Modelling of soil nitrogen dynamics within the decision support system DANUBIA

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ABSTRACT

Within the GLOWA-Danube project, the integrated decision support system DANUBIA was developed to address effects of global change on water resources of the Upper Danube watershed (~80,000 km^2). Key components of DANUBIA in respect to water quality and plant growth modelling are nitrogen turnover, nitrogen fluxes and storages. This paper discusses an approach to model soil nitrogen dynamics in a mesoscale watershed. Within the model, the soil column is represented by three soil layers. The model components for water fluxes, nitrogen uptake and nitrogen transformation are process-based. To validate the model, field data from four locations were used. Nitrogen modelling results are in good agreement with measured data. Statistical analysis for soil nitrogen and water content resulted in satisfactory indices of agreement. The study demonstrated that the coupled soil moisture and soil nitrogen transformation model is suitable to simulate the fate of mineral nitrogen within the soil profile on the field scale. Sensitivity studies indicate that the model quality for large scale modelling depends particularly upon the appropriate representation of sandy soils, the accurate parameterization of the saturated hydraulic conductivity and the precise initialization of soil mineral nitrogen content.

1. Introduction

Human impact on ecological cycles is highly evident in the industrial capture of atmospheric nitrogen for use in agricultural fertilizers. Nearly all ecosystems (especially agroecosystems) show an imbalance of nitrogen receipts and subsequent losses to surface waters (Schlesinger et al., 2006). Excessive nitrate availability within ecosystems affects the environment due to leaching through soils to groundwater and streams, thereby depleting soil minerals, acidifying soils and altering downstream freshwater and coastal marine ecosystems (Vitousek et al., 1997). Negative implications also arise from exaggerated nitrogen fertilization which contributes to rising N_2O-emissions affecting the climate system (Jungkunst et al., 2006). While the basic processes of nitrogen turnover are well understood, there is still plenty of uncertainty in magnitude and rates of nitrogen cycling at the watershed and river basin scale (Schlesinger et al., 2006), which prevents effective watershed nitrogen management. To improve and protect water quality on the watershed scale, EU member states are obliged to meet the requirements of the Water Framework Directive (EC, 2000). Following the Nitrate Directive (EC, 1991), critical zones for water quality must be identified and action programmes initiated.

To improve the understanding of N-cycling in agricultural landscapes, numerous models have been developed, addressing different environmental situations on various scales (plot to watershed). As previous studies have shown (Diekkrüger et al., 1995; Kroes and Roelsma, 2007; Post et al., 2007), process-oriented ecosystem models such as: ANIMO (Rijtema and

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Kroes, 1991), CERES (Jones and Kiniry, 1986), ECOSYS (Grant, 1995), EXPERT N (Priessack et al., 2001), DAISY (Svendsen et al., 1995), HERMES (Kersebaum, 1995) or LEACHN (Johnson et al., 1999) simulate soil nitrogen dynamics for advisory purposes (e.g. optimizing N-fertilization, predicting crop yield, preventing nitrate leaching to the groundwater) mainly on the field scale. Model validation with experimental data demonstrated the suitability of models for effective nitrogen management on the field scale facilitating the derivation of management options for potential stakeholders such as farmers or politicians (Kersebaum et al., 2006).

For the assessment of global change impacts on the regional scale, process-based and spatially distributed modelling approaches are required. Simple statistical or conceptual deterministic models are not appropriate to investigate future water quality development due to their lack of sensitivity to climate changes. Various studies with models that are based on statistical modelling approaches combined with GIS-bases were conducted to simulate actual N-dynamics on the regional scale, e.g. MAGPIE (Lord and Anthony, 2000) and STONE (Wolf et al., 2005). In recent years, some process-based regional models dealing with water quality have also been developed, often combining state-of-the-art hydrological models with N-model components, e.g. SHETRAN (Birkinshaw and Ewen, 2000), MIKE-SHE/Daisy (Styczen and Storm, 1993; Refsgaard et al., 1999), SWIM (Krysanova and Haberlandt, 2002; Krysanova et al., 2007) or PROMET-V (Schneider, 2003). These process-based models have demonstrated their capability to model N-cycling on the watershed scale and facilitate temporal extrapolation.

For a broader view on effects of climate change on the water- and nitrogen-cycle in mesoscale watersheds, models should not only be driven by changes in climatic inputs, but also by human interaction. Against this background, the decision support system DANUBIA was developed within the GLOWA-Danube project (Mauser and Ludwig, 2002; Ludwig et al., 2003; Barth et al., 2003). DANUBIA combines models from socioeconomics and natural sciences to evaluate the consequences of global climate change on water-, carbon- and nitrogen-fluxes in the 80,000 km^2 watershed of the Upper Danube.

To integrate the N-cycle into DANUBIA, a process-based N-model suitable for mesoscale modelling was implemented. The soil water and nitrogen model (SOIL-SNT) uses the geocomplex concept (Ludwig et al., 2003) to bridge the gap between DANUBIA's mesoscale grid resolution (1 km $\times$ 1 km) and the field scale. Due to the lack of appropriate data, model validation on the large scale is difficult. However, for field scale validation, data are readily available in many cases. Hence, for a successful application on the regional scale, it is necessary to utilize a concept that is valid on the field as well as on the large spatial scale and to test the model rigorously on the field scale, where detailed validation data is available.

The objectives of this paper are (i) to describe the soil water and nitrogen model (SOIL-SNT), (ii) to test and validate the model according to several field data sets and (iii) to evaluate the model's sensitivity in regard to uncertainties of the parameterization, input data and climate change issues.

2. Material and methods

2.1. *Modelling framework*

DANUBIA is a component-based, object-oriented and raster-based modelling framework that couples numerous ecological and socioeconomic models. Model implementation is realized in the programming language JAVA. During an integrative simulation, information is exchanged dynamically between the model components ACTORS (representing human activity), ATMOSPHERE, GROUNDWATER, LANDSURFACE and RIVERNETWORK (Fig. 1, left).

Soil processes, e.g. N-turnover, are modelled within the LANDSURFACE component. The LANDSURFACE component contains models to calculate all essential water, energy and matter fluxes at the land surface, including vegetation and soil (Barth et al., 2003). Interfaces control data transfer between the models of LANDSURFACE (Fig. 1, right) and with other DANUBIA components (e.g. GROUNDWATER, RIVERNETWORK, ACTORS).

The soil column is represented by a three-layered profile and soil properties are specified for each soil layer. SOIL-SNT calculates all processes on an hourly time step. It uses water and nitrogen uptake provided by the dynamic plant growth model. Soil evaporation and effective precipitation are important additional model drivers. The latter are calculated by a surface model that computes, among others, the energy balance at the land surface. An interface to the agroeconomic model ensures input data of agricultural management (e.g. fertilization information). SOIL-SNT provides data for the plant growth model (e.g. soil nitrogen content, soil moisture), the surface model and the farming model. Complex feedback mechanisms influence modelling results mutually. The interdisciplinary and integrative modelling approach used in the

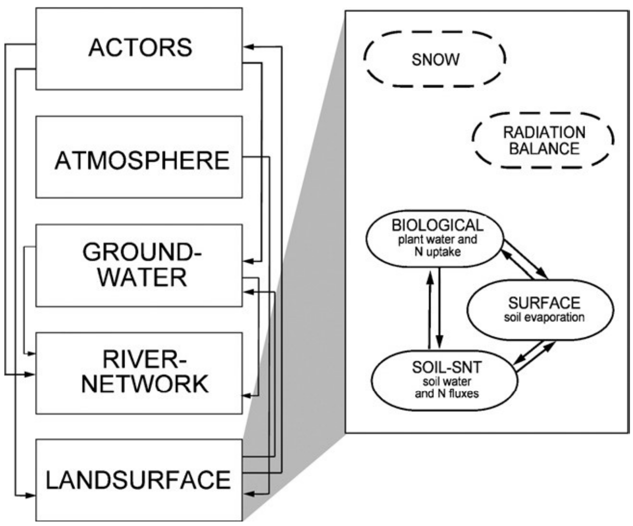

Fig. 1 – Relationships of the components of DANUBIA and of models within the LANDSURFACE component. Only interrelations used for this study are illustrated. Models shown with dashed lines were not coupled for the analyses of this study.

context of GLOWA-Danube particularly requires a thorough validation of all models.

