

Assessment of nitrogen leaching from arable land in large river basins

Part I. Simulation experiments using a process-based model

Valentina Krysanova *, Uwe Haberlandt

Potsdam Institute for Climate Impact Research, Telegrafenberg, P.O. Box 601 203, 14412 Potsdam, Germany

Received 28 March 2001; received in revised form 6 November 2001; accepted 26 November 2001

Abstract

A two-step procedure for analysing nitrogen leaching from arable land in large river basins is suggested: (1) application of a process-based dynamic model for a set of representative conditions in a large river basin to simulate water and nitrogen fluxes and (2) development of a fuzzy-rule based metamodel using the simulated nitrogen fluxes in Step 1 as a training set. After that the metamodel can be used for rapid assessment of water quality inside the considered ranges of parameters, describing natural conditions and management practices. This paper describes Step 1 of the procedure. Step 2 is described in an accompanying paper (Haberlandt et al., *Ecological Modelling* 150 (3) (2002) 277–294). The advantage of this approach is that it combines the ‘process-based foundation’ with the resulting simplicity of the metamodel. Simulation experiments for analysing nitrogen (N) leaching from arable land were performed using the Soil and Water Integrated Model (SWIM) for a set of representative conditions in the Saale basin (23 687 km²) in Central Europe. The Saale River is one of the main tributaries of the Elbe. In advance, hydrological validation of the model was done for the whole Saale basin and validation of nitrogen dynamics was fulfilled in two mesoscale sub-basins of the Elbe. For the simulation experiments the drainage basin area was sub-divided into five climate zones and nine representative soil classes were chosen. The basic rotation and fertilisation schemes were established using regional information obtained from literature. In addition, the effects of changing the basic rotation to more/less intensive ones and changing fertilisation rates by 50% increase/decrease were studied. The ranges of simulated nitrogen fluxes for the basic rotation and fertilisation schemes are comparable to available regional estimates and differences between sub-regions and soils are plausible. The relative importance of natural and anthropogenic factors affecting nitrogen leaching for the Saale River basin was as follows: (1) soil, (2) climate, (3) fertilisation rate and (4) crop rotation. The simulation experiments provide a basis for a fuzzy-rule based metamodel approach, which aims at rapid water quality assessment of large regions. © 2002 Elsevier Science B.V. All rights reserved.

Keywords: Ecohydrological modelling; Diffuse pollution; Nitrogen wash-off; Nitrogen leaching to groundwater; Water quality; River basin

* Corresponding author. Tel.: +49-331-288-2515; fax: +49-331-288-2600.

E-mail address: krysanova@pik-potsdam.de (V. Krysanova).

1. Introduction

Rational management of water quality and provision of sufficient water of high quality at affordable costs belong to the most important issues of the EC policy in the coming decades. Nutrient pollution is no longer considered as a local matter, but as a serious problem in many large river basins in Europe and worldwide. In the case of phosphorus, point sources (municipal and industrial) still contribute a bulk of the riverine load in many European river basins. In the case of nitrogen, diffuse or non-point sources of pollution in the rural landscape (mainly arable fields) contribute a significant part of the total riverine load. It is obvious that quantification and control of point sources are much easier than those for the diffuse sources. Therefore the evaluation and quantification of the impacts of natural conditions (soil, climate and topography) and land management practises (crop rotation, fertilisation rate and time of application) on nitrogen wash-off to surface water and leaching to groundwater are very important. The evaluation of the impacts of different factors can be helpful for defining the effectiveness of measures aimed at reduction of diffuse nutrient pollution. Modelling tools can essentially contribute to that kind of assessment.

There are at least three different types of models dealing with the assessment of water quality at the river basin scale: (a) simple statistical models of riverine load for quantification of nutrient load from different sources (Grimvall and Stålnacke, 1996; de Wit, 1999), (b) simplified conceptual deterministic models, which are partly based on outputs from other models (MIR—van Herpe et al., 1998; HBV-N—Arheimer and Brandt, 2000), or try to couple several models (Beaujouan et al., 2001; Arhonditsis et al., 2000); and (c) deterministic continuous process-based models coupling hydrological, biogeochemical and ecological processes at the river basin scale (SWAT—Arnold et al., 1994; MIKE SHE—Refsgaard, 1997; Soil and Water Integrated Model (SWIM)—Krysanova et al., 1998). Besides, there are continuous process-based models coupling hydrochemical and ecological processes for the assessment of water quality at the patch or field

scale (EPIC—Williams et al., 1984; SOILN—Johnsson et al., 1987; THESEUS—Wegehenkel, 2000).

