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Description of an application with SOILNDB at the Mellby experimental station in south-west Sweden simulating nitrate leaching between 1984 and 1998 for 10 different management practices

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Teknisk rapport 71 **Uppsala 2003**
Avdelningen för vattenvårdslära
Swedish University of Agricultural Sciences
Division of Water Quality Management

Preface

This work was carried out within the Swedish Water Management Research Programme (VASTRA) that is funded by the Foundation for Strategic Environmental Research (MISTRA), which is gratefully acknowledged. Additional funding was received from SLU (Swedish University of Agricultural Sciences). We would like to thank Hans Johansson, Department of Soil Sciences, Division of Hydrotechniques, for skilful programming, and Gunnar Torstensson for help with providing data from the experimental site, and for fruitful discussions in relation to the model application.

Contents

Summary

For an efficient abatement of diffuse N pollution from arable land, it is important to have practical and reliable tools, which can quantify the effect of different management practices on leaching, and also analyse the effect of alternative management scenarios aimed at reducing leaching. We present here an application of SOILNDB, a management-oriented model for quantifying nitrate leaching from arable land. Simulations with SOILNDB were compared with measurements of N in harvested products and tile-drain discharge of nitrate taken in a 14-year field experiment on a sandy loam soil in south-west Sweden. Following adjustment of parameters connected to litter and faeces decomposition and mineralization, the model gave satisfactory predictions of nitrate leaching for all 10 treatments. The temporal pattern was mostly well captured by the model, which is also indicated by high model efficiency values (average = 0.59). This application also gave promising results regarding the model's ability to simulate the long-term influence of different crops and catch crops as well as different manure strategies on leaching. However, further studies should be done to evaluate the model under additional agro-environmental conditions (e.g. soils, climates, and crops).

Introduction

Diffuse N pollution from agriculture remains a serious threat to many groundwater aquifers, coastal waters and the sea, and diffuse sources are currently the major source of N input to the aquatic environment in many regions (e.g. Stålnacke, 1996; Larsen et al., 1999; De Wit and Bendoricchio, 2001; Naturvårdsverket, 2002). Analysis of 23 small agricultural catchments in Sweden and Norway during the 1990s reveals that there is no clear trend regarding N losses stemming from changes in agricultural management practices (Kyllmar, 2000; Stålnacke and Bechmann, 2002). Of the 23 catchments, 3 showed evidence of downward trends, 17 showed no trends and 3 exhibited increased N losses. This is supported by Stålnacke et al. (1999), who state that in many agricultural river basins in Sweden, most of the N-transport curves exhibited a weak positive trend during the past 15 years and no significant downward trends can be confirmed.

In order to find the most efficient measures to decrease nitrogen leaching from agriculture it is important to understand and to be able to quantify the effect of different agro-environmental conditions (e.g. soils, climates, and cultivation practices). For this purpose, models can be valuable tools since extrapolating or making general statements about N leaching on the basis of results from a limited number of field experiments may have a high degree of bias. However, to be useful as management tools, models should be flexible, easy to operate and 'validated', i.e. tested under conditions appropriate for the intended use.

Recently, Johnsson et al. (2002) presented SOILNDB, a management-oriented decision support tool to quantify nitrate leaching that is based on the mechanistic research-oriented models SOIL and SOILN, a parameter database, and parameter estimation algorithms. With SOILNDB, the time-consuming process of parameterization, administrating model runs, and presenting model results is reduced, allowing a large number of calculations for various agro-environmental conditions (e.g. scenario calculations) to be made efficiently. The mechanistic research-oriented models SOIL and SOILN have been applied for a variety of agro-environmental conditions (see compilation by Hoffmann, 1999), and could therefore be considered operationally validated. However, all applications have involved a parameter selection process, often combining measurements, literature values and calibration. Calibrations are typically performed against measurements of N concentration in drainage water, soil mineral N content at different depths, plant N uptake and N in grain exported at harvest. Since one of the main purposes of SOILNDB is to simplify parameterization, it should be possible to keep time-consuming iterative calibration to a minimum.

The functional applicability of SOILNDB was demonstrated by Hoffmann and Johnsson (2003) in a 3-year study simulating N leaching from a 900 ha agricultural catchment with 150 fields. Only a rough evaluation of the model behaviour could be made in that application because of the short period simulated and the lack of detailed measurements (e.g. field-scale drainage and leaching, retention in the stream etc.).

This paper describes an application of the SOILNDB model where simulation results were compared with 14 years of measured nitrate leaching at an experimental site where the effects of catch crops and different manure application strategies have been studied. Leaching in this area is, for Swedish conditions, comparatively high due to a combination of mild winters, high precipitation, coarse-textured soils and relatively high animal densities, and it is therefore essential to correctly quantify the effect of practical measures aimed at reducing nitrate leaching in the region. The main goal was to evaluate the robustness of the automatic parameterization routines and test if the current selection of parameters in the database could give acceptable results at this site.

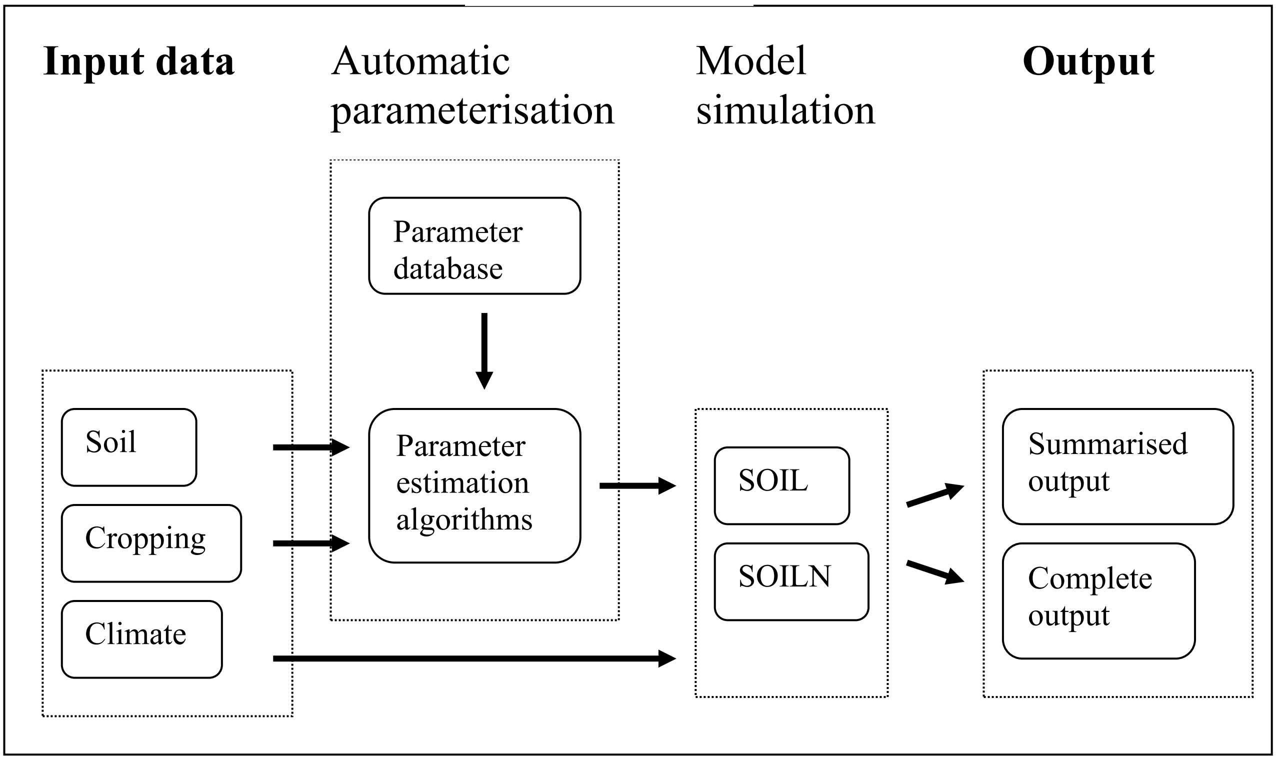

Fig. 1. Schematic description of the SOILNDB model system.

Materials and Methods

The SOILNDB model

SOILNDB (Fig. 1) is a shell program which links user input data and data from databases to automatic parameterization procedures for the water and heat model SOIL (Jansson and Halldin, 1979) and the nitrogen model SOILN (Johnsson et al., 1987). The simulation results are presented on a yearly basis for a selected number of important variables. Since the model is presented in detail elsewhere (Johnsson et al., 2002; Larsson et al., 2002), we will give a brief overview of the model here and only describe in detail the parts that are relevant to this study.

The modelling approach consists of a coupling in series of a soil water and heat model, SOIL and a nitrogen transport and transformation model, SOILN. The SOIL model, using standard daily meteorological data as input, provides driving variables for the SOILN model (e.g. infiltration, water flow between layers and to drainage tiles, soil water content and soil temperature). The models have a one-dimensional vertical structure, with the profile divided into layers representing distinct physical and biological characteristics of the soil. Both SOIL and SOILN include the possibility of choosing between different sub-models for some processes. In such cases, the best tested sub-models, or in some cases those that require least parameterization, have been chosen for SOILNDB.

The SOIL model (Jansson and Halldin, 1979) describes heat and water transport in a soil profile, including snow dynamics, frost, evapotranspiration, infiltration and surface runoff using standard daily meteorological data as input. In the SOIL model, either free drainage or horizontal flow to groundwater and tile drains can be selected as bottom boundary conditions. With free drainage, a unit gravitational gradient is assumed as the driving force for vertical flow out of the lowest soil layer. No groundwater level is then simulated within the soil profile. With the other option, a groundwater level, net horizontal groundwater flow and flow to tile drains can be simulated. Saturated water flow to tile drains, q_{pipe}, is calculated when the groundwater table rises above the depth of the tile drains, z_{pipe}, according to the hydraulic gradient:

$$q_{pipe} = k_s A_{rel} \frac{z_{pipe} - z_{gw}}{L}$$

where k_{s} is the saturated hydraulic conductivity, A_{rel} is the ratio between the vertical area of the soil layer and the unit horizontal area, z_{gw} represents the depth of the water table and L the distance between the tile drains. Horizontal groundwater flow, q_{gr}, out of the one-dimensional soil profile is described with an empirical first order recession equation, so that when there is a groundwater level, z_{sat}, in the soil profile, outflow is given as:

$$q_{gr} = q_1 \frac{z_1 - z_{gw}}{z_1}$$

where q_1 represents a potential maximum flow rate per day and z_1 the depth where flow ceases (Jansson, 1991). Water flow between soil layers is described by Darcy's law and the law of mass balance, while the description of heat flow is derived from Fourier’s law. Parameter values in the SOIL model connected to hydraulic properties are assigned by the pedo-transfer functions described by Rawls et al. (1982) in SOILNDB, in which soil texture is given as input.