2.2. *Soil hydrology modelling*

SOIL-SNT models water fluxes in three layers (0–30, 30–60 and 60–90 cm) based on a modified Eagleson (1978) approach. Assuming an unsaturated homogeneous textured soil column, with uniform soil moisture at the beginning of each storm and interstorm period and a water table depth much greater than soil column depth, Eagleson (1978) calculated the changes in volumetric soil moisture θ and the matric potential $\Psi(\theta)$ according to the one-dimensional concentration dependent diffusivity equation (Philip, 1960):

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left[D(\theta)\frac{\partial \theta}{\partial z}\right] - \frac{\partial K(\theta)}{\partial z} \tag{1}$$

where $K(\theta)$ is the effective hydraulic conductivity (cm s^{-1}), t is time (s), z is depth (cm), $D(\theta)$ is diffusivity (cm^2 s^{-1}), which is a function of hydraulic conductivity, matric potential and volumetric water content:

$$D(\theta) = K(\theta)\frac{\partial \Psi(\theta)}{\partial \theta} \tag{2}$$

For the simplified boundary conditions mentioned above, Eagleson (1978) presented an analytic solution of Eq. (1) for different processes of soil water movement, namely for infiltration (Eq. (3)), exfiltration, percolation (Eq. (4)), and capillary rise (Eq. (5)). For the simulation of independent processes, the solution of the different equations is superimposed linearly.

Infiltration capacity into the soil column is calculated according to Eq. (3). If the intensity of the effective precipitation exceeds the infiltration capacity, surface runoff occurs:

$$f_i^*(t, s_0) = \left[(1-s_0)\left(\frac{5n\,\Psi_{sat}\,\Phi_i(d, s_0)}{3\pi m t\,K_{sat}}\right)^{1/2} + \frac{(1+s_0^c)}{2} - \frac{w}{K_{sat}}\right]K_{sat} \tag{3}$$

Percolation is expressed as:

$$v(s_0) = s_0^c\;K_{sat} - w \tag{4}$$

And capillary rise is calculated from:

$$w = K_{sat}\left[1 + \frac{2}{3(mc-1)}\right]\left[\frac{\Psi_{sat}}{Z}\right]^{mc} \tag{5}$$

where f_i^* is infiltration capacity (cm s^{-1}), t is time (s), s_0 the initial degree of saturation in surface boundary layer, n is effective medium porosity, which is the effective volume of voids divided by total volume (cm^3 cm^{-3}), Ψ_{sat} is soil matric potential at saturation (cm), Φ_i is dimensionless infiltration diffusivity, d is a diffusivity index, m is pore size distribution index, K_{sat} is saturated effective hydraulic conductivity (cm s^{-1}), c is a pore disconnectedness index ($c = (2 + 3m)/m$), w is upward apparent pore fluid velocity representing capillary rise from the water table (m s^{-1}), v is apparent fluid velocity out of lower boundary of soil moisture zone due to gravitational percolation (cm s^{-1}), and Z is depth of water table (cm).

To derive the pore size distribution index from water retention curves representing the relationship between hydraulic conductivity θ and the matric potential $\Psi(\theta)$, the approach developed by Brooks and Corey (1964) is used.

The vertical distribution of soil moisture is represented in DANUBIA with three soil layers, thus accounting for the temporal course of water availability for evaporation and transpiration as well as vertical fluxes of water and nitrogen. For each soil layer, the Eagleson approach is applied, assuming that percolation (Eq. (4)) from an upper soil layer equals effective precipitation for the downward layer. If a soil layer is saturated, part of the percolating water is taken as interflow, whereas the proportion of interflow is calculated using the slope α of the land surface (interflow = $v(s_0)\tan(\alpha)$).

Below the lowest soil layer (>2 m), soil moisture is assumed to be constant and therefore the percolation rate can be directly related to the specific soil hydraulic conductivity (Eq. (4)). Moreover, a deep ground water table is assumed to prevent unrealistic exchange rates across the capillary fringe. Capillary rise is modelled only for the third soil layer and limited to conditions, where root water uptake has depleted this layer below the assumed constant soil moisture of the soil zone below 2 m depth. Upward movement of soil water within the three layers is not considered.

Evaporation from bare soil is limited to the uppermost soil layer. The amount of water that can be withdrawn from the soil is controlled by a soil resistance parameter r_{soil} (Kondo et al., 1992), the moisture deficit in the atmosphere and an empirical plant cover factor, which considers the reduction of evaporation in the case of a more or less closed plant canopy. Assuming that evaporation is most active in the uppermost 7.5 cm of the soil column, evaporation (EP_{soil}) in the uppermost soil layer (0–0.3 m) is restricted to 25% of the volume of this layer:

$$EP_{soil} = \Delta_v H \frac{1}{r_{soil}}\frac{1}{4}(E - E_{sat})(1 - P_{fac}) \tag{6}$$

where $\Delta_v H$ is the heat of vaporisation (W m^{-2}), r_{soil} is the soil resistance (s m^{-1}) calculated according to Kondo et al. (1992), E is actual water vapour pressure (kg m^{-3}), E_{sat} is saturated water vapour pressure (kg m^{-3}) and P_{fac} is a dimensionless plant cover factor, which at most equals 1 and is calculated according to an empirical relation to leaf area index ($P_{fac} = LAI^2 0.44$).

In DANUBIA's crop growth model, actual water uptake of plants is simulated according to CERES (Jones and Kiniry, 1986), based on soil water supply, root length density and transpiration. First, soil-limited water uptake per unit of root length is determined as a function of root length density and available soil water in each soil layer (Eq. (7)). Root water uptake is limited to soil water contents exceeding the wilting point. Considering soil layer thickness and root length density, water uptake per unit of root length is converted to potential water uptake in each soil layer (Eq. (8)):

$$U_{Wr} = \frac{0.0027\;\exp(62(\theta_i - \theta_{WP}))}{6.68 - \ln(R_{LD})} \tag{7}$$

$$U_{Wp} = U_{Wr}\;R_{LD}\,z \tag{8}$$

where U_{Wr} is water uptake per unit of root length ($cm^3\,cm^{-1}\,d^{-1}$), R_{LD} is root length density ($cm\,cm^{-3}$), θ_i is the soil water content ($cm^3\,cm^{-3}$) in layer i, θ_{WP} is the water content at wilting point ($cm^3\,cm^{-3}$), U_{Wp} is the potential water uptake ($cm\,h^{-1}$), z the soil depth of the specific soil layer (cm). Water uptake and transpiration are interrelated processes. Thus, the actual total water uptake is given by the minimum value of the total potential water uptake from the rooted soil profile (sum of values of potential water uptake in all layers) and the potential transpiration rate. If the latter is less than the potential water uptake, actual water uptake in each layer is reduced proportionally:

$$U_{Wa,i} = U_{Wp,i}\left(\frac{T_p}{U_{Wp,P}}\right) \tag{9}$$

where $U_{Wa,i}$ is the actual total water uptake ($cm\,h^{-1}$) in layer i, T_p is the potential transpiration rate ($mm\,s^{-1}$), $U_{Wp,i}$ is the potential water uptake ($cm\,h^{-1}$) in layer *i* and $U_{Wp,P}$ is the sum of values of U_{Wp} in all layers ($cm\,h^{-1}$). The calculation of the potential transpiration rate is adopted from the model GECROS (Yin and van Laar, 2005) and is based on the Penman–Monteith equation (Monteith, 1973). For further details, see Lenz (2007) and Yin and van Laar (2005).

2.3. *Soil nitrogen modelling*

Crop nitrogen uptake is determined in the crop growth model according to the CERES model (Jones and Kiniry, 1986). The potential nitrate and ammonium uptake rates for each rooted soil layer are modelled as a function of soil mineral nitrogen reservoirs, soil water content and root length density, using a crop-specific maximum nitrogen uptake rate per unit length of root. The actual uptake rates are obtained through comparison of the total potential nitrogen uptake with the current crop nitrogen demand. In accordance to the concept used for defining actual water uptake, the interrelation of nitrogen demand and uptake is considered. If the crop demand exceeds the potential nitrogen supply, actual uptake is equal to potential uptake. If the demand is less than the potential uptake, the latter is reduced to actual uptake in each layer. Current crop nitrogen demand in relation to plant growth is dynamically modelled according to the GECROS model (Yin and van Laar, 2005). This modelling concept distinguishes deficiency-driven and growth activity-driven demand. The first guarantees the maintenance of the actual plant nitrogen concentration above a critical concentration, whereas the second is modelled based on the functional-balance theory. According to this theory, plants maximize their relative carbon gain through optimum nitrogen concentration (Hilbert, 1990). For details, see Yin and van Laar (2005).

