 0.21 ha was affected by urine, with an input of 88.2 kg N, or 420 kg ha⁻¹. Thus, the chosen dosage rate of urine-N in Figure 5.3 (420 kg ha⁻¹) was about 12 % less than it should have been.

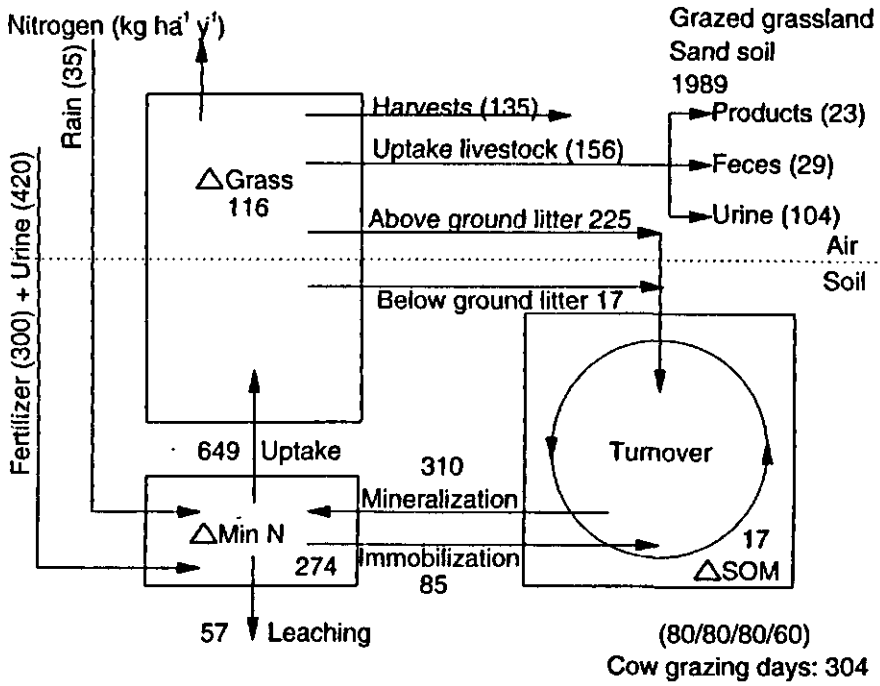


Figure 5.3. Nitrogen balance of urine spots in a grazed pasture on a sandy soil for the year 1989.

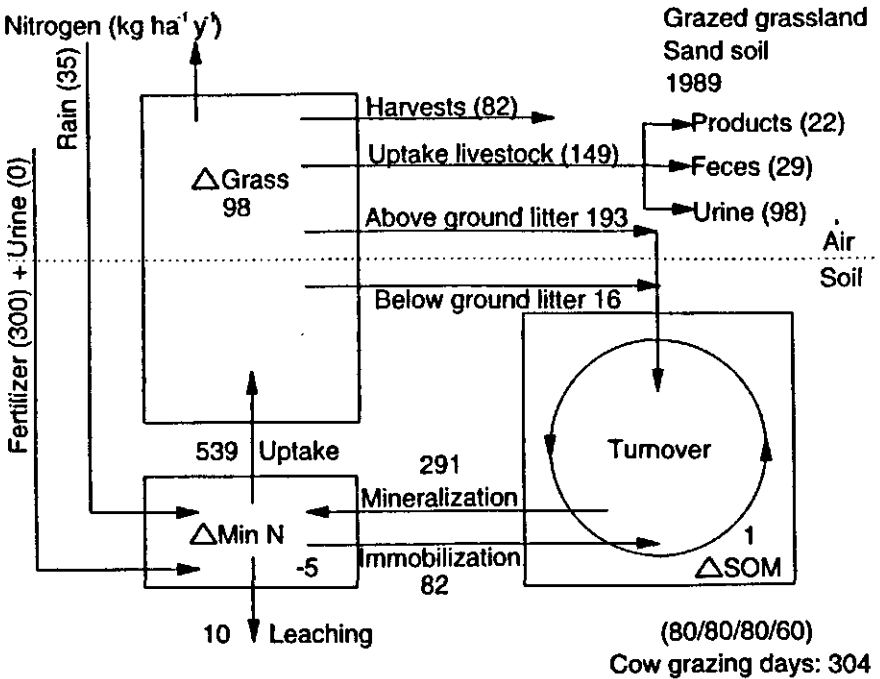


Figure 5.4. Nitrogen balance of the area in a grazed pasture that is not affected by urine on a sandy soil for the year 1989.

Parameter values

Parameter values used in modeling effects of grazing are given in Table 5.1.

Table 5.1. Summary of parameter values used to simulate grazing

Parameter values		Units	Description
G_{max}	18.	kg DM animal ⁻¹ day ⁻¹	maximum daily intake
$DUGR$	10.	day	minimum length of grazing period
k_g	1.	m ² m ⁻²	determines the half-maximum response
q	3.	-	sigmoidicity parameter
a_i	0.4, 0.3, 0.2, 0.1	-	affinity index for leaf class i
$\lambda_{CN,ret}$	3.42	kg C [kg N] ⁻¹	C/N ratio of retained biomass
Y_{animal}	0.5	kg C prod. [kg C substr.] ⁻¹	carbon yield of assimilated C
$f_{N,ret}$	0.15	-	nitrogen fraction retained in milk and meat

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