The SOILN model (Johnsson et al., 1987) includes all the major processes determining transport and transformations of nitrogen in arable soils. Inputs of nitrogen can be in the form of fertilizer, manure and atmospheric deposition, while harvest, leaching and denitrification constitute the output. Litter, faeces and humus comprise the organic-N fractions. The litter fraction represents non-decomposed material (e.g., crop residues, dead roots), microbial biomass and metabolites. The faeces component represents the digested fraction in manure, i.e., excluding bedding material, and humus is characterized as stabilized organic material derived from litter and faeces decomposition. To regulate nitrogen mineralization and decomposition, organic carbon pools are connected to the N pools of litter and faeces. Mineralization of soil organic carbon and humus nitrogen is calculated as a first-order rate process. A Q_{10}-expression is used for the soil temperature response function regulating all biological processes in the model. For all biological activity except denitrification, the effect of soil moisture is calculated based on the assumption that the activity decreases on both sides of an optimum soil moisture content range. In SOILN, plant uptake of N is calculated from a time-dependent empirical function requiring specific parameter values for the different crops. A logistic growth curve, defined by the coefficients u_{b} and u_{c}, is used to define a potential uptake demand, u_{a}, during the growing season, which is distributed in the soil profile according to an assumed root distribution (i.e. root biomass decreases exponentially from the soil surface to the root depth, where the exponential decrease is governed by the parameter, r_{frac}). Accordingly, in SOILNDB, N uptake and crop growth is not simulated explicitly, and the harvested crop yield, S, is used to calculate the target N uptake, N_{totup}:

$$N_{totup} = \frac{S * c_{N1} + f_a * S * c_{N2}}{1 - f_r}$$

and the potential uptake demand, u_a, is then estimated as:

$$u_a = N_{totup} * \frac{1 - e^{-u_c * t_{UP}}}{1 - \frac{N_{totup}}{u_b} * e^{-u_c * t_{UP}}} + u_b$$

where c_{N1} is the nitrogen concentration in the harvested product (i.e. grain, seed or tuber) while c_{N2} is the nitrogen concentration in above-ground residues (i.e. straw, tops, stubble, chaff, stalks etc.), f_a is the ratio of above-ground residues to grain biomass, and f_r is the fraction of N in roots of total plant N (Johnsson et al., 2002). The target harvest yield, *S*, and the length of the uptake period, t_{UP}, are the only parameters in these two equations specified by the user, the remaining parameters are all included in the SOILNDB database. The length of the uptake period is calculated simply by subtracting the start of the uptake period from the time of harvest, or if no harvest takes place, the end of the uptake period.

Roots and harvest residues (if the straw is not harvested) are incorporated into the soil litter pool at ploughing. Denitrification is calculated as a function of potential rate, soil temperature, soil oxygen status and soil nitrate content. Nitrate transport is calculated as the product of water flow and nitrate concentration in the soil layer from which the water flow originates, while ammonium is considered to be immobile in the soil profile.

The requirements for input data in SOILNDB are more general, less detailed and less extensive than for the SOIL and SOILN models. The input can be categorized into soil properties, local hydrology, climatic data and crop management. Soil properties are either selected from a list of texture classes (USDA) for topsoil and subsoil, or from a soil database. To calculate initial amounts of litter and humus, the organic matter content must be specified for both topsoil and subsoil, or alternatively, the user may create an own file containing initial amounts of mineral N and organic C and N for the different pools and layers. Under local hydrology, two options for the bottom boundary condition is given: free drainage or flow to tile drains and groundwater. In the latter case, the distance between tile drains, the depth to tile drains and the potential lateral groundwater flow must be specified. Climate data is selected from a database maintained by the user, containing daily values of rainfall, air temperature, solar radiation (or solar duration or cloudiness), wind speed and vapour pressure (or relative humidity) and the latitude of the meteorological station. Nitrogen deposition rates can either be taken from a database by selecting a county in Sweden or the dry deposition rates and N concentration in rainfall can be given as input by the user. Yearly input of crop and management information includes the following: crop type and sowing date, harvest date and yield, fertilization amount and time, time and amount of manure applications, soil cultivation time and, if a catch crop is simulated, the expected N uptake of the catch crop. Crop type is selected from a database, and can be combined without restraint in the crop rotation. A choice can be made between a number of the most common types of manure, whereby values for NH_4-N concentration, c_{ammN}, organic N concentration, c_{orgN}, and C-N ratio are given in a database. Alternatively, the user may specify the composition of the manure applied. Volatilization of NH_3 can either be specified by the user or estimated by SOILNDB by selecting between a number of common types of manure application techniques. Input data given to SOILNDB, as described above, determines the parameter values used for the underlying SOIL and SOILN models. This parameterization is done automatically by the use of a parameter database and parameter estimation algorithms included in SOILNDB. Details about the specific values contained in the parameter database, and the parameter estimation algorithms can be found in the SOILNDB technical description (Larsson et al., 2002).

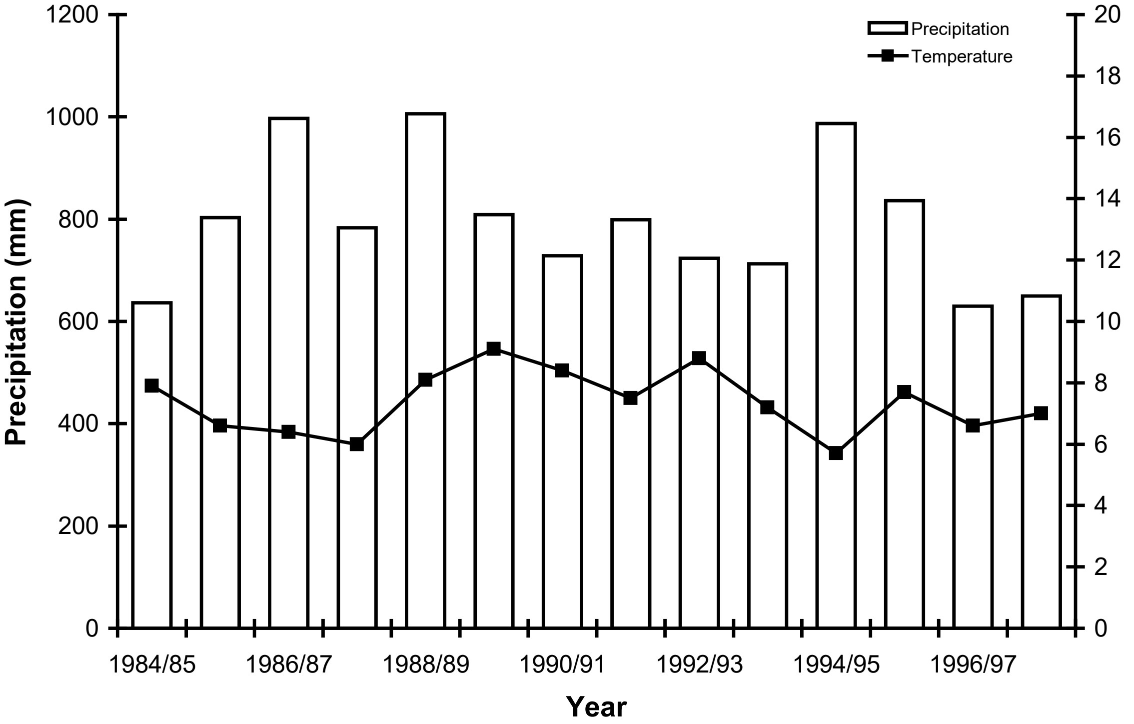

Fig. 2. Accumulated yearly precipitation and annual mean temperatures for the agrohydrological years (i.e. 1st July to 30th June) during the period studied.

Experimental site details and measurements

The experiments were carried out at the Mellby field site (lat. 56°29′N, long. 13°E, alt. 10m) in south-west Sweden where the climate is cold temperate and semi-humid. The mean temperature was 7.4°C and the mean annual precipitation was 790 mm during the period studied. Figure 2 shows the accumulated yearly precipitation and annual mean temperatures for the agrohydrological years (i.e. July to June). Meteorological data (i.e. precipitation, air temperature, vapour pressure, wind speed and global radiation) were obtained on site from a standard automatic weather station.

The soil at the experimental site consists of sand deposits to a depth of 90-130 cm, covering a glacifluvial clay. The topsoil is a weakly structured sandy loam with an organic matter content of ca. 4%, and the subsoil is a structureless loamy sand with an organic matter content of less ca. 1%. The upper topsoil has been recognized as water repellent when dry (Dekker et al., 1999), and experiments with a dye tracer and a Br^- tracer showed that preferential flow under certain conditions can influence the flow and transport at this site (Larsson et al., 1999).

The part of the experimental site used in this study consists of 10 experimental plots each 40 by 40 m in size. The plots are surrounded by a single discard drainage pipe located 2.5 m from the border at 90 cm depth. This secondary drain, which was not monitored, is intended to minimize lateral inflow to the plots. The primary drainage system consists of perforated plastic pipes at a spacing of 7 m and at a depth of ca. 90 cm. Each plot is monitored separately, and drainage flow from the plots was measured continuously with a calibrated tipping bucket system. From 1982 to 1989 the number of tips was recorded by a counter and registered every second week, while from 1989 to 1998 flow was recorded continuously by a datalogger and the accumulated daily amounts were registered. Drainage water from each plot was sampled manually every two weeks and weekly during periods with high discharge. Concentrations of NO_3-N were measured by flow injection analysis (Tecator, 1983; Swedish Standards, 1991). A linear interpolation between measured concentration values was used to calculate the daily transport of NO_3-N in drainage water. Instead of using the individual discharge rates for each plot to calculate the NO_3-N transport, a mean value of the water flow for all plots was used. The reason for this is that variation in tile-drain discharge of water between plots was assumed to be caused mainly by intrinsic differences between plots and to a considerably smaller extent by actual effects of the different treatments.

The amount of grain and straw, and potatoes was determined by harvesting three sub-plots (20-50 m^2) in each plot. Until 1988 straw was only harvested in the catch crop treatment, while from 1989 the straw was harvested from all treatments, except from the potatoes (1992) and spring rape (1995) where all residues were left in the field. The amount of catch crop material was determined just before ploughing by collecting above-ground material from eight randomly chosen microplots (0.25 m^2) in each plot. For calculation of total N uptake in catch crop, sampled above-ground material was assumed to represent 40% of the total plant N content (Sjösvärd and Svensson, 1990). Total N contents in plant material were analysed with an elemental analyser (LECO CS 125), according to Kirsten and Hesselius (1983).