Soil nitrogen transformation processes are modelled for each soil layer. The implemented algorithms are based upon the CERES maize model (Jones and Kiniry, 1986). CERES algorithms are used because (i) they can be executed based on input parameters available in mesoscale watersheds such as the Upper Danube and (ii) the approach was already extensively tested and validated under a wide variety of environmental conditions (e.g. Allison and Entenmann, 1993; Jones et al., 2003; Popova and Kercheva, 2005; Nain and Kersebaum, 2007). Modelled N-transformation processes are: (i) mineralization from two soil organic carbon pools (easily

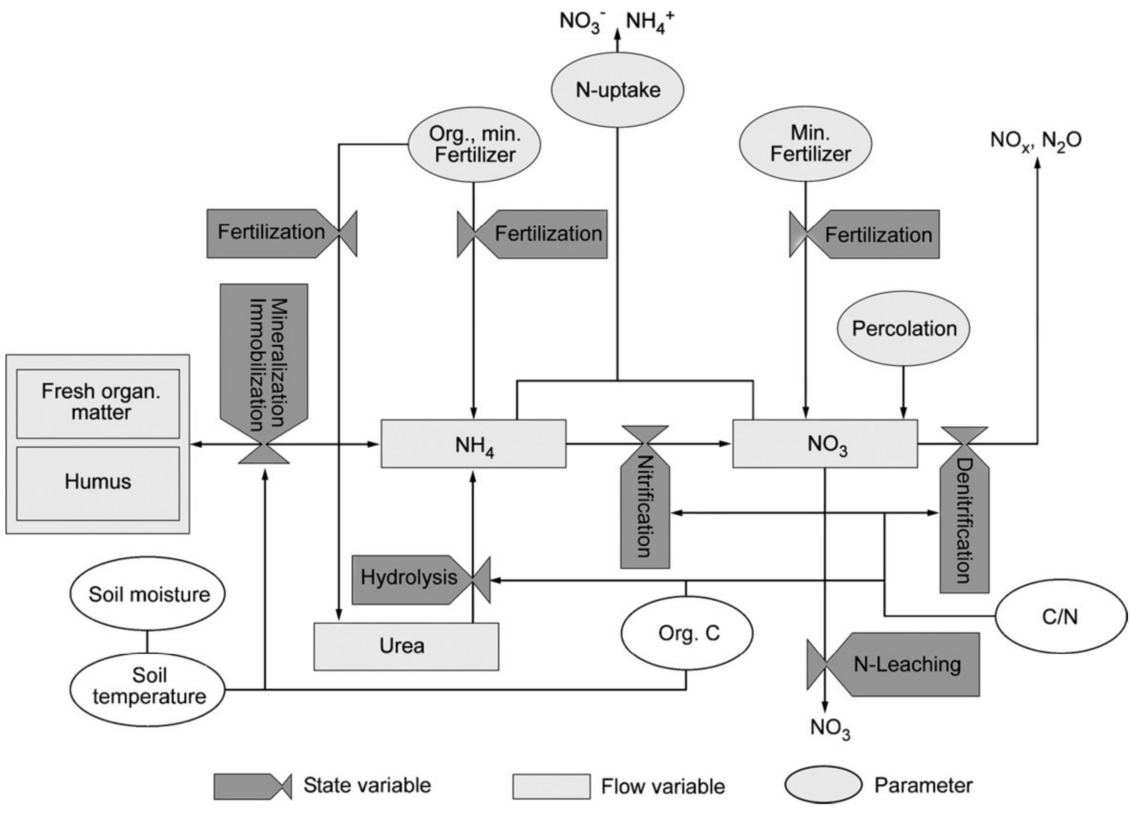

Fig. 2 – Schematic diagram of the nitrogen cycle as modelled in SOIL-SNT.

decomposable fresh organic matter and stable humus pool), (ii) immobilization, (iii) nitrification, (iv) denitrification and (v) urea hydrolysis (Fig. 2). Only a brief overview about the main algorithms implemented in SOIL-SNT is given here. More details can be found in Godwin and Jones (1991) and Jones and Kiniry (1986).

N-mineralization is calculated separately for the two different soil organic matter pools. The mineralization approach is based on a modified version of the PAPRAN model (Seligmann and van Keulen, 1981). N-mineralization from the fresh organic matter pool is described taking into account the different decay rates of plant tissue constituents (carbohydrates, cellulose and lignin) and the C/N ratio in the pool and considers soil temperature and moisture:

$$N_{\text{m-FOM}} = [CN_{\text{FOM}}\, T_{\text{m}}\, M_{\text{m}}\, (DR_{\text{ch}} + DR_{\text{cl}} + DR_{\text{li}})] N_{\text{FOM}} \tag{10}$$

where $N_{\text{m-FOM}}$ is the N-mineralization rate of fresh organic matter (kg ha^{-1} d^{-1}), CN_{FOM} is a factor based on the ratio of carbon in fresh organic matter to nitrogen available for decay (0–1), T_{m} and M_{m} are a soil temperature and moisture factor affecting mineralization (0–1), N_{FOM} is the nitrogen content in the fresh organic matter pool (kg ha^{-1}), and DR are the potential decay rates in the fresh organic matter pool for the different plant tissue constituents, whereas the subscripts ch, cl and li represent carbohydrates, cellulose and lignin, respectively. N-mineralization from the stable humus pool is calculated according to Eq. (11):

$$N_{\text{m-HUM}} = T_{\text{m}}\, M_{\text{m}}\, DR_{\text{m-HUM}}\, N_{\text{HUM}} \tag{11}$$

where $N_{\text{m-HUM}}$ is the mineralization rate from the stable humus pool (kg ha^{-1} d^{-1}), $DR_{\text{m-HUM}}$ is the potential decay rate of the humus pool (kg C kg^{-1} humus), N_{HUM} is the nitrogen content of the humus pool (kg ha^{-1}). To derive $N_{\text{m-HUM}}$ a fixed potential decay rate is used for modelling (Table 1).

Based on Seligmann and van Keulen (1981), N-immobilization as incorporation of nitrogen into the microbial biomass is calculated as the minimum of the soil-extractable mineral nitrogen and the demand for nitrogen by decaying fresh organic matter:

$$N_{\text{im}} = \text{Min}\left(N_{\text{t}}, R_{\text{c}}\ 0.02 \frac{N_{\text{FOM}}}{\text{FOM}}\right) \tag{12}$$

Table 1 – Decomposition rates (DR), soil humus C:N ratio and soil-pH used for model application; subscripts ch, cl, li and m-Hum indicate decomposition of carbohydrates, cellulose, lignin and humus

Parameter	Symbol	Value
Residue decomposition rates	DR_{ch}	0.2
	DR_{cl}	0.05
	DR_{li}	0.0095
Humus decomposition rate	$DR_{\text{m-Hum}}$	8.3×10^{-5}
Soil humus C:N ratio	CN	10
Soil-pH	pH	7

where N_{im} is the gross rate of nitrogen immobilization (kg ha^{-1} d^{-1}), N_{t} is the amount of nitrogen available for immobilization (kg ha^{-1}), R_{c} is the gross release of carbon with decay (kg ha^{-1}), N_{FOM} is the nitrogen in fresh organic matter (kg ha^{-1}), FOM the fresh organic matter (kg ha^{-1}) and 0.02 represents the nitrogen requirement for microbial decay of a unit of FOM. The value results from the product of the fraction of carbon in FOM (0.4), the biological efficiency of microbial carbon transformation (0.4) and the N:C ratio of microbial biomass (0.125).

Actual nitrification rates N_{nit} (kg ha^{-1} d^{-1}) in each soil layer depend on the soil-NH_4^+-concentration and some limiting factors including substrate-NH_4^+, oxygen, soil-pH, temperature, moisture and nitrification capacity taking into account an index of the nitrification potential:

$$N_{\text{nit}} = \frac{A 40\, C_{NH_4^+}}{(C_{NH_4^+} + 90\, M_{NH_4^+})} \tag{13}$$

where A is the index of nitrification potential (0–1), $C_{NH_4^+}$ is ammonium concentration in soil (mg kg^{-1}) and $M_{NH_4^+}$ the amount of ammonium (kg ha^{-1}). Further details can be found for example in McLaren (1970) and Focht and Verstraete (1977).

An equation by Rolston et al. (1980) describing denitrification was adopted to model gaseous nitrogen losses. Denitrification occurs under anaerobic conditions ($\theta > \theta_{\text{FC}}$) commencing when 60% of all pores are filled with water. As described in Linn and Doran (1984), denitrification increases linearly up to 100% filled pore space. A temperature factor is determined and the amount of total water extractable carbon as well as nitrate content and layer thickness are included in the calculation of denitrification:

$$N_{\text{de}} = 6 \times 10^{-5} C_{\text{AW}}\, C_{NO_3^-}\, T_{\text{de}}\, M_{\text{de}} D \tag{14}$$

where N_{de} is the denitrification rate (kg ha^{-1} d^{-1}), C_{AW} is a carbon availability factor, $C_{NO_3^-}$ is the nitrate concentration (mg kg^{-1}), T_{de} is a temperature factor, M_{de} a moisture factor (0–1) and D represents the soil layer thickness (cm).