The experimental site was established in 1982 to study the influence of different cropping practices on N leaching. The crops during the period studied were spring sown cereals plus two years with potatoes and two years with spring rape. Because of the increasing interest for catch crops during the 1980s, a new experimental plan was introduced in 1989 that increased the number of plots with catch crops. From 1984 to 1988 the field included eight treatments, one without any added N, one with only mineral fertilizer, and six with different strategies for adding manure (see table 1). Only one of the treatments included a catch crop. Rye (*Secale cereale*) was then used as the catch crop, planted one to three weeks after harvest of the main crop, and incorporated the subsequent year, before sowing of the next main crop. From 1989 to 1998 the number of treatments was 10, with the main difference that six treatments now included a catch crop (table 1). When cereals and spring rape were grown, the catch crop was perennial ryegrass (*Lolium perenne*) undersown in spring. In 1990 though, Italian ryegrass (*L. multiflorum*) was used, and after the potato harvest 1992, winter rye was used as a catch crop. From 1989 to 1998 the treatments without catch crops were stubble-cultivated once immediately after harvest in August or September and then ploughed in November, which is a common practice for spring cereal crop production in south-west Sweden. The treatments including catch crops were ploughed in spring before sowing. Further details of the first period of the experiment can be found in Torstensson et al. (1992), and Torstensson and Johnsson (1996) and of the period from 1989 to 1998 in Lindén et al. (1993), Hessel Tjell et al. (1999), and Torstensson and Aronsson (2000).

Modelling strategy and parameterization

The purpose of this study of SOILNDB at a field site with complete registration of management operations, harvest yields, N uptake by catch crops and measured NO_3-N leaching was not to perform a comprehensive generic evaluation of the model. Rather, this application was aimed at evaluating the long-term behaviour of the model, with current automatic parameterization routines

Table 1. Experimental plan showing application rate of fertilizer and manure, time for ploughing and manure application, and cultivation of catch crop for the ten plots and for the two periods with different treatments. The treatment acronyms can be explained as: *0F* denote no fertilization, *1F* denote normal dose mineral fertilizer, *cc* denotes cultivation of catch crops, *1/2M*, *1M*, *2M* denotes half, normal and double dose manure, respectively, and *ea*, *la*, *s* denotes early autumn, late autumn and spring application of manure, respectively.

Treatment acronym	Plot No	Catch crop	Mineral fertilizer	Liquid manure	Time for manure application	Ploughing
			From 1984 to 1988			
0F	5, 7		0	0		Autumn
1F	2, 10		normal rate [a]	0		Autumn
½M ea	9		half rate	Half rate	early autumn	Autumn
1M ea	8		half rate	Normal rate [b]	early autumn	Autumn
2M ea	3		half rate	Double rate	early autumn	Autumn
1M la	4		half rate	Normal rate	late autumn	Autumn
1M s	1		half rate	Normal rate	Spring	Autumn
1M s cc	6	√	half rate	Normal rate	Spring	Spring
			From 1989 to 1998			
0F	7		0	0		Autumn
0F cc	5	√	0	0		Spring
1F	2		Normal rate	0		Autumn
1F cc	10	√	Normal rate	0		Spring
1M ea cc	8	√	half rate	Normal rate	early autumn	Spring
2M ea cc	3	√	half rate	Double rate	early autumn	Spring
1M s	1		half rate	Normal rate	Spring	Autumn
1M s cc	6	√	half rate	Normal rate	Spring	Spring
2M s	9		half rate	Double rate	spring	Autumn
2M s cc	4	√	half rate	Double rate	spring	Spring

[a] Normal rate mineral fertilizer corresponds approximately to the recommended amount for the specific crop (i.e. 90 kg N ha^{-1} for cereals and 110 kg N ha^{-1} for spring rape and potato).

[b] Normal rate manure corresponds approximately to a production of slurry resulting from the maximum allowed number of animals per ha^{-1} (i.e. 10.5 hogs ha^{-1}, which generate ca. 95 kg N ha^{-1} with 2.5 batches per year Claesson and Steineck, 1991; Steineck et al., 2001).

and selection of parameters, at one place with a wide range of management strategies resulting in large differences in leaching.

The strategy for application of SOILNDB was (i.) to simulate the water discharge, comparing simulation results with accumulated tile-drain discharge, (ii.) to simulate N uptake by the crops and catch crops, comparing simulation results with N content in the harvested products and N uptake in the catch crops, and (iii.) to simulate NO_3-N leaching, comparing simulation results with accumulated annual tile-drain discharge of NO_3-N. Continuous simulations were conducted from 1 January 1983 to 30 June 1998. The model predictions for the first one and a half years are not presented here since these are strongly influenced by the uncertain initial conditions. Water discharge and NO_3-N leaching are presented for agrohydrological years (i.e. from 1st July to 30th June). It should be noted that simulation results for nitrate leaching are presented both before (denoted 'database' parameterization) and after (denoted 'alternative' parameterization) site-specific adjustment of parameters connected to litter turnover.

Table 2. Input data used in SOILNDB related to quantity and quality of manure for the different plots (plot numbers given below column heads)

Year	Amount Manure (ton ha^{-1})					Ammonium content (kg N ton^{-1})				Org-N content (kg N ton^{-1})				CN-ratio			
	1, 6	3	4	8	9	1, 6	3, 8	4	9	1, 6	3, 8	4	9	1, 6	3, 8	4	9
1984	20	40	20	20	10	3.5	3.4	4.0	3.4	1.9	1.8	1.5	1.8	28	15	15	15
1985	20	40	20	20	10	2.7	3.9	3.0	3.9	0.7	2.0	0.8	1.9	25	14	16	14
1986	20	40	20	20	10	2.8	3.5	3.4	3.5	1.5	2.0	2.1	2.0	20	22	19	22
1987	20	40	20	20	10	3.2	2.6	3.3	2.6	2.2	1.2	2.0	1.2	18	17	20	17
1988	20	40	-	20	-	2.5	2.4	-	-	1.9	0.9	-	-	20	11		
1989	20	40	42	20	42	2.6	3.3	2.6	2.6	1.6	0.8	1.6	1.6	16	12	16	16
1990	23	46	39	23	39	3.4	3.2	3.4	3.4	1.4	0.6	1.3	1.3	13	12	13	13
1991	23	44	49	22	49	3.1	3.3	3.1	3.1	0.6	1.1	0.6	0.6	11	10	11	11
1992	23	40	47	20	47	3.5	3.0	3.7	3.7	2.0	0.8	2.0	2.0	22	10	22	22
1993	25	58	49	30	49	3.0	2.5	3.0	3.0	2.6	1.4	2.7	2.7	18	12	18	18
1994	25	80	52	40	52	2.6	1.6	2.6	2.6	0.6	0.4	0.6	0.6	20	12	20	20
1995	30	120	53	60	53	2.7	1.0	2.7	2.7	1.3	0.4	1.3	1.3	13	12	13	13
1996	31	42	60	24	60	3.1	3.4	3.4	3.4	1.0	1.3	0.7	0.7	17	12	17	17
1997	34	56	80	28	80	3.4	2.3	2.3	2.3	0.6	0.8	1.2	1.2	17	12	17	17
1998	20	80	38	40	38	3.8	2.2	3.8	3.8	1.5	0.9	1.5	1.5	17	12	17	17

[a] For plot 6 the ammonium content was 3.0 and 3.4 kg N ton^{-1} for 1997 and 1998, respectively.

The input data for SOILNDB were mainly based on measurements. The soil was defined as a loamy sand topsoil and a sandy loam subsoil, according to the USDA soil texture classification. For initial content of humus, litter C and N, NH_4-N and NO_3-N in the different soil layers, an earlier application by Torstensson and Johnsson (1996) was used instead of the internal SOILNDB values and calculations based on the organic matter contents given as input. The reason for this was that the estimations by Torstensson and Johnsson (1996) based on a methodical model calibration were considered to be more reliable than the incomplete measurements available. Deposition for Halland county was selected from the database. The application amounts and concentrations of NH_4-N and organic-N of manure used in SOILNDB are shown in table 2. Volatilization losses of N from manure at application were set equal to earlier model applications at Mellby (Torstensson and Johnsson, 1996; Torstensson and Aronsson, 2000). Fertilization amounts and uptake of N by the catch crops are shown in table 3, while all dates used as input in SOILNDB related to cultivation activities are presented in the Appendix (table A1) and harvest yields and corresponding N concentrations are presented in table A2 in the Appendix.

Since this was a site-specific application, and SOILNDB was originally developed for a more generic use, some changes in SOILNDB were introduced. The current bottom boundary condition free drainage was not applicable at Mellby, and the option of choosing from the alternatives free drainage or flow to tile drains in the SOIL and SOILN models was also introduced in SOILNDB. The parameters governing the horizontal groundwater flow rate were set so that the simulated outflow from the tile drains roughly matched the measured accumulated tile-drain discharge (i.e. the potential flow rate, q_1 was set to 0.4 mm d^{-1} and the depth where groundwater flow ceases, z_1 was set to 1.5 m, corresponding to the bottom of the soil profile). The depth to the tile drains, z_{pipe} was set to 0.9 m and the distance between the tile drains, L to 5m corresponded to an earlier application at the site (Torstensson and Johnsson, 1996).

Table 3. Input data used in SOILNDB for fertilization and uptake of N by the catch crop for the different plots (plot numbers given below column heads)

Year	Fertilization (kg N ha^{-1})			Target N uptake by the catch crop (kg N ha^{-1})					
	Plot number			Plot number					
	5, 7	2, 10	1, 3, 4, 6, 8, 9	3	4	5	6	8	10
1984	0	220	55	–	–	–	23	–	–
1985	0	90	45	–	–	–	27	–	–
1986	0	90	45	–	–	–	18	–	–
1987	0	110	55	–	–	–	5	–	–
1988	0	90	45	–	–	–	25	–	–
1989	0	90	45	94	78	15	81	84	35
1990	0	110	55	46	52	28	45	53	39
1991	0	90	45	126	41	32	57	95	32
1992	0	110	55	85	34	22	38	70	36
1993	0	90	45	126	55	25	42	88	38
1994	0	84	42	31	18	14	17	35	20
1995	0	110	55	116	45	22	35	52	25
1996	0	110	55	45	29	15	25	34	18
1997	0	90	45	67	48	20	38	39	29
1998	0	95	47	31	31	31	31	31	31

In SOILNDB, the soil profile is divided in 5 layers that are, from top to bottom, 25, 25, 25, 25, and 50 cm thick, respectively. However, to adequately account for surface runoff after a period with frost in 1985/86, it was necessary to divide the 25-cm topsoil layer in two layers of 10 and 15 cm thickness.