The conversion of urea in ammonium is described by the urea hydrolysis process. Based on a variety of experiments (McGarity and Myers, 1967; Myers and McGarity, 1968; Tabatabai and Bremner, 1972; Zantua et al., 1977; Linn and Doran, 1984), the potential rate of hydrolysis is estimated according to Godwin (1987):

$$AK_{\text{pot}} = -1.12 + 1.31\, OC_A + 0.203\, \text{pH} - 0.155\, OC_A\, \text{pH} \tag{15}$$

where AK_{pot} is the potential rate of hydrolysis (kg ha^{-1} d^{-1}) and OC_A is the amount of organic carbon in urea (kg ha^{-1}). The soil-pH value is constantly set to 7 (Table 1). The actual hydrolysis rate is calculated as follows:

$$AK_{\text{act}} = AK_{\text{pot}}\ \text{MIN}(T_{\text{FU}}, M_{\text{FU}}) U \tag{16}$$

where AK_{act} is the actual hydrolysis rate (kg ha^{-1} d^{-1}), T_{FU} and M_{FU} are soil moisture and temperature factors (0–1), respectively, and U is the amount of urea (kg ha^{-1}).

Table 2 – Field characteristics and management information for all experimental sites

	Nienwohlde (NW)				Neuenkirchen (NK)					Feienberg (FB)							
Depth (cm)	Soil texture	C_{org} (%)	N_{tot} (%)	Bulk density ($g\,cm^{-3}$)	Depth (cm)	Soil texture	C_{org} (%)	N_{tot} (%)	Bulk density ($g\,cm^{-3}$)	Depth (cm)	Soil texture	C_{org} (%)	N_{tot} (%)	Bulk density ($g\,cm^{-3}$)	C_{org} (%)	N_{tot} (%)	Bulk density ($g\,cm^{-3}$)
00–25	Loamy sand	1.22	0.07	1.6	00–30	Silty loam	1.02	0.12	1.4	00–30	Silty loam	1.72	0.11	1.4[a]	2.00	0.13	1.4[a]
25–40	Loamy sand	0.01	0.006	1.6	30–80	Silty loam	0.31	0.05	1.5	30–60	Silty loam	0.52	0.05	1.5[a]	0.64	0.07	1.5[a]
40–80	Sand	0.01	0.003	1.6	80–90	Silty loam	0.13	0.03	1.6	60–90	Silty loam	0.27	0.04	1.5[a]	0.24	0.02	1.5[a]
80–220	Sand	0.00	0.001	1.7	–	–	–	–	–	–	–	–	–	–	–	–	–

Management				
Crop	Summer barley	Winter wheat	Winter wheat	Maize
Cultivar	*Alexis*	*Kanzler*	*Vivant*	*Cerutti*
Sowing	20 March 1991	16 November 1990	15 October 2004	01 May 2005
Harvesting	8 October 1991	26 August 1991	2 August 2005	12 October 2005
Previous crop	Sugar beet	Sugar beet	Maize	Winter wheat

Fertilization	Date	N ($kg\,ha^{-1}$)	Type	Date	N ($kg\,ha^{-1}$)	Type	Date	N ($kg\,ha^{-1}$)	Type	Date	N ($kg\,ha^{-1}$)	Type
1st	21 March	49		–	–	–	15 March	60	KS[e]	17 April	50	PM[c]
2nd	6 April	50	60	–	–	–	21 April	60	KS[e]	25 June	60	AHl[d]
3rd	26 May	16	DAP[b]	–	–	–	29 June	60	KS[e]	6 June	25	PM[c]

[a] Ad-hoc- Boden (2005).
[b] Diammoniumphosphate.
[c] Poultry manure.
[d] NH_4^+ NO_3^- urea solution.
[e] Ammonium nitrate.

Modelling of nitrate movement within the soil column is closely connected to modelling of water fluxes. Nitrate discharge is assumed to be proportional to the amount of percolated water. First, the fraction of percolated water in relation to the soil water content of the whole layer is determined. The layer-specific downward translocation rate of nitrate is calculated as product of the fraction of percolated water and the nitrate content in each layer (Godwin and Singh, 1998):

$$N_{out} = C_{NO_3^-} \frac{F}{\theta + F} \tag{17}$$

where N_{out} is the amount of percolated nitrate (kg ha^{-1}), $C_{NO_3^-}$ is the nitrate content (kg ha^{-1}), F is the amount of percolated water (mm), and θ is the water content (mm). Downward directed nitrate flux increases the nitrate pool of the layer beneath. Nitrate flux from the deepest layer is the amount of leachate.

2.4. *Field data*

For model validation, data sets from three locations in Germany were used containing 2 years of winter wheat and 1 year of summer barley and maize, respectively. A data set for winter wheat and for maize was measured at Feienberg, Germany by the authors; the other data sets were provided by the Technical University of Braunschweig and are published in detail in McVoy et al. (1995).

Feienberg is located about 15 km southeast of Cologne in the Rhenish Slate Mountains (50°52′N, 13°00′E). The test site has two adjacent fields at an elevation of 165 m a.s.l. with a slight slope (0–1%). The predominant soil for both fields is a Luvisol (FAO, 1998) on loess with a silty loam texture. Due to the fertile soils and the location close to the agglomeration of Cologne/Bonn, the area is intensively used agricultural land.

On one field, winter wheat was monitored from October 2004 to September 2005 (subsequently referred as winter wheat year), while in the other, maize was cultivated between January and December 2005 (subsequently referred as maize year). During the winter wheat year, a rainfall amount of 917 mm and an average temperature of 11.7 °C were measured, whereas rainfall was 894 mm and the average temperature was 11.2 °C during the maize year. For winter wheat and maize, N-fertilization was spread in three periods with a total N supply of 180 and 135 kg ha^{-1}, respectively (Table 2).

During the growing season, soils were sampled bi-weekly at 10 locations within the fields extracting samples from three depths (0–30, 30–60, 60–90 cm). The distribution of the sampling points was selected according to official directives (LUFA, 2005) to cover spatial variability of the mineral nitrogen content within each field.

All samples from each soil layer within one field and sampling date were mixed up and homogenized. Afterwards NO_3^--, NH_4^+- and water contents were determined layer-specifically. Soil moisture was determined gravimetrically.

NO_3^-- and NH_4^+-contents were determined with a German standard laboratory method using a spectrometer (UV2 Spectrometer, Unicam) (DIN 38406, 1995; VDLUFA, 1997) and with a simpler method in the field using the RQflex plus analyser (RQflex plus Reflektometer, Merck, Darmstadt, Germany). The latter method is based on the principle of reflectometry where the reflected light is measured in a cuvette. Differences in intensity of emitted and reflected radiation are used to measure the respective concentrations.

Parallel measurements were carried out for 144 samples. Statistical analysis (F-test, rejection probability 0.01) showed no significant difference between the laboratory measurements and the RQflex plus analyser-method. The Pearson correlation coefficient of $r = 0.99$ also shows the strong relationship between both results. Since the RQflex plus analyser method is significantly less time demanding than the laboratory method, it was used for further analysis.

Layer-specific soil texture was determined according to the sieve–pipette method (DIN 19683-2, 1997). C_{org}- and N_{tot}-contents were also measured by an elemental analyser (CNS Elementaranalysator VARIO EL, Elementar, Hanau, Germany).

Above ground biomass samples (1 m^2) were taken three times during the growing period at three different locations along a transect within the fields. An organ-specific representative aliquot of all plants per sampling point was taken to determine average dry biomass after drying for 24 h at a temperature of 105 °C. Biomass carbon and nitrogen contents were obtained by elemental analysis.

Meteorological data (rainfall, air and soil temperature, radiation, wind speed, air pressure and humidity) were provided by the German weather service (DWD) station Cologne–Wahn, which is located 5 km to the west of the test sites at an elevation of 80 m a.s.l.

A second data set for winter wheat (Neuenkirchen) was provided by the TU Braunschweig (McVoy et al., 1995). Within the Krummbach watershed, the Neuenkirchen test site (52°01′N, 10°27′E) is located in the northern forelands of the Harz mountain range. The elevation is 151 m a.s.l. and the slope of the field is 1%. Predominant soils are Orthic and Gleyic Luvisol on loess (FAO, 1998). Between November 1990 and October 1991, a rainfall of 500 mm was measured and the average air temperature was 8.3 °C. No N-fertilization was applied (Table 2).