Initially, the simulated crop uptake of N was underestimated for some years. This could partly be attributed to erroneous estimations of N concentration in the harvested product, c_{N1}. In SOILNDB, specific values for c_{N1} are set for each crop type (Larsson et al., 2002). However, the measured N concentrations at Mellby showed a considerable variation between different treatments and years within each crop type (Torstensson et al., 1992; Lindén et al., 1993; Hessel Tjell et al., 1999). As a consequence, the SOILNDB model was modified regarding N concentration in the harvested product, c_{N1}, which was transferred from the database to the crop input menu to allow for use of measured data. To increase plant N uptake, the root depths for sandy loam for the crops included in this application were somewhat increased, from 0.6 to 0.7 m in agreement with the application by Torstensson and Johnsson (1996). In addition, the parameter r_{frac}, governing the fraction of roots below the root depth, was changed from 0.001 to 0.05 to increase plant N uptake, and the date for maximum root depth, $t_{\mathrm{root}(2)}$, was altered from $(t_{\mathrm{root}(1)} + t_{\mathrm{root}(3)})/2$ to $(t_{\mathrm{root}(1)} + t_{\mathrm{root}(3)})/2.4$, where $t_{\mathrm{root}(1)}$ is the date for emergence, and $t_{\mathrm{root}(3)}$ is the harvest date (Larsson et al., 2002). This resulted in an average change of the date for maximum root depth from 1 July to 1 June in this application. Similarly, uptake of N by the catch crops was underestimated for some years, and the root depth for catch crops were increased from 0.26 to 0.76 m in agreement with Torstensson and Johnsson (1996), in order to increase the N uptake.

The simulated leaching was at first significantly overestimated for all plots and treatments. This was most likely caused by erroneous timing of litter and faeces mineralization and underestimation of the humification. A parameter setting similar to an earlier application by Aronsson and Torstensson (1998) at Mellby, with a relatively high turnover rate of the litter pool and a relatively large fraction of the litter transferred to the humus pool was adopted. Consequently, the specific litter decomposition rate, k_l (set to 0.035 d^{-1} in the database) was increased to 0.055 d^{-1} and the litter carbon humification fraction, f_h (set to 0.2 in the database) was changed to 0.3. The SOILN parameter values related to faeces mineralization can not be considered well established since they are based on a single application (Borg et al., 1990), therefore it proved necessary to adapt the faeces turnover parameters according to the more recent application by Aronsson and Torstensson (1998). Consequently, the faeces decomposition rate, k_f, was decreased from 0.035 to 0.02 d^{-1}, and the related efficiency constant, f_{efe}, was increased from 0.5 to 0.7, and the faeces carbon humification fraction, f_{chf}, was set to 0.4 instead of 0.2. It was also found that SOILNDB uses a remarkably low C-N ratio for roots (set to 20). This value was changed to 30 as a rough mean of measured data (Hansson et al., 1987; Sjödahl Svensson and Clarholm, 1994; Kätterer and Andrén, 1996). The N content in potato residues in SOILNDB was high compared to existing measurements at Mellby (Hessel Tjell et al., 1999), and was changed accordingly (from 0.78 to 0.42).

Model evaluation

In addition to graphical displays of simulated and measured results, a statistical measure of model efficiency (EF) was used to evaluate the ability of the model to simulate NO_3-N leaching, as suggested by Loague and Green (1991):

$$EF = \frac{\sum_{1}^{N}(O-\overline{O})^2 - \sum_{1}^{N}(P-O)^2}{\sum_{1}^{N}(O-\overline{O})^2}$$

where P and O represent predicted and observed NO_3-N amounts respectively, and $\overline{O}$ is the mean of the observed values. The maximum and ideal value for EF is 1.0, while a negative value for EF indicates a poor fit, whereby the model predictions are worse than they would be using the observed mean as an estimate.

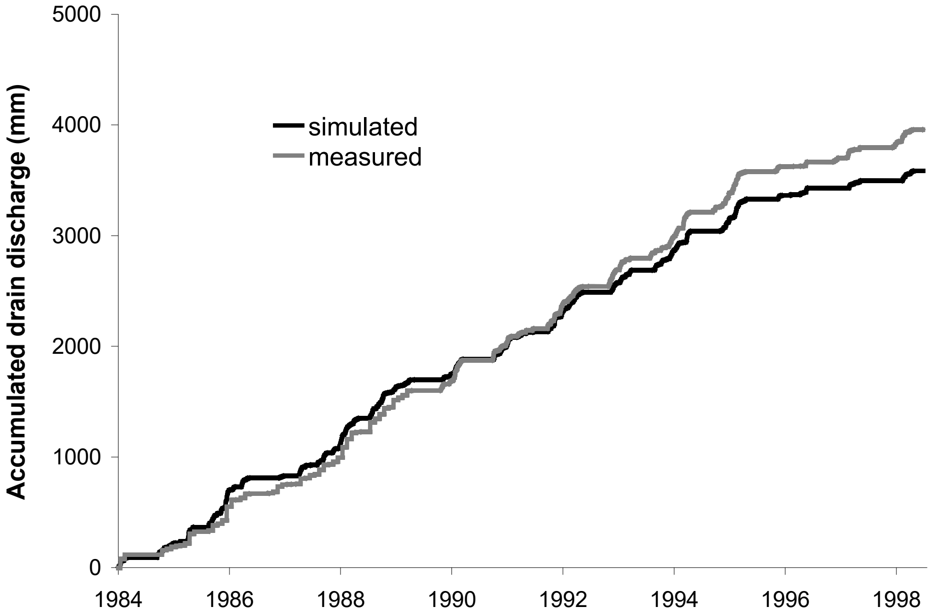

Fig. 3. Simulated and measured accumulated drain discharge (mean of all plots).

Table 4. Simulated mass balance per year (showing only the 'alternative' litter turnover parameterization, with k_l=0.055 d^{-1} and f_h=0.3) for the most important flows from July 1984 to June 1998 for the different treatments (as defined from 1989 to 1998). Denitrification and surface runoff are not shown separately since those flows where insignificant

Flows and storages	Treatment and plot number									
	0F *7*	0F cc *5*	1F *2*	1F cc *10*	1M eacc *8*	1M s cc *6*	1M s *1*	2M s *9*	2M eacc *3*	2M s cc *4*
	kg ha^{-1} yr^{-1}									
Deposition	10.4	10.4	10.4	10.4	10.4	10.4	10.4	10.4	10.4	10.4
Fertilization	0	0	97.1	97.1	49.1	49.1	49.1	49.1	49.1	49.1
Manure NH4-N	0	0	0	0	46.7	67.7	68.6	93.9	95.8	104.4
Manure Org-N	0	0	0	0	26.0	32.4	32.9	51.6	51.3	56.3
Σ Inputs	**10.4**	**10.4**	**107.5**	**107.5**	**132.2**	**159.6**	**161.0**	**205.0**	**206.6**	**220.2**
Harvest export [a]	23.4 (26.7)	22.9 (30.0)	75.3 (77.5)	72.6 (73.8)	55.9 (58.1)	78.9 (79.7)	85.1 (86.7)	77.9 (78.4)	72.8 (77.9)	80.7 (81.6)
Denitrification	0.5	0.4	0.5	0.5	0.5	0.4	0.5	0.6	0.6	0.6
Tile drains discharge [a]	22.8 (24.5)	16.4 (15.5)	34.2 (42.7)	27.6 (24.9)	39.7 (38.1)	25.1 (19.8)	35.5 (45.2)	61.0 (56.2)	59.8 (61.5)	54.1 (47.0)
To groundwater	4.2	3.0	5.7	4.6	6.9	4.5	6.2	11.0	10.3	9.5
Surface runoff	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.2
Σ Outputs	**51.0**	**42.8**	**115.8**	**105.4**	**103.1**	**109**	**127.4**	**150.6**	**143.6**	**145.1**
Mineral-N storage	1.4	0.4	3.8	2.0	2.4	7.0	9.1	18.9	3.9	15.4
Organic-N storage	-42.5	-32.7	-3.3	8.7	26.6	44.0	24.9	36.1	60.2	60.9
Plant-N storage	0.7	-0.1	-8.8	-8.5	-0.1	-1.2	-1.0	0.6	-1.2	-1.4
Σ Storage	**-40.4**	**-32.4**	**-8.3**	**2.2**	**28.9**	**49.8**	**33.0**	**55.6**	**62.9**	**74.9**
Net mineralization	69	69	80	85	95	93	84	86.0	111	96

Results

Water discharge

Figure 3. shows a comparison of simulated and measured accumulated drain discharge (mean of all plots). On the whole, the model closely reproduces the amount of water flowing through the tile drains. However the discharge is overestimated by about 30% compared with the measured mean discharge of all plots for the agrohydrological year 1985/86, and for 1997/98 the discharge is underestimated by about 45%. Tile-drain flow represents 81%, bypass flow to groundwater 16 % and surface runoff 3% of the simulated total discharge, respectively.

Mass balance and nitrogen uptake

Simulated nitrogen balances for the 14-year period are shown in table 4. The N export in harvest closely matched measured values except in the two non-fertilized treatments (*0F* and *0F cc*), where N removal is underestimated by 3 and 7 kg N ha-1 yr-1 (12 and 24%), respectively. It can be noted that in the *0F* and *0F cc* treatments, simulated total N outputs are 4 to 5 times higher than the inputs, while in the fertilized treatments (*1F* and *1F cc*) the outputs and inputs are quite similar, and in the treatments with added manure, the simulated inputs are always larger then the outputs. This was compensated for by a corresponding decrease of the organic N pool in the non-fertilized treatments (with 7% in the *0F* treatment) and an increase in the treatments with manure applications (with 9%

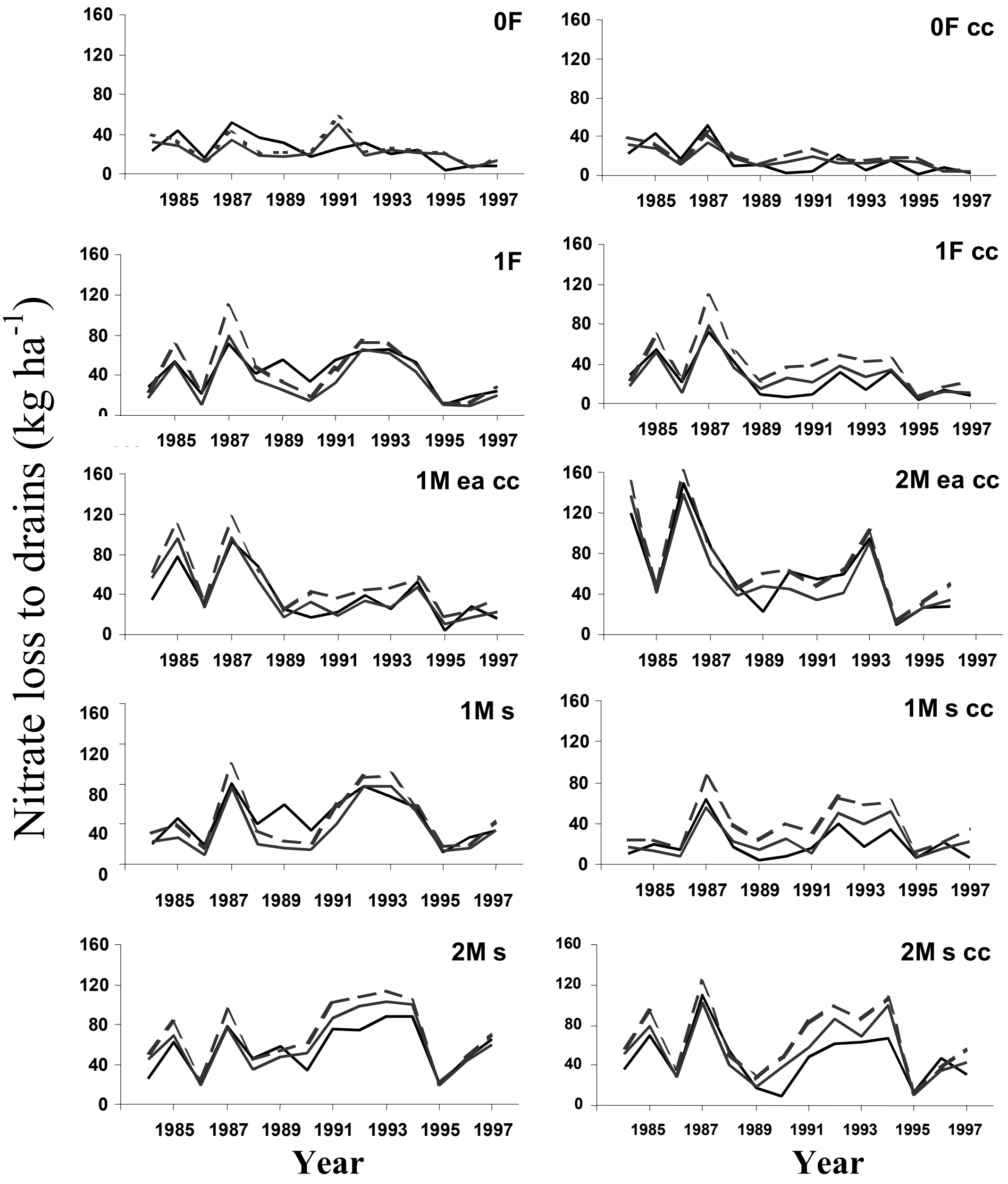

Fig. 4. Simulated with 'database' (grey broken lines), 'alternative' parameterization (grey full lines) and measured (black lines) mean annual NO_3-N discharge to drains for the 10 plots. The treatment acronyms can be explained as: *0F* denote no fertilization, *1F* normal dose mineral fertilizer, *cc* denotes cultivation of catch crops, *1M* denotes normal dose manure, *2M* double dose manure and *ea*, *la*, *s* denotes early autumn, late autumn and spring application of manure, respectively.

in the *2M s cc* treatment). The simulated N uptake of the catch crops is in close agreement with the measured uptake (not shown).

Table 5. Model efficiency (EF) for tile-drain discharge of NO3-N for the two simulations applying the 'database' and the alternative parameterization

Treatment	Model efficiency	
	parameter setting for litter turnover	
	'database'	'alternative'
0F	0.08	0.09
0F cc	0.41	0.53
1F	0.48	0.54
1F cc	0.06	0.79
1M ea cc	0.51	0.82
2M ea cc	0.78	0.84
1M s	0.59	0.44
1M s cc	-1.03	0.44
2M s	0.36	0.73
2M s cc	0.12	0.64
Mean	0.24	0.59

Nitrate leaching

As shown in Figure 4, the simulations match measured NO_3-N discharge for most treatments reasonably for both the described parameterization approaches. However, with the original 'database' parameterization (i.e. with the specific litter decomposition rate, k_l set to 0.035 d^{-1} and the litter carbon humification fraction, f_h set to 0.2) the average NO_3-N leaching for all plots is overestimated by almost 10 kg ha^{-1} compared to the measured leaching of 38 kg ha^{-1}. Using the ('alternative' parameterization with k_l set to 0.055 d^{-1} and f_h set to 0.3) both the average leaching (38 kg ha^{-1}) and the temporal pattern are nicely captured by the model, which is also indicated by the high model efficiency values (table 5). The simulated NO_3-N discharge (applying the 'alternative' parameterization) is especially close to measured discharge for the last three years, with a mean *EF* of 0.80. However, for the agrohydrological year 1989/90, the model underestimates leaching by 30 kg ha^{-1} for plot 2 (treatment *1F)* and by 42 kg ha^{-1} for plot 1 (treatment *1 M s*). As an average for all plots, with the 'alternative' parameterization, the simulated NO_3-N discharge to drains represents 85% and bypass flow to groundwater 15% of the total leaching, while NO_3-N losses via surface runoff is negligible.

Discussion

This comprehensive application of SOILNDB at the plot scale shows that leaching in this sandy loam/loamy sand textured soil can be satisfactorily described for a number of contrasting management practices and for a relatively long period (i.e. 14 years). However, to match measured leaching in this application, it was necessary to change some parameters connected to litter and faeces decomposition and mineralization. It is difficult to give a definite reason for the need of the site-specific adaptation of the litter turnover parameters. One reason may be that the decomposition and mineralization processes are not adequately described in the model, so that the specific mineralization constants are related to characteristics not accounted for. For example, the litter pool may need to be separated in different constituents within the plant litter, e.g. lignin, cellulose and hemicellulose (see review by Paustian et al., 1997). In such multi-pool decomposition models, specific decomposition rate constants are defined for each pool. However, refinement of the description of processes can only be justified if the processes do have a well-defined impact on the model output; and from a limited comparison with five nitrate leaching models, it could not be concluded that multi-pool decomposition models gave better predictions than models with only three organic N pools (Vereecken et al., 1991). Another reason may be that in SOILN, the effect of substrate availability is assumed to be negligible. However, soil tillage, repeated freezing and thawing, and wetting and drying may disrupt soil organic matter and increase substrate availability to the microbes (e.g. Soulides and Allison, 1961; Groffman and Tiedje, 1988; Scott et al., 1996). Additionally, erroneous values for the sensitive parameters governing the influence of temperature and moisture on the biological processes (Larocque and Banton, 1994) or of the initial size of the N and C pools may force a modification of other parameters connected to litter and faeces decomposition. As some parameters are interdependent, non-unique parameter sets may arise, and it can therefore be difficult to discover erroneous values for single parameter values. SOILN was applied by different modellers at 16 locations in the Nordic countries, resulting in 10 different parameter settings being used for organic matter turnover (Kätterer et al., 1999). This could either be interpreted as a result of the model not being generic, or as being due to a variation between different model users. The cause for this inconsistency in variation of parameter settings related to organic matter turnover should be further scrutinized.

The relatively poor match between simulated (with ‘alternative’ parameterization) and measured N removal with grain for the non-fertilized treatments (*0F* and *0F cc*) and the poorly simulated leaching for the *0F* treatment (EF=0.09) can probably be attributed to the parameter settings root development and N concentration in crop residues. For example, it is observed that fertilization promotes root development in cereals (Hansson and Andrén, 1987), and that rooting depth increases when N is supplied to soils with low natural fertility (Fehrenbacher et al., 1969). Hansson et al. (1987) found in a study with barley that a greater proportion of the production was localized below ground in the 0-fertilized treatment compared to the fertilized treatment receiving 120 kg N yr^{-1}. Measurements between 1990 and 1997 of the nitrogen concentration in the crop residues from the non-fertilized treatments (*0* and *0cc*) also showed significantly lower values, 0.67% N of dry mass, compared to an average of 0.79% for the fertilized treatments (Hessel Tjell et al., 1999). This is not explicitly accounted for in SOILNDB, which applies the same values for each crop type independent of fertilization level for the parameters governing root distribution, r_{frac}, and the maximum root depth, z_r, fraction of N in roots of total plant N, f_r, and concentration of N in residues, c_{N2}. Consequently, with extreme management practices such as in the non-fertilized treatment, deviations from the database parameter values can be significant and result in relatively poor simulated dynamics of the NO_3-N leaching. However, if data are available the ‘advanced user’ can easily change the appropriate parameters in the SOILNDB database for specific simulations.

The large discrepancies between simulated and measured leaching for plot 1 and 2 for the agrohydrological years 1988/89 to 1991/92 (see Fig. 4) may be explained by excavation work close to plot 1 in the summer 1988 that disturbed flows to tile drains. It is unclear how this influenced the NO_3-N concentrations, but it is evident that rather large tile-drain flows were recorded for plot 1 and 2 for this period. For example, from 1 July 1983 to 30 June 1986, before the excavation work, the tile-drain discharge was almost equal for plot 1 and 6 (682 and 673 mm, respectively). After the excavation work, from 1 July 1988 to 30 June 1992, the tile-drain discharge was 34% larger for plot 1 (1626 mm) compared to plot 6 (1217 mm). From 1 July 1995 to 30 June 1998, the differences were smaller again (14%).

It should be noted that in this study, the N applied in manure could be regarded as net input. That is, the volatilization losses are estimated from measurements and expert judgements combined with model calibrations (Torstensson and Johnsson, 1996; Torstensson and Aronsson, 2000) instead of using the values contained in the incomplete SOILNDB database (Larsson et al., 2002). Since manure-derived NH_4-N can contribute to a significant part of the total N input in areas with high animal densities (e.g. see table 6), great care should be employed to obtain a sound estimation of the volatilization losses when quantifying the impact of different strategies for application of manure on leaching.

In addition, the estimation routines and values contained in SOILNDB for initial content of humus, litter, NH_4-N and NO_3-N in the different soil layers were not employed. These data are instead taken from Torstensson and Johnsson (1996). Consequently, the estimation routines and values contained in SOILNDB are not tested in this respect. However, since the initial amount of humus is most critical, and the routine for calculation of initial amount of humus from soil organic matter is quite straightforward, the problem may rather be related to obtaining correctly measured amounts of soil organic matter.