To test SOIL-SNT for summer barley, a 1-year data set of the TU Braunschweig (Nienwohlde) was available. Nienwohlde

Table 3 – Water content at field capacity θ_{FC} and wilting point θ_{WP}, saturated hydraulic conductivity K_{sat}, matrix potential Ψ, effective medium porosity n, and pore size distribution index m (Brooks and Corey, 1964) used to parameterize the soil hydrology model for the three test sites

	Nienwohlde		Neuenkirchen	Feienberg
Soil depth (cm)	0–30	30–90	0–90	0–90
θ_{FC} (m^3 m^{-3})	14	8	40	29
θ_{WP} (m^3 m^{-3})	3	1	18	8
K_{sat} (cm h^{-1})	0.89	20.35	0.09	0.054
n (%)	44.9	41.9	45.1	42.7
Ψ (cm)	10.9	7.6	80	74.9
m	0.394	0.517	0.133	0.295

Table 4 – Layer-specific initial conditions of soil water (θ) and mineral nitrogen content (N_{min}) of the whole profile for the test sites in Nienwohlde (NW), Neuenkirchen (NK) and Feienberg (FB)

	Summer barley (NW)		Winter wheat (NK)		Winter wheat/maize (FB)	
Depth (cm)	θ ($m^3\,m^{-3}$)	N_{min} ($kg\,ha^{-1}$)	θ ($m^3\,m^{-3}$)	N_{min} ($kg\,ha^{-1}$)	θ ($m^3\,m^{-3}$)	N_{min} ($kg\,ha^{-1}$)
00–30	14		30			
30–60	7	17	30	80	29/29	45/33
60–90	7		20			

Values for summer barley and winter wheat (NK) were taken from measurements, in Feienberg values for θ were initialized as described and N_{min} was estimated based on farmer's statements.

is located in the north of Braunschweig within the German Pleistocene sand plain (52°50′N, 10°35′E). The test site is at an elevation of 103 m a.s.l. The predominant soil is a Luvisol, which developed on sandy parent material (FAO, 1998) and has a very slight slope of 0–1%. Former land use of the field was forest, which is still noticeable in irregular soil humus content. In 1991, average air temperature was 9.5 °C and annual rainfall was 590 mm. Summer barley was grown applying three rates of N-fertilizer with a total amount of 130 kg ha^{-1} (Table 2). As already indicated in other studies (Kersebaum, 1995; Svendsen et al., 1995), there is evidence that the amount of irrigation (106 mm) given in management information was not valid for the plot where measurements were conducted. A detailed description about field measurements, observation techniques and the settings of experimental sites is given in McVoy et al. (1995). Both external data sets were used for N-modelling validation in various studies (e.g. Diekkrüger et al., 1995).

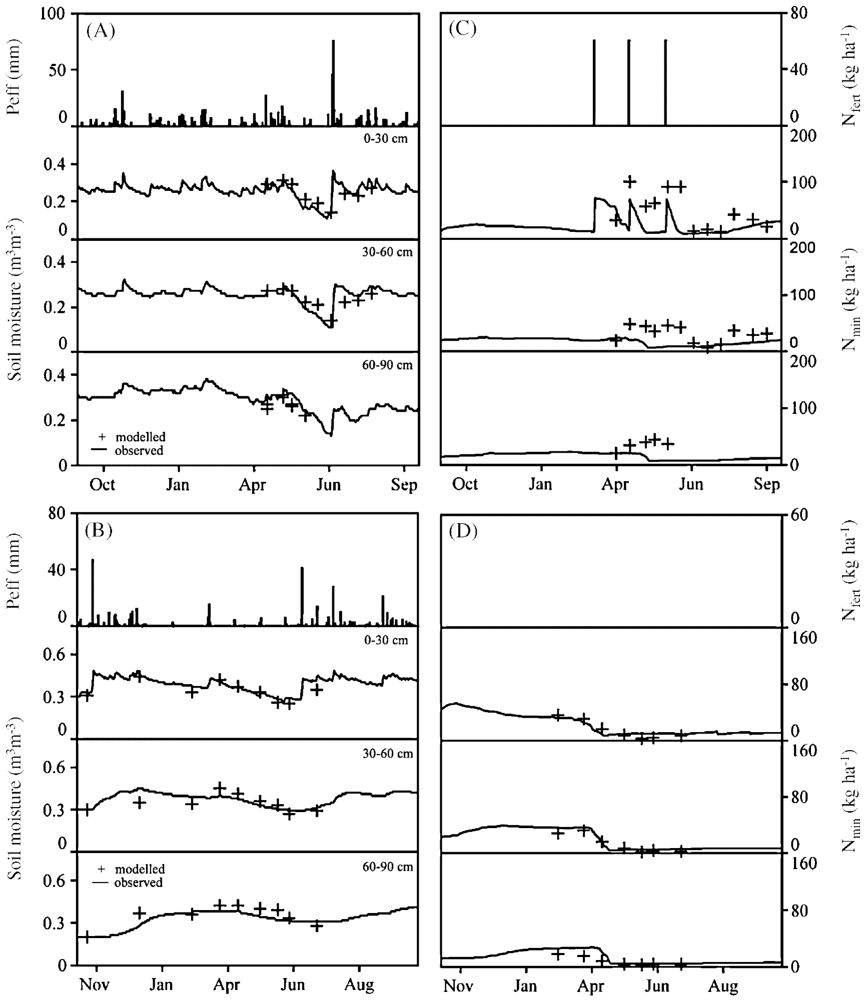

Fig. 3 – Simulated and observed water (part A and B) and nitrogen (part C and D) dynamics for each soil layer under winter wheat in Feienberg (above) (1 October 2004 to 30 September 2005) and Neuenkirchen (below) (1 November 1990 to 31 October 1991). N_{min} is mineral nitrogen, P_{eff} is effective precipitation (precipitation–interception), no N-fertilization (N_{fert}) was applied in Neuenkirchen.

2.5. *Model parameterization and validation*

Model runs started on the 1st of January for summer crops (barley and maize) and winter wheat simulations began on the 1st of September (Feienberg) and the 1st of November (Neuenkirchen). The modelling periods for all crops were one whole year. It is assumed that for the rest of the simulation period, no further crops than the described were cultivated on the test sites. Model calculations in Feienberg were initialized assuming a soil suction value [pF] of 2.3 from which the initial pore filling and hence the initial soil moisture are retrieved. For the test sites in Nienwohlde and Neuenkirchen, initial water contents were adjusted to field measurements. N_{min}-contents at the beginning of the simulation were set according to literature values (AID, 2002) for Feienberg. For the Nienwohlde data set, field measurements were used and for the Neuenkirchen data set, N_{min}-content was estimated (harvesting of previous crop on November 10th) according to literature values (AID, 2002). Initial values of N_{tot}- and C_{org}-contents were taken from field observations (Table 2). Tables 3 and 4 give an overview of soil hydrological parameters and initial conditions of soil moisture and N_{min} for all test sites, respectively.

To validate modelled water and nitrogen fluxes in a controlled environment, only the plant growth and the surface model were coupled to SOIL-SNT. Other interaction and feedback mechanisms, which are available within DANUBIA, were disabled. A meteorological input database was generated to provide the required meteorological input data from measurements taken by the German weather service (DWD). Model runs are based on hourly input data (precipitation, air temperature, air humidity, global radiation and wind speed). Management and cultivation information obtained by the farmers were applied (Table 2). Model efficiency was quantified according to the Index of Agreement (IA) (Willmott, 1981) (Eq. (18)) and the root mean square error (RMSE):

$$IA = 1 - \frac{\sum_{i=1}^{n}(M_i - O_i)^2}{\sum_{i=1}^{n}[|M_i - \bar{O}| + |O_i - \bar{O}|]^2} \tag{18}$$

where M_i and O_i are defined as simulated and observed values. $\bar{O}$ is the observed mean value. An IA value of 1 is defined as total conformity between measurement and model.

3. Results and discussion

3.1. *Winter wheat*

The modelled soil water dynamics at the Feienberg test site are in very good agreement with the observed values (Fig. 3A). Percolation from the lowest soil layer ceased in April since the water content did not exceed field capacity due to the water demand by evapotranspiration. In May, some minor deviations in soil moisture ($0.05\,m^3\,m^{-3}$) in the deeper layers are noticeable. In early July, a strong rainfall event refilled the top layer up to saturation and also increased soil moisture significantly in the middle layer. Particularly the soil moisture in the topmost soil layer was reduced subsequently due to plant water uptake. The model simulates this drying process after the extreme rainfall (e.g. July 4th) event fairly accurate. Comparing the measured with modelled soil moisture values for each soil layer resulted in IA values ranging from 0.69 to 0.94 and a RMSE < $0.03\,m\,m^{-3}$ (Table 5). The modelled values of evapotranpiration and total runoff are in the expected range as compared to long-term measurements given in the literature (BMU, 2000). The modelled percolation amounts are in agreement with typical groundwater recharge rates (Table 6). Overall, modelled water dynamics at the Feienberg test site show satisfactory results for nitrogen modelling validation.

The model underestimated the observed N_{min}-value at the date of the second fertilizer application. The difference between the N_{min}-content modelled for the time between the second fertilization and the next day of field measurements (May 8th, 2005) was $54\,kg\,ha^{-1}$. This modelled value agrees well with the observed decrease in soil nitrogen content ($59\,kg\,ha^{-1}$). This indicates a realistic nitrogen uptake by the model, although the modelled N_{min}-content is $46\,kg\,ha^{-1}$ less than the measured content on May 8. A likely reason for this difference is a higher fertilization amount than assumed. Total annual mineralization within the soil profile is $125\,kg\,ha^{-1}$, which represents a typical value for the Feienberg region (AID, 2002). The measured increase in soil nitrogen amounts at the end of the vegetation period indicates a stronger decomposition of root biomass as compared to the model results. A possible reason for this effect is accelerated mineralization after ploughing. Ploughing is not considered by the model. A different reason might be the modelled low root nitrogen content or intertillage. Conditions suitable for denitrification were rare. As indicated by the storage change of $19\,kg\,ha^{-1}$ (Table 7), the system is in balance with its environment. A statistical analysis showed the greatest discrepancies in the deepest layer (Table 5) where IA was 0.23, which is also due to the limited number of samples. Probably, the soil compaction, which is not explicitly considered by the model, also impacted nitrogen modelling results. The range of model efficiency IA for the middle and upper soil layer (IA = 0.46 and 0.65, respectively) is acceptable. However, some of the model results deviate significantly from the measurements.

The modelled and measured soil moisture at the winter wheat site in Neuenkirchen (Fig. 3B) is in good agreement with the measurements. At the end of the growing season, the modelled soil moisture was slightly higher than observations in the top layer. In June, the upper layer was refilled after a heavy precipitation event. Until the end of October, modelled water contents increased and almost reached field capacity. RMSE between measured and modelled soil moisture ranged between 0.04 and $0.05\,m^3\,m^{-3}$ (Table 5) with the strongest discrepancies in the deeper layers. The IA of modelling results varies within a range of 0.68 (30–60 cm) up to 0.86 (0–30 cm). Due to nitrogen limited plant growth, only 138 mm (Table 6) were extracted by evapotranspiration. The low amount of precipitation resulted in less than average total runoff (BMU, 2000). Overall, the modelled soil water dynamics provide a good basis for the nitrogen model validation.

Modelling results for mineral nitrogen within the soil profile at the Neuenkirchen site agreed very well with measurements (Fig. 3D). Statistical analysis shows a high IA (0.81–0.98) (Table 5). Observed N-uptake of $102\,kg\,N\,ha^{-1}$ was untypical for winter wheat. The plant growth model thereby

Table 5 – Layer specific statistical analysis of model results for soil water (θ) and mineral nitrogen (N_{min}) at the four test sites in Nienwohlde (NW), Neuenkirchen (NK) and Feienberg (FB)

Depth (cm)	Summer barley (NW)				Winter wheat (NK)			
	θ		N_{min}		θ		N_{min}	
	RMSE ($m^3 m^{-3}$)	IA	RMSE ($kg ha^{-1}$)	IA	RMSE ($m^3 m^{-3}$)	IA	RMSE ($kg ha^{-1}$)	IA
0–30	<0.01	0.31	9.6	0.97	0.04	0.86	1.2	0.93
30–60	0.03	0.33	2.7	0.79	0.05	0.68	1.2	0.98
60–90	0.01	0.13	2.1	0.35	0.05	0.84	0.5	0.81

Depth (cm)	Winter wheat (FB)				Maize (FB)			
	θ		N_{min}		θ		N_{min}	
	RMSE ($m^3 m^{-3}$)	IA	RMSE ($kg ha^{-1}$)	IA	RMSE ($m^3 m^{-3}$)	IA	RMSE ($kg ha^{-1}$)	IA
0–30	0.03	0.94	3.3	0.65	< 0.01	0.83	9.3	0.87
30–60	0.03	0.89	3.8	0.46	< 0.01	0.77	0.5	0.71
60–90	0.03	0.69	25.0	0.23	0.01	0.56	4.1	0.42

demonstrates its responsiveness to nitrogen stress. Net mineralization of 57 kg N ha^{-1} indicated low microbial activity due to lack of nitrogen and low organic matter content (1%). Modelled nitrate leaching was small due to low nitrate contents in the deepest layer. Denitrification occurred only on a few days with an almost saturated soil. Hence, modelled release of nitrogen as gaseous compounds was quite low with 7 kg N ha^{-1}. After harvesting, the soil mineral nitrogen content increased due to mineralization of plant residues as indicated by field measurements and modelling results. The annual soil nitrogen balance was negative (55 kg ha^{-1}).

In general, the modelled nitrogen and water dynamics for different soils under winter wheat were satisfactory. The analysis of the modelling results shows the strong dependency of the mineral nitrogen content upon plant nitrogen uptake and growth.

3.2. *Maize*

Overall, the dynamics of soil water content under maize in 2005 was relatively small. It varied only between 0.20 and 0.35 $m^3 m^{-3}$. The model captured the water dynamics reasonably well (Fig. 4A). Calculated layer-specific IA ranged between 0.56 for 60–90 cm and 0.83 for the top layer. RMSE was always <0.01 $m^3 m^{-3}$. The modelled total runoff of 622 mm (Table 6), agrees well with long-term observations (600–800 mm) (BMU, 2000). The small amount of modelled evapotranspiration corresponds to field observations which indicated reduced plant growth due to water stress in the spring.

Mineral nitrogen content during the spring was slightly underestimated, especially for the second and third soil layer (Fig. 4B). IA for the different soil layers was 0.87 (0–30 cm), 0.71 (30–60 cm), and 0.42 (60–90 cm), respectively. The measured

Table 6 – Modelled annual water balance (mm) for the four test sites in Nienwohlde (NW), Neuenkirchen (NK) and Feienberg (FB)

Crop	Year	P_{eff}	=	E_a	+	R_{tot}	+	ΔS	q_w	R	I
Winter wheat (NK)	1991	383	=	138	+	112	+	133	27	85	0
Summer barley (NW)	1991	511	=	218	+	242	+	51	136	0	106
Maize (FB)	2005	821	=	226	+	622	+	−27	348	274	0
Winter wheat (FB)	2005	776	=	248	+	560	+	−32	293	267	0

Depicted are sums of effective precipitation (P_{eff}), evapotranspiration (E_a), total runoff (R_{tot}) and change in soil water storage (ΔS). Additionally, amounts of percolation (q_w), surface runoff (R) and irrigation (I) are shown.

Table 7 – Modelled annual mineral nitrogen balances (kg ha^{-1}) for the four test sites in Nienwohlde (NW), Neuenkirchen (NK) and Feienberg (FB)

Crop	Year	$N_{min, initial}$	$N_{min, end}$	N_m	N_f	N_u	N_l	N_d	ΔN_s
Winter wheat (NK)	91	80	25	57	0	102	3	7	−55
Summer barley (NW)	91	17	28	58	130	159	16	2	11
Maize (FB)	05	33	66	147	160	228	42	4	33
Winter wheat (FB)	05	45	64	125	180	242	44	0	19

Depicted is the initial mineral nitrogen (N_{min}) and N_{min} at the end of the year as well as the sums of mineralization (N_m), fertilization (N_f), uptake (N_u), leaching (N_l), denitrification (N_d) and storage change (ΔN_s).