Since this is a study with only one soil type and a limited variety of crops, additional applications under contrasting agro-environmental conditions (e.g. soils, climates, crop types etc.) are required to evaluate the general functionality of the SOILNDB model. However, this application gave promising results, especially regarding the ability to mimic the dynamics in accumulated yearly leaching, and also to correctly simulate the influence of different crops and catch crops as well as different manure strategies on leaching. If the model description or the parameterization related to humus mineralization or litter decomposition had been incorrect, this would almost certainly have resulted in an erroneous increase or decrease of the humus pool, and as a consequence, erroneous leaching. Hence, the excellent agreement between simulated and measured NO_3-N discharge for the last three years is particularly encouraging, indicating insignificant deviations in the calculated long-term changes in organic-N storage.

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APPENDIX

Table A1. Input data used in SOILNDB related to cultivation activities for the different plots (plot numbers given below column heads)

Year	Crop	Fertilization	Manure application				Sowing	Harvest	Ploughing		
			1, 6	4	9	3, 8			6	3, 4, 5, 8, 10	1, 2, 7, 9
1984	Spring rape	5 Apr.	3 April	12 Nov.	20 Sept.	20 Sept.	13 Apr.	2 Sept.	m.d., 3 Apr.	15 Nov.	15 Nov.
1985	Spring barley	22 Apr.	18 April	14 Nov.	25 Sept.	25 Sept.	6 May	26 Aug.	6 Sept.	18 Nov.	18 Nov.
1986	Oats	25 Apr.	28 April	10 Nov.	1 Oct.	1 Oct.	3 May	26 Aug.	16 Sept.	14 Nov.	14 Nov.
1987	Potatoes	8 May	7 May	17 Nov.	15 Oct.	15 Oct.	10 May	10 Sept.	12 Oct.	20 Nov.	20 Nov.
1988	Spring barley	25 Apr.	20 April	-	-	16 Sept.	27 Apr.	10 Aug.	22 Aug.	4 Nov.	4 Nov.
1989	Oats	19 Apr.	18 Apr.	18 Apr.	18 Apr.	20 Sept.	20 Apr.	18 Aug.	No ploughing	No ploughing	20 Nov.
1990	Spring wheat	7 Apr.	6 Apr.	6 Apr.	6 Apr.	11 Oct.	9 Apr.	24 Aug.	6 Apr. [a]	6 Apr. [a]	20 Nov.
1991	Spring barley	12 Apr.	9 Apr.	9 Apr.	9 Apr.	18 Sept.	13 Apr.	22 Aug.	10 Apr. [a]	10 Apr. [a]	29 Nov.
1992	Potatoes	20 May	13 May	13 May	13 May	27 Oct.	21 May	17 Aug.	15 May [a]	15 May [a]	16 Nov.
1993	Spring barley	10 Apr.	29 Mar.	29 Mar.	29 Mar.	16 Sept.	13 Apr.	18 Aug.	31 Mar. [a]	31 Mar. [a]	16 Nov.
1994	Oats	20 Apr.	7 Apr.	7 Apr.	7 Apr.	14 Sept.	21 Apr.	9 Aug.	8 Apr. [a]	8 Apr. [a]	14 Nov.
1995	Spring rape	26 Apr.	10 Apr.	10 Apr.	10 Apr.	13 Sept.	27 Apr.	24 Aug.	12 Apr. [a]	12 Apr. [a]	9 Nov.
1996	Spring wheat	26 Apr.	17 Apr.	17 Apr.	17 Apr.	19 Sept.	24 Apr.	5 Sept.	18 Apr. [a]	18 Apr. [a]	12 Nov.
1997	Spring barley	15 Apr.	9 Apr.	9 Apr.	9 Apr.	12 Sept.	16 Apr.	11 Aug.	11 Apr. [a]	11 Apr. [a]	15 Nov.
1998	Oats	22 Apr.	20 Apr.	20 Apr.	20 Apr.	10 Oct.	22 Apr.	25 Aug.			18 Nov.

Table A2. Input data used in SOILNDB for harvest yields with concentration of N in the harvested product given in parenthesis. The yields are given for the ten plots at water contents of 15, 9 and 79%, for cereals, rape, and potatoes, respectively, whereas the N concentration is given for dry matter

Year	Crop	Harvest yield (kg ha^{-1}) and N concentration in the harvested product (%) for the ten plots									
		1	2	3	4	5	6	7	8	9	10
1984	Spring rape	1810	2760	1860	1660	950	1540	950	1430	1210	2760
		(3.38)	(3.75)	(3.16)	(2.91)	(2.72)	(3.28)	(2.72)	(2.96)	(2.92)	(3.75)
1985	Spring barley	5640	5530	4820	4080	2640	5620	2640	4030	3730	5530
		(1.77)	(1.64)	(1.73)	(1.59)	(1.69)	(1.65)	(1.69)	(1.55)	(1.55)	(1.64)
1986	Oats	5000	4940	4930	4340	2600	4900	2600	4180	3800	4940
		(1.76)	(1.55)	(1.74)	(1.65)	(1.13)	(1.73)	(1.13)	(1.46)	(1.55)	(1.55)
1987	Potatoes	38600	36900	36900	37600	22300	39900	22300	36500	32600	36900
		(1.25)	(1.21)	(1.16)	(1.11)	(0.81)	(1.37)	(0.81)	(0.99)	(1.01)	(1.21)
1988	Spring barley	4430	3980	3570	3450	1810	3930	1810	3160	2970	3980
		(2.15)	(1.95)	(1.88)	(1.81)	(1.75)	(2.19)	(1.75)	(1.71)	(1.74)	(1.95)
1989	Oats	5010	4400	4220	3780	2920	3190	2170	3360	4300	4400
		(2.26)	(1.95)	(2.03)	(2.35)	(1.59)	(1.98)	(1.55)	(1.91)	(2.03)	1.95)
1990	Spring wheat	6570	5940	4710	4970	1350	5140	2100	3340	5970	4520
		(2.02)	(2.03)	(1.86)	(2.39)	(1.86)	(1.97)	(1.7)	(1.76)	(2.13)	(1.69)
1991	Spring barley	5850	5900	6180	5150	2720	6150	1240	5600	5130	5720
		(1.66)	(1.32)	(1.82)	(2.32)	(1.23)	(1.58)	(1.14)	(1.43)	(2.29)	(1.28)
1992	Potatoes	24000	28000	30000	29000	19000	32000	21000	28000	33000	32000
		(1.66)	(1.56)	(1.48)	(1.69)	(0.94)	(1.49)	(1.0)	(1.18)	(1.51)	(1.17)
1993	Spring barley	3200	3060	3700	3850	2430	3690	1900	3130	3740	3400
		(2.43)	(2.28)	(2.27)	(2.75)	(1.54)	(2.40)	(1.49)	(2.18)	(2.72)	(2.25)
1994	Oats	3850	3360	3650	2460	1960	3050	1270	3220	3050	2980
		(1.59)	(1.47)	(1.90)	(2.05)	(1.25)	(1.89)	(1.31)	(1.57)	(1.93)	(1.66)
1995	Spring rape	2000	2160	2250	2740	50	1980	50	1410	2560	1850
		(3.48)	(3.04)	(3.03)	(3.65)	(2.63)	(3.51)	(2.66)	(2.89)	(3.50)	(3.17)
1996	Spring wheat	4720	4950	4200	3900	2200	4160	2350	3910	3890	4040
		(2.71)	(1.99)	(2.00)	(2.80)	(1.58)	(2.56)	(1.50)	(1.78)	(2.83)	(1.99)
1997	Spring barley	5160	4060	4330	4780	1620	4760	890	3750	4980	4480
		(1.65)	(1.41)	(1.74)	(2.34)	(1.61)	(1.79)	(1.63)	(1.49)	(2.22)	(1.43)
1998	Oats	6200	5310	6440	5650	2600	5450	1840	5550	5050	5780
		(1.87)[a]	(1.66)[a]	(1.89)[a]	(2.02)[a]	(1.32)[a]	(1.87)[a]	(1.33)[a]	(1.65)[a]	(1.84)[a]	(1.72)[a]

[a] Calculated for each plot as the mean of measured N concentration in oats the other years.

APPENDIX II

List of symbols

Symbol	parameter defenition	value	unit in source	equation number	source	name in SOILNDB	name in SOIL/SOILN
	SOIL-soil hydrology and plotpf						
k_s	saturated hydraulic conductivity	table 3	cm hr^{-1}	4	autopar.mdb	SATC	SATC
k_{sm}	saturated hydraulic conductivity including macropores	table 3	cm hr^{-1}	5	autopar.mdb	SATCT	SATCT
λ	pore size distribution index	table 3	—	2, 4	autopar.mdb	LAMBDA	LAMBDA
θ_r	residual water content	table 3	vol %	2	autopar.mdb	RES	RES
θ_s	porosity	table 3	vol %	2, 3, 5	autopar.mdb	PORO	PORO
ψ_a	air entry pressure	table 3	cm water	2, 4	autopar.mdb	PSIE	PSIE
θ_w	water content at wilting point (at pF 4.2)	table 3	vol %	1	autopar.mdb	WILT	WILT
ψ_x	upper limit for use of the Brooks & Corey expression	table 3	cm water	1, 2	autopar.mdb	XPSI	XPSI
A_{0T}	empirical coefficient	0.54	—	—	autopar.mdb	A0T	A0T
A_{1T}	empirical coefficient	0.025	—	—	autopar.mdb	A1T	A1T
n_{var}	tortuosity factor in the Mualem equation	1; 5	—	4	autopar.mdb	NVAR	NVAR
ψ	calculated soil water tension	—	cm water	1, 2, 4, 5	—	—	—
θ	calculated water content	—	vol %	1 - 3	—	—	—
ψ_{wilt}	soil water tension at wilting point	15000	cm water	1, 4	—	—	—
θ_x	calculated water content at ψ_x	—	vol %	1	—	—	—
ψ_m	threshold tension for the use of the Brooks & Corey expression	—	cm water	2 - 5	—	—	—
ψ_0	lower range in the linear expression in the retention function	0	cm water	3, 5	—	—	—
k_w	calculated unsaturated hydraulic conductivity	—	cm hr^{-1}	4, 5	—	—	—
	upper depth of the soil layer, used in 'soilp.dat'	—	cm	—	autopar.mdb	UDEP	UDEP
	lower depth of the soil layer, used in 'soilp.dat'	—	cm	—	autopar.mdb	LDEP	LDEP
	replicate number of soil profile, used in 'soilp.dat'	—	—	—	autopar.mdb	UNUM	UNUM
	profile number, used in 'soilp.dat'	—	—	—	autopar.mdb	UPROF	UPROF

SOIL – evapotransp.

$t_{\mathrm{day}}(\mathrm{i})$	day number for specification of temporal variation within year	6	julian day	autopar.mdb	daynum(i)	DAYNUM(i)
$d_{\mathrm{h}}(t_{\mathrm{day}}(\mathrm{i}))$	displacement height	7	m	autopar.mdb	displv(i)	DISPLV(i)
$l_{\mathrm{ai}}(t_{\mathrm{day}}(\mathrm{i}))$	leaf area index	7	—		laiv(i)	LAIV(i)
$z_0(t_{\mathrm{day}}(\mathrm{i}))$	roughness length	8	m	autopar.mdb	roughv(i)	ROUGHV(i)
$r_{\mathrm{s}}(t_{\mathrm{day}}(\mathrm{i}))$	surface resistance	8	s m^{-1}	autopar.mdb	rsv(i)	RSV(i)
r_{sint}	surface resistance for intercepted water	5,0	s m^{-1}	autopar.mdb	intrs	INTRS
a_{r}	albedo of vegetation and soil	20	—	autopar.mdb	albedo	ALBEDO
$c_{\mathrm{form}}(t_{\mathrm{day(i)}})$	shape coefficient	1	—	autopar.mdb	cform(i)	CFORM
i_{LAI}	interception storage capacity of canopy	0.2	mm LAI^{-1}	autopar.mdb	intlai	INTLAI
d_{lat} (s)	latitude of site			climate.mdb	latitud	LATID
	SOIL –water uptake					
r_{frac}	root fraction	0.05	—	SOIL	RFRACLOW	RFRACLOW
$z_{\mathrm{r(i)}}$	root depth (at different dates defined by $t_{\mathrm{root(i)}}$)	table 9, 10	m	autopar.mdb VB-code	rootdep(i)_soil nrootdep2	ROOTDEP(i)
$t_{\mathrm{root(i)}}$	dates defining root development stages	table 10	julian day	VB-code	rootti(i)	ROOTT(i)
f_{umov}	degree of compensatory uptake of water	0.5	—	SOIL	UPMOV	UPMOV
t_1	temperature coefficient	0.8	—	autopar.mdb	wupate	WUPATE
t_2	temperature coefficient	0.4	—	autopar.mdb	wupbte	WUPBTE
ψ_{c}	critical soil water tension where reduction of transpiration begins	table 5	cm water	autopar.mdb	wupcri	WUPCRI
p_1	parameter in water tension respons function for transpiration	0.2	day mm^{-1}	autopar.mdb	wupf	WUPF
p_2	parameter in water tension respons function for transpiration	0	—	autopar.mdb	wupfb	WUPFB
	SOIL – soil evapaporation					
r_{alai}	aerodynamic resist.	50	s m^{-1}	autopar.mdb	ralai	RALAI
k_{rn}	extinction coefficient		LAI^{-1}	autopar.mdb	rntlai	RNTLAI
r_{ψ}	empirical coefficient used to calculate soil surface resistance	200 sand; 100 loamy sand	s m^{-1}	autopar.mdb	psirs	PSIRS
	SOIL - temperature					
T_{ini}	initial soil temperature	8	°C	VB-code	ITEMPS	ITEMPS
y_{cycle}	length of cycle of analytical air temperature	365	days	VB-code	YCH	YCH
t_{ph}	phase shift of analytical air tempemperature	18	days	VB-code	YPHAS	YPHAS
T_{amean}	mean value in the analytical air temperature function	8	°C	VB-code	YTAM	YTAM

T_{aamp}	amplitude in the analytical air temperature function	10	°C		VB-code	YTAMP	YTAMP
	SOIL -Frost						
fc_{i}	decrease of unsat. hydraulic conductivity due to freezing	table 5	—		autopar.mdb	fcond	FCOND
d_1	fraction of wilting point remaing as unfrozen water at –5°C	table 5	—		autopar.mdb	fwfrac	FWFRAC
d_2	coefficient in the freezing point depression function	table 5	—		autopar.mdb	fdf	FDF
	SOIL -Snow						
T_{max}	rain temp. threshold	2	°C		VB-code	PRLIM	PRLIM
T_{min}	snow temperature threshold	-2	°C		VB-code	PSLIM	PSLIM
S_1	radiation melt factor for old snow	2.5	—		VB-code	SAGEM1	SAGEM1
S_2	snow age coefficient in radiation melt respons on snow	0.1	—		VB-code	SAGEM2	SAGEM2
P_{samin}	limit for snow age updating	5	mm day^{-1}		VB-code	SAGEZP	SAGEZP
Q_{samin}	thermal quality limit for snow age updating	0.9	—		VB-code	SAGEZQ	SAGEZQ
S_{dl}	liquid water coefficient in snow density function	100	kg m^{-3}		VB-code	SD1OL	SD1OL
S_{dw}	water equivalent coefficient in snow density funct.	0.9	m^{-1}		VB-code	SD2OM	SD2OM
ρ_{smin}	snow density of newly formed snow	100	kg m^{-3}		VB-code	SDENS	SDENS
S_{wlmin}	threshold liquid water storage of snow	3	kg m^{-2}		VB-code	SLWL0	SLWL0
m_{f}	refreezing efficiency coefficient in snow melt function	0.1	m		VB-code	SMAFR	SMAFR
m_{Rmin}	minimum value of global radiation influence in snow melt funct.	1e-007	mm J^{-1}		VB-code	SMRIS	SMRIS
m_{T}	temperature coefficient in snow melt function	3	mm day^{-1} °C^{-1}		VB-code	SMTEM	SMTEM
f_{ret}	retention capacity of snow	0.07	—		VB-code	SRET	SRET
s_{k}	thermal conductivity coefficient for snow	2.86e-006	Wm^4 kg^{-2}		VB-code	STCON	STCON
	SOIL – other						
ψ_{ini}	initial soil tension	100	cm water		VB-code	IPOT	IPOT
T_{ini}	initial soil temperature	?			?	?	IPOT
n^{o}	number of layers	5	—		VB-code	NUMLAY	NUMLAY
$z(l)$	layer thickness	0.25/0.25/ 0.25/0.25/ 0.5	m	6, 7, 8	VB-code	thick(i)	THICK(i)
$c_{\mathrm{rain\ (s)}}$	correction coefficient for rain precipitation	1.18	—	—	climate.mdb	preca0	PRECA0
$c_{\mathrm{snow\ (s)}}$	addition correction coefficient for snow precipitation	0.20	—	—	climate.mdb	preca1	PRECA1
	thickness of layers 1 to 5 used in ‘soilp.dat’	0	—	—	VB-code	UTHICK(i)	UTHICK(i)
	multiplicative factor for all layer thicknes	1	—	—	VB-code	VC	VC

	technical: division factor in time step integration calculation	2	—	—	VB-code	XADIV	XADIV
	lower limit to calculate convective heat flow	10	—	—	VB-code	XINFLI	XINFLI
	technical: recalculation frequency	2	—	—	VB-code	XLOOP	XLOOP
	technical: number of layers for recalculation frequency	4	—	—	VB-code	XNLEV	XNLEV
		20		—	VB-code	STPMAX 20	STPMAX
		50		—	VB-code	STXTGD 50	STXTGD

SOILN-Plant N uptake and management

u_{a1}	N uptake parameter for main uptake period for all crops but ley	—	g m^{-2} yr^{-1}	12	VB-code	upa1(i)	UPA(i)
u_{a2}	N uptake parameter for catch crop	—	g m^{-2} yr^{-1}		indata	upa2	UPA(i)
u_{a3}	N uptake parameter for winter crops during the autumn period	table 15	g m^{-2} yr^{-1}	13	autopar.mdb	upa3	UPA(i)
u_{b1}	coefficient in plant N uptake function	table 15	g m^{-2} yr^{-1}	12	autopar.mdb	upb1	UPB(i)
u_{b2}	coefficient in plant N uptake function for catch crops during the autumn period	table 16	g m^{-2} yr^{-1}		autopar.mdb	c_upb2	UPB(i)
u_{b3}	coefficient in plant N uptake function for winter crops during the autumn period	table 15	g m^{-2} yr^{-1}	13	autopar.mdb	upb3	UPB(i)
u_{c1}	coefficient in plant N uptake function	table 15	d^{-1}	12	autopar.mdb	upc1	UPC(i)
u_{c2}	coefficient in plant N uptake function for catch crops during the autumn period	table 16	d^{-1}		autopar.mdb	c_upc2	UPC(i)
u_{c3}	coefficient in plant N uptake function for winter crops during the autumn period	table 15	d^{-1}		autopar.mdb	upc3	UPC(i)
$u_{a(i)L}$	N uptake parameter for the first and second uptake period for ley	—	g m^{-2} yr^{-1}	15	VB-code	upa1(i)	UPA(i)
N_{L3up}	potential N uptake of ley after the last harvest each year or if no harvest is specified	table 16	g m^{-2} yr^{-1}	14	autopar.mdb	upa	UPA(i)
u_{aiL}	N uptake parameter for undersown ley	7	g m^{-2}		VB-code	upa2(i-1)	UPA(i)
$u_{b(i)L}$	coefficient in plant N uptake function, ley	0.3	g m^{-2} yr^{-1}	15	autopar.mdb	upb1(i)	UPB(i)
u_{biL}	coefficient in plant N uptake function, undersown ley	0.3	g m^{-2} yr^{-1}		autopar.mdb	i_upb	UPB(i)
$u_{c(i)L}$	coefficient in plant N uptake function, ley	0.045; 0.09;0.09	d^{-1}	15	autopar.mdb	upc1	UPC(i)
$u_{c(i)L}$	coefficient in plant N uptake function, ley	0.06;0.09	d^{-1}	15	autopar.mdb	upc2	UPC(i)
$u_{c(i)L}$	coefficient in plant N uptake function, ley	0.09	d^{-1}	15	autopar.mdb	upc3	UPC(i)
u_{ciL}	coefficient in plant N uptake function, undersown ley	0.08	d^{-1}	15	autopar.mdb	i_upc	UPC(i)
u_{au}	pot. N uptake of insown ley in the autumn after harvest of the main crop	7	g m^{-2} yr^{-1}		autopar.mdb	i_upa	UPA(i)
$u_{st(i)}$	start of plant uptake period, spring crops	—	julian day		VB-code	s_tdp(i)+12	UPST(i)
$u_{st(i)}(s)$	start of plant uptake period, winter crops (w.c.) and ley	100 (w.c.)	julian day		climate.mdb	w_(i)_upst1	UPST(i)