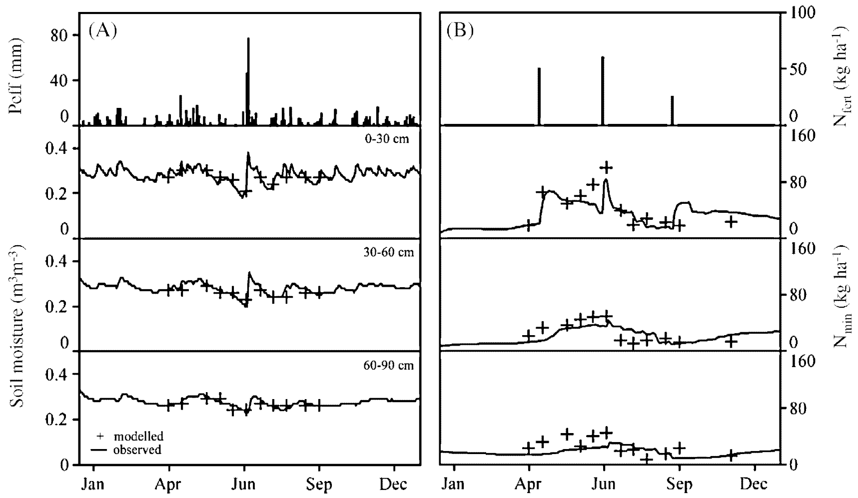

Fig. 4 – Simulated and observed water and nitrogen dynamics for each soil layer under maize in Feienberg (1 January to 31 December 2005). P_{eff} is effective precipitation (precipitation–interception), N_{min} is mineral nitrogen, N_{fert} is N-fertilization.

continuous increase of nitrogen in the uppermost layer previous to the second fertilizer application was not captured by the model. During this period, good mineralization conditions might have accelerated the decomposition of poultry manure. As indicated by nitrogen measurements at the end of June, nitrogen uptake was very high. This effect was modelled well by the coupled plant growth—soil nitrogen model. The heavy rainfall event at the end of June resulted in a short but strong nitrate leaching event from the top layer. The total amount of mineralized N (147 kg N ha^{-1}, see Table 7) is quite typical for this soil type and climate conditions (AID, 2002). Modelled nitrate leaching under maize was 42 kg ha^{-1}. Despite the shorter growing period, maize often increases the loss of nitrate to the saturated soil zone due to its phenological development and cultivation practice. As for all investigations, denitrification losses were small (1 kg N ha^{-1}) due to aerated soil conditions (AID, 2002). In conclusion, nitrogen dynamics agreed well with measurements.

3.3. *Summer barley*

Modelling results of water fluxes for summer barley on the sandy soil were not of the same quality as the other data sets (Fig. 5A). This was mainly due to an uneven distribution of irrigation water. An additional model run assuming no irrigation showed that the measured soil water contents are usually in between the results for irrigated and not irrigated conditions (assuming full irrigation and no irrigation). Thus, it is very likely that not all irrigation water reached the sampling point. During winter, soil water content was recharged to field capacity. Whereas in spring and summer, water uptake as well as percolation resulted in a decrease of the water contents close to the wilting point. From October onwards, measurements as well as simulated soil moisture show the refill of the soil profile. Model efficiencies range between 0.13 (60–90 cm) and 0.33 (30–60 cm) for layer-specific values (Table 5). Considering the fact that no site-specific calibration of the soil water

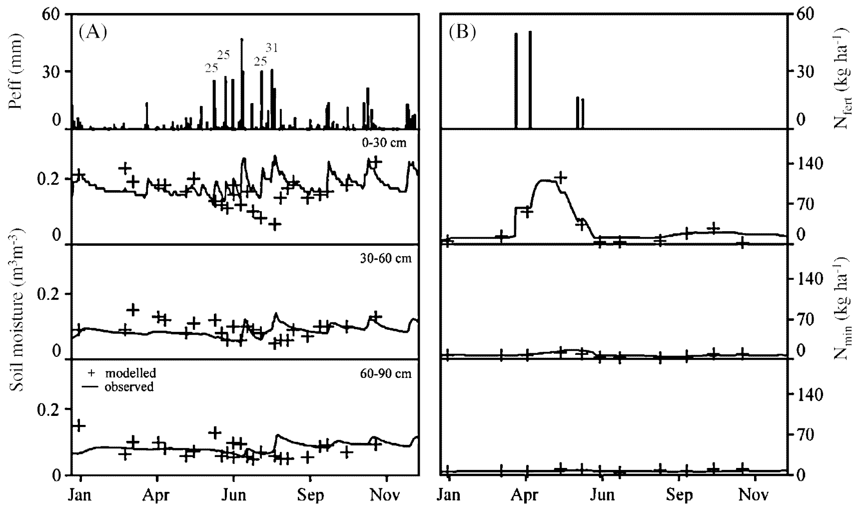

Fig. 5 – Simulated and observed water and nitrogen dynamics for each soil layer under summer barley in Nienwohlde (1 January to 31 December 1991). P_{eff} is effective precipitation (precipitation-interception), N_{min} is mineral nitrogen, N_{fert} is N-fertilization; small numbers above precipitation represent the irrigation amount.

model was carried out and the imponderability of representatively measuring soil water under inhomogeneous irrigation, the model results are quite acceptable.

Mineral nitrogen dynamics of the upper soil layers (0–60 cm) showed good agreement with observed nitrogen amounts (Fig. 5B), with an IA ranging from 0.79 (30–60 cm) to 0.97 (0–30 cm) (Table 5). For the deepest layer, the IA was 0.35. This was due to very low mineral nitrogen content, where minor deviations result in a large effect upon the IA value. As measurements indicated, mineral nitrogen contents beneath 30 cm were almost constant. Hence, nearly the complete amount of nitrogen uptake was extracted from the upper layer. Total net mineralization (58 kg ha^{-1}) was low due to less soil organic matter content (Table 7). Fertilization of 130 kg ha^{-1} mineral nitrogen combined with its initial amount covered the crop's demand quite well. Nitrate leaching was marginal due to very low mineral nitrogen contents in the lowest layer. In the top layer, field capacity was never exceeded, whereas in the layers below, nitrate supply was too small for significant denitrification.

In comparison with the results of former studies (e.g. Kersebaum, 1995; Svendsen et al., 1995), the quality of the presented results for modelled water and nitrogen dynamics are of comparable quality. Nitrogen as well as water balance components (Tables 6 and 7) are within the expected ranges of the regional long-term observations (BMU, 2000). The course of N_{min}-content was modelled well by SOIL-SNT with an IA varying between 0.23 and 0.98 (Table 5). Also, the modelled soil water contents are fairly accurate (IA between 0.13 and 0.94) despite the previously mentioned problems. For most data sets, a trend of quality loss from the upper to the lower layers was noticeable. The average IA for nitrogen modelling results was slightly higher (0.68) than the IA for water contents (0.65), but both provide a modelling quality suitable for climate change research.

4. Sensitivity analysis

Knowledge about the sensitivity of modelled nitrate leaching to (i) parameterization, (ii) initialization and (iii) input data quality is of major importance for applications in an integrated global change study on the regional scale. For the regionalization from field scales to a 1 km × 1 km grid, accurate parameterization of sensitive parameters is an essential precondition. Due to the reduction of data quality on the larger scale, knowledge about model sensitivity is therefore fundamental. A further aspect is to investigate the model's sensitivity to parameterization and initialization in order to distinguish these implications from those of climatic changes.

Hence, a sensitivity study that evaluated the influence on model performance was conducted for SOIL-SNT with regards to the parameterization of saturated hydraulic conductivity and field capacity as well as the initial values of N_{tot} and N_{min}. Due to the importance for nitrogen modelling, the effects resulting from climatic changes were investigated, additionally. Therefore, mean annual temperature and precipitation patterns in terms of the annual rainfall amount and rainfall intensity were also evaluated (assuming that extreme rainfall events become even more severe). All parameters and input data were selected because of their expected influence on nitrate leaching. Since in DANUBIA, N-leaching from soils serves as input for the groundwater model, evaluation of modelled nitrate leaching is important. Sensitivity to parameters and input data related to plant growth was not considered in this study.

To account for soil texture-specific differences, sensitivity analyses for each main soil texture class (S, U, C) were conducted. Soil parameters of the test sites were varied within their range of typical values for each soil texture class (Table 8) to investigate the effects of the parameter variability given in the literature [?] (Hillel, 1998; Dingman, 2002).

Initial values of the nitrogen pools were modified within the range of typical values for agriculturally used mineral soils in the investigation area. As given, for example by Scheffer and Schachtschabel (1998) and own field measurements, typical total soil organic nitrogen contents within our test sites in Feienberg vary between 0.7 and 3.8%. It was assumed that all organic matter is concentrated within the top layer. Empirical data of N_{min}-contents after harvesting under various previous crops (AID, 2002) indicate a realistic spectrum ranging from 0 to 100 kg ha^{-1} distributed over the whole profile.

Microbial activity is strongly influenced by soil temperature. To assess the temperature effect on soil nitrogen transformation processes and its implications on N-leaching, mean soil temperature was varied ±2 °C (Table 8).

N-leaching strongly depends on infiltration due to rainfall. Therefore, the sensitivity to the amount of precipitation was also evaluated. In DANUBIA, regional precipitation patterns are interpolated between meteorological station data. Due to uncertainties of calculated precipitation, sensitivity was determined for variations of the rainfall amount between ±60% (errors of 60% may occur for single events) from the reference (observed data). Additionally, the amount of extreme rainfall events (>40 mm d^{-1}, which equals an average one year reoccurrence interval in the Feienberg region) was increased up to 50% to investigate the potential effects of climate change on nitrate leaching.