$u_{\mathrm{st(i)}}$	start of plant uptake period, undersown ley and catch crops	95 (ley)	julian day		VB-code	ley_upst1 upst1, upst2(i)	UPST(i)
$t_{\mathrm{sk(i)}}$	harvest date, all crops but ley	—	julian day		indata	sk_tdp(i)	UPET(i)
$u_{\mathrm{et(i)}}$	end of plant uptake period, catch crops	365	julian day		VB-code? autopar.mdb	upet3 i_upet c_upet2	UPET(i)
$u_{\mathrm{et(i)}}(\mathrm{S})$	end of plant uptake period, winter crops (w.c.) and ley	364 (w.c.) 334 (ley)	julian day		climate.mdb	w_(i)_upet3 ley_upet3 ley_i_upet3	UPET(i)
f_{ma}	fraction of N available for plant uptake	0.08	d^{-1}		autopar.mdb	upma	UPMA
f_{harv}	harvested fraction of plant N	—	—	19	calculated	harhp1(i)	HARHP(i)
f_{harvL}	harvested fraction of plant N, ley and catch crops (c.c.)	0.5 ley 0 (c.c.)	—	14, 15	autopar.mdb	harhp(i); ploughing of ley harhp(i) c_harhp2	HARHP(i)
f_{s}	above ground residue fraction of plant N at harvest	—	—	20	calculated	HARAR	HARAR(i)
f_{sL}	above ground residue fraction of plant N at harvest and at the end of the uptake period, ley and catch crops	table 16	—		autopar.mdb	harar(i); ploghing of ley harar(i); i_harar c_harar2	HARAR(i);
f_{lr}	regulating plant death during winter, for winter crops	1	—	13	autopar.mdb	harlr3	HARLR(i)
f_{reslr}	fraction of living root-N remaining after harvest	0	—	20	autopar.mdb	harlr1 C_harlr2	harlr1
$C/N_{\mathrm{hres(y,c)}}$	C/N ratio of above ground residues	—	—	21	calculated	cnares(i)	CNARES
$C/N_{\mathrm{root(c)}}$	C/N ratio of roots	20	—		calculated	cnroot	CNROOT
r_{fracN}	root fraction	0.001	—		autopar.mdb	rfraclow	RFRACLOW
f_{umov}	degree of compensatory uptake of N	1	—		autopar.mdb	upmov	UPMOV
$t_{\mathrm{root(i)}}$	dates defining root development stages	table 10	julian day		VB-code	nrootti(i)	ROOTT(i)
	SOILN-mineralisat. and immobilisation						
r_{o}	C-N ratio of microorganisms and humified products	10	—	6, 7	autopar.mdb	cnorg	CNORG
f_{efe}	effic. in intern. synth. of micro. biomass and metabolites in faces	0.5	—		autopar.mdb	feceff	FECEFF
f_{chf}	faeces carbon humification fraction	0.2	—		autopar.mdb	fechf	FECHF
k_{f}	rate constant for faces decomposition	0.035	d^{-1}		autopar.mdb	feck	FECK
k_{h}	rate constant for humus mineralisation	0.00006	d^{-1}		autopar.mdb	humk	HUMK
f_{e}	effic. in intern. synth. of micro. biomass and metabolites in litter	0.5	—		autopar.mdb	liteff	LITEFF

f_h	litter carbon humification fraction	0.2	—		autopar.mdb	lithf	LITHF
k_l	rate constant for litter decomposition	0.035	d^{-1}		autopar.mdb	litk	LITK
k_n	specific nitrification rate	0.2	d^{-1}		autopar.mdb	nitk	NITK
n_q	NO_3-N:NH_4-N ratio in nitrification function	6	—		autopar.mdb	nitr	NITR
	ploughdepth	0.25	m		VB-code	PLOUGHDEP	PLOUGHDEP
	date for ploughing	—	julian day		VB-code	j_tdp(i)	PLOUGHDAY
	SOILN-soil moisture respons						
$\Delta\theta 1$	water cont. related to soil moisture respons on biological activity	table 12	%		autopar.mdb	mos1	MOS(1)
$\Delta\theta 2$	water cont. related to soil moisture respons on biological activity	table 12	%		autopar.mdb	mos2	MOS(2)
xm	empirical const. in soil moist funct.	table 12	—		autopar.mdb	mosm	MOSM
e_s	coef. defining the relative effect of moist. when the soil is satur.	table 12	—		autopar.mdb	mossa	MOSSA
	SOILN-denitrification						
$\theta_d(z)$	water content range in funct. for soil moist effect on denitrificat.	17	vol %		autopar.mdb	mosden	MOSDEN
d	empirical constant	2	—		autopar.mdb	dend	DEND
c_s	half-saturation constant, gives the effect of nitrate concentration	10	mg N l^{-1}		autopar.mdb	denhs	DENHS
d_{frac}	fraction of potential denitrification in soil layers	0.7/0.3/0/0/0	—		VB-code	DFRAC(i)	DFRAC(i)
k_d	potential rate of denitrification	0.1	gN m^{-2} d^{-1}		autopar.mdb	denpot	DENPOT
	SOILN-soil temperature respons						
t_b	temp. at which the temp. effect in the Q_{10}- function equals 1	20	°C		autopar.mdb	tembas	TEMBAS
Q_{10}	respons to a 10°C temperature change on biological activity	2	—		autopar.mdb	temq10	TEMQ10
	SOILN-manure						
CN_{fec}	C-N ratio of faeces in manure	table 1			input data to SOILNDB; autopar.mdb	C-N ratio	CNFEC
t	date of manure application	—	julian day	10	input data to SOILNDB	MANET(i) MANST(i)	MANET(i) MANST(i)
N_{faeces}	amount N in faeces in manure	—	gN m^{-2}	9	VB-code	xmanfn(i)	MANFN(i)
N_{amm}	amount N in ammonium in manure	—	gN m^{-2}	10	VB-code	xmannh(i)	MANNH
	amount N in bedding in manure	0	gN m^{-2}		VB-code	MANLN(i)	MANLN(i)
	C-N ratio of bedding in manure	40	—		VB-code	CNBED	CNBED
	mixing depth of applied manure in to the soil	0.1	m		VB-code	MANDEPTH	MANDEPTH

SOILNDB-manure

$c_{\mathrm{ammN}}(\mathrm{m})$	concentration of NH_4-N in manure	table 1	kg N ton^{-1}	10	input; autopar.mdb	Ammonium content	—
$c_{\mathrm{orgN}}(\mathrm{m})$	concentration of organic N in manure	table 1	kg N ton^{-1}	9	input; autopar.mdb	Organic N-content	—
F_{sloss}	volatilisation loss of NH_3	table 2	%	10	input; autopar.mdb		—
m	type of manure	table 1	—	9, 10	input; autopar.mdb		—
M	applied amount of manure	—	ton	9, 10	input	st_giva(i)	—
a	application technique of manure	—	—	10	input; autopar.mdb		—

SOILNDB-plant uptake and harvest

N_{harv}	target N yield	—	kg ha^{-1}	16, 17, 19	VB-code	malskord(i)	—
N_{harvL}	target N yield for ley	—	kg ha^{-1}	18	VB-code	malskord(i)	—
N_{totup}	target N uptake	—	g m^{-2}	11 – 15, 19	VB-code	U	—
S_1	target harvest yield of all crops excluding ley	—	kg ha^{-1}	11, 13, 16, 17	input	sk_avk1(i)	
$S_{\mathrm{L(i)}}$	target ley yield for first and second harvest	—	kg ha^{-1}	14, 15, 18	input	sk_avk1(i)	
c_{N1}, c_{N3}	nitrogen concentration in the harvested product	table 14	%	11, 13-18	autopar.mdb	grain N content	—
c_{N2}	nitrogen concentration in above ground residues	table 14	%	11, 13, 17, 21	autopar.mdb	residues N content	—
C_{C2}	carbon concentration in plant biomass	0.5		21	autopar.mdb	residues_C_content	—
wc_2	water content in above ground residues	table 14	%	21	autopar.mdb	water content for residues N content values	—
f_{a}	ratio of above ground residues to grain biomass	table 14	—	11, 13, 20	autopar.mdb	residues: grain ratio	—
f_{b}	straw/grain ratio	table 14	—	17	autopar.mdb	straw:grain ratio	—
f_{r}	fraction of N in roots of total plant N	table 14	—	11, 13, 20	autopar.mdb	rootN:plantN fraction	—

$t_{s(i)}$	sowing date	—	julian day		indata to SOILNDB	s_tdp(i)	
t_{up}	length of the uptake period	—	days	12, 15	VB-code	t	—
y	year	—	—	11, 13-19, 21	indata to SOILNDB	—	—
c	crop type	—	—	11, 13, 17, 19, 21	indata to SOILNDB	—	—
	SOILN-initial conditions						
—	initial content of NO3-N for each soil layer	1, 0.5, 0.3, 0.2, 0	g m^{-2}		VB-code	no3(i)	NO3(i)
—	initial content of NH4-N for each soil layer	1, 0.5, 0.3, 0.2, 0	g m^{-2}		VB-code	nh4(i)	NH4(i)
$N_{lom}(l)$	initial content of litter N for each soil layer	—	g m^{-2}	6	VB-code	nlit(i)	NLIT(i)
$N_{hom}(l)$	initial content of humus N for each soil layer	—	g m^{-2}	7	VB-code	nh(i)	NH(i)
$C_{lom}(l)$	initial content of litter C for each soil layer	—	g m^{-2}	8	VB-code	cl(i)	CL(i)
—	initial content of C in faeces	0	g m^{-2}	—	VB-code	CF(i)	CF(i)
—	initial content of N in faces	0	g m^{-2}	—	VB-code	NF(i)	NF(i)
—	initial accumulcted denitrification	0	g m^{-2}	—	VB-code	DENIT	DENIT
—	initial accumulcted N leaching	0	g m^{-2}	—	VB-code	DLOSST	DLOSST
—	initial content of N in plant	0	g m^{-2}	—	VB-code	PLANT	PLANT
—	initial content of N in fertilizer pool	0	g m^{-2}	—	VB-code	FERT	FERT
—	initial content of N in above ground residues	0	g m^{-2}	—	VB-code	LITABOVE	LITABOVE
	SOILNDB-initial conditions						
r_{lh}	litter-humus ratio	0.01		6 - 8	autopar.mdb	ini_lit_hum_ratio	—
		0.1			autopar.mdb	sub_SOM_Content	
$c_{Com(l)}$	fraction of C in soil organic matter	0.58		8	autopar.mdb	SOM_C_Content	
		10			autopar.mdb	SOM_CN_Ratio	CNORG???
$\rho(l)$	dry bulk density for the top soil (0-25 cm)	1.35	g cm^{-3}	6 - 8	autopar.mdb	db_dens_top	
$\rho(l)$	dry bulk density for the top soil (25-150 cm)	1.45	g cm^{-3}	6 - 8	autopar.mdb	db_dens_sub	
$SOM(l)$	soil organic matter content	—	%	6 - 8	input data to SOILNDB	top_SOM_Content	
$SOM(l)$	soil organic matter content	—	%	6 - 8	input data to SOILNDB	sub_SOM_Content	