For each set of parameters and input data, a separate 1-year simulation run was performed for the Feienberg winter wheat test site (01 September 2004 to 31 August 2005) using the standard parameterization for the other model parameters and input data. Table 3 gives an overview about soil parameterization of the reference run. To ensure the evaluation without interaction with the plant growth model, a non-vegetated test site was modelled. Reference modelling results for annual nitrate leaching under the sand, silt and clay soil were 77, 35 and 18 kg ha^{-1}.

The sensitivity analysis that the prediction of nitrate leaching is strongly dependent on the initial amount of mineral nitrogen in the soil profile (Fig. 6). The highest deviations can be found for the maximum initial N-content of 100 kg ha^{-1} for the heavier soils. Here, the result for nitrate leaching was more than doubled (120%) due to the low absolute reference value. Sand is not as strongly effected (75%) because it already exhibits high leaching amounts in relation to the increase of initial N_{min}.

Sensitivity to C_{org}-content for silt is higher (128%) than for the sand and clay soil. Mineralization was strongest in the silt soil due to favourable conditions for microbial activity.

Table 8 – Minimum (Min), reference (Ref) and maximum (Max) values of water content at field capacity (θ_{FC}) and saturated hydraulic conductivity (K_{sat})

Parameter	S			U			C		
	Min	Ref	Max	Min	Ref	Max	Min	Ref	Max
θ_{FC}[a] ($m^3\,m^{-3}$)	2	7	16	26	29	40	33	40	47
K_{sat}[b] ($cm\,s^{-1}$)	10^{-3}	3.4×10^{-3}	10^{-1}	10^{-3}	5×10^{-4}	10^{-5}	10^{-4}	2.6×10^{-5}	10^{-6}
N_{min} ($kg\,ha^{-1}$)	0				40				100
C_{org}[c] (%)	0.75[d]				2.0[d]				3.75[d]
Temp (°C)	9.7				11.7				13.7
P (mm)	367				917				1440

Variation of soil independent initial mineral nitrogen (N_{min}), organic matter content (C_{org}), annual mean air temperature (Temp) and precipitation sum (P) used for model parameterization in the sensitivity analysis.

[a] Rawls et al. (1993).

[b] Hillel (1998).

[c] Ad-hoc- Boden (2005).

[d] Assuming a constant humus CN ratio of 10.

The buffering capacities of clay reduce the effect of an accelerated release of nitrogen from organic matter. In general, sensitivity to C_{org}-content tends to be less than for the initial N_{min}-content (max. 71%).

The influence of field capacity is small but non-linear and depends on the relation of precipitation to water retention. Under given conditions, leaching from sand is reduced by 30% when increasing field capacity to the maximum (Fig. 6). The heavier soils show a different behaviour, which is due to their high water holding capacity. There, minor effects on modelled leaching are noticeable (<20%).

Most soil models are sensitive to the parameterization of K_{sat} controlling vertical water fluxes in the soil profile. Due to the dependence of N-leaching from water movement, also nitrogen fluxes can be strongly influenced. Here, the maximum deviation of 95% indicates a high sensitivity for K_{sat}, especially in clay, where the minimum K_{sat}-value almost prevents N-leaching due to poor permeability (Fig. 6). A non-linear reaction of model output is due to degrading mineralization conditions. Around a soil specific soil water optimum, conditions for mineralization become too dry or saturated, influencing decomposition negatively. However, even rising values of K_{sat} can lead to reduced N-leaching while percolation increases.

Changing soil temperature affects N-leaching but in comparison to other factors model sensitivity is small (max. 13%). Due to accelerated microbial activity, mobilization from organic compounds and nitrification support nitrate leaching. Lower temperature slows mineralization and reduces nitrate leaching (Fig. 6).

Sensitivity to total precipitation is high for all soils. An almost linear increase or decrease of model output up to 78% demonstrates the impact of rainfall as input data (Fig. 6). In contrast, the increment of just the extreme events shows

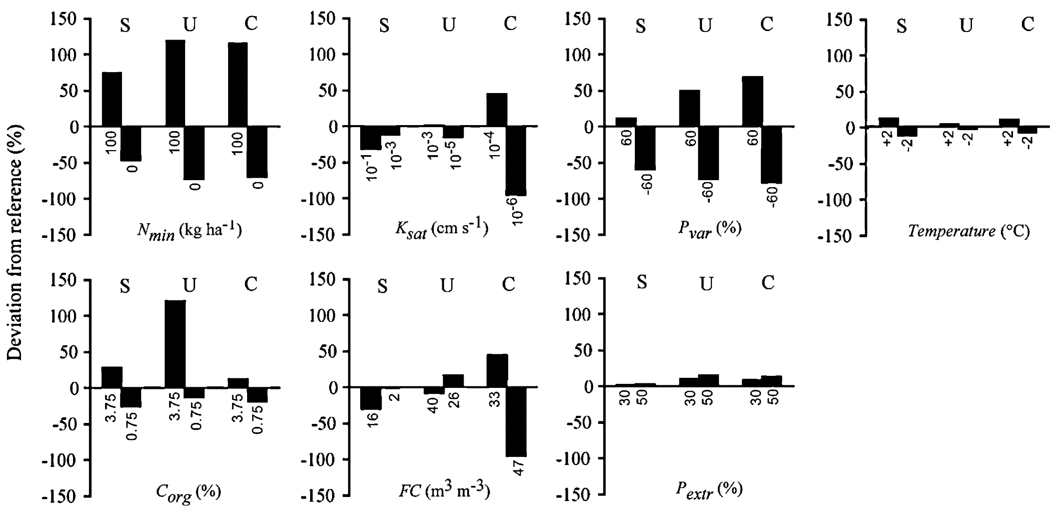

Fig. 6 – Results of the sensitivity analysis; illustrated are relative deviations (%) of modelled nitrate leaching from the reference; results are shown for a sand (S), a silt (U) and a clay (C) soil; small numbers below the bars represent maximum and minimum values of each parameter used for the sensitivity analysis. N_{min} is mineral nitrogen content, C_{org} is organic carbon content, K_{sat} is saturated hydraulic conductivity, FC is field capacity, P_{var} is variation of precipitation amount, P_{extr} is variation of precipitation amount of extreme events.

negligible variation (max. 15%) in simulated N-leaching. A combination of exceeded infiltration capacity (and increasing runoff) and the low amount of nitrogen in the soil at the moment when rainfall occurred were responsible for low variation in modelled nitrate leaching.

Overall, the sensitivity analysis shows that modelling of nitrate leaching depends mainly on the initial N_{min}-content, K_{sat} and the amount of precipitation. Also, sandy soils with a high hydraulic conductivity and a low water retention capacity are prone to nitrate leaching, especially in intensively used agricultural regions where high rates of precipitation occur. Thus, in the absence of spatially explicit accurate initialization data for the large scale modelling, (i) a model spin-up over a few years is important in order to begin the study with initial values that show realistic soil conditions resulting from the interaction of crop growth and soil conditions, (ii) emphasis must be put on an accurate parameterization of K_{sat} due to spatial variability, as well as its variability within one soil texture class and (iii) consideration of highly sensitive combinations of land use and soil (e.g. sugar beet or maize on sandy soils) for nitrate leaching is very important for large scale modelling.

Considering the model efficiency, regionalization of the soil model to 1 km^2 grid cells for the whole Upper Danube basin according to the geocomplex concept (Ludwig et al., 2003) should lead to an improvement of modelling results for regional applications. With the geocomplex concept, the spatial heterogeneity of processes and parameters within a 1 km^2 raster grid is represented by different combinations of subgrid land use-soil classes. In accordance to the model parameterization used here for the validation of field measurements, these subgrid classes allow the assignment of model parameters to a raster cell based upon rules. Results of the sensitivity analysis will be utilized to derive subgrid classes which represent spatial variability of parameters and processes within one raster cell. Thus, the parameterization used here is directly transferable to large scale modelling using the geocomplex approach.

5. Conclusion

In general, the soil nitrogen model provides reasonable results for N- and water dynamics under winter wheat, summer barley and maize for a variety of different soils without site-specific model calibration. The best model performance for nitrogen and water dynamics was found for maize. For summer barley and one of the winter wheat test sites, some problems occurred in modelling water dynamics. Despite this, N-dynamics were simulated very reasonably for all test sites. As indicated by the sensitivity analysis, rules to aggregate small scale heterogeneity for large scale modelling need to consider particularly sandy soils because of their great sensitivity for nitrate leaching. Although the effects of global change may be less than the effects of imperfect model parameterization and uncertain input data, global change effects can nevertheless be evaluated with the model, since uncertainties of parameterization and input data affect both, the reference as well as the scenario results. Due to the process-based model description and the adequate model results without local parameter fitting, the presented modelling concept showed its suitability to model soil water and nitrogen dynamics for large scale modelling.

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