Among those, the deterministic continuous process-based models SWAT, MIKE-SHE and SWIM are appropriate tools to investigate the complex chain of interrelated factors defining nitrogen wash-off to surface water and leaching to groundwater in large heterogeneous basins. Nevertheless, due to their complexity and high data requirements, such models are not best suited for *rapid assessment of water quality* in large-scale applications aimed at policy support. Therefore, a two-step procedure is suggested:

- Step 1: after appropriate validation a process-based model (in our case—SWIM) is applied for a set of representative conditions in a large river basin to simulate water and nitrogen fluxes;
- Step 2: a fuzzy-rule based metamodel is created using the simulated nitrogen fluxes in Step 1 as a training set and the results are compared to those of Step 1.

After that the fuzzy-rule based metamodel can be used for the rapid assessment of water quality in the same or similar basins inside the considered ranges of parameters, describing natural conditions and management practices. This paper describes Step 1 of the procedure. Step 2 is described in Haberlandt et al. (2002). The advantage of this approach is that it combines the ‘process-based foundation’ with the resulting simplicity of the metamodel, which is comparable to that of the statistical and simplified conceptual models. Besides, the metamodel can be efficiently included in decision support systems for integrated assessment. A similar integrated approach was used by Børgesen et al. (2001) to investigate the effect of legislation on nitrogen leaching, where a statistical model was set up on the basis of simulation results obtained with the deterministic model DAISY (Hansen et al., 1991).

The process-based ecohydrological modelling system SWIM (Krysanova et al., 1998) was used as a dynamic tool in our case study. The simulation experiments with SWIM were performed, considering a set of representative natural conditions and land management practices in the Saale

River basin, with two main objectives: (1) to evaluate natural and anthropogenic factors influencing nitrogen wash-off to surface water and leaching to groundwater and (2) to provide a basis for a fuzzy-rule based metamodel approach for water quality assessment in large river basins.

In the paper the terms ‘N losses with water’ and ‘N leaching’ are used for the total N losses from soil with surface runoff, lateral subsurface flow and percolation to groundwater; the term ‘N wash-off’ is used for N losses from soil with surface runoff and subsurface flow; and the term ‘N leaching to groundwater’ refers only to N losses with percolation to groundwater.

2. Case study basin and choice of representative conditions

2.1. Basin description

The Saale River is one of the main tributaries of the Elbe River located in Central Europe. Practically the whole Saale drainage basin is located in Germany. In general, the German part of the Elbe drainage area is subdivided into three typical sub-regions based on relief and soils, namely: the Pleistocene lowland, the loess sub-region and the mountainous sub-region. The Saale basin occupies large parts of the loess and mountainous sub-regions. The total length of the Saale River is about 320 km and the drainage basin area is about 24 000 km². The main tributaries of the Saale are the Unstrut, the Weiße Elster and the Bode. The basin includes the cities of Leipzig, Halle, Erfurt, Gera and Jena. Topography of the basin is heterogeneous with elevation varying between 50 m a.m.s.l. and about 1100 m a.m.s.l. Highland areas are represented by the Harz Mountains and the Thüringer Wald.

The long-term mean annual precipitation in the Saale basin is about 700 mm. The long-term mean discharge of the Saale River is 115 m³ s⁻¹ at the mouth and the specific discharge is 4.85 l s⁻¹ km⁻², which corresponds to the mean annual discharge of 3.63 × 10⁹ m³. The river discharge is characterised by winter and spring high water periods. There are several regulating reservoirs in the upper part of the basin.

Nutrient pollution (nitrogen and phosphorus) is one of the most widespread forms of water pollution in the basin. Agriculture land occupies about 63% of the total Saale drainage area with its very productive loess soils and represents the most important source of diffuse nitrogen pollution. The Saale and its tributaries are intensively used for fresh water supply for domestic, industrial and agricultural purposes. Though since the beginning of the nineties the emissions from point sources were notably decreased in the basin due to closing of some industries, reduction of others and introduction of new and better sewage treatment facilities, the diffuse sources of pollution represented mainly by agriculture are still not sufficiently controlled.

The intended simulation experiments had to incorporate a wide range of representative natural and management conditions, but the number of variants and the length of the time series had to be restricted. Therefore, not all possible combinations of natural conditions and management practices in the Saale basin were considered in the simulation runs. Nevertheless, the intention was to include a set of conditions representative for the basin. The conditions incorporated in the simulations included five different climate conditions (represented by climate stations), nine soil classes (represented by soil types according to soil map BÜK-1000, Hartwich et al., 1995), five elevation classes (represented by slope steepness) and nine agriculture practices (combinations of three crop rotations and three fertilisation schemes).

2.2. Choice of representative natural conditions

The choice of climate stations in the region was based on a graphical cluster analysis of the long-term average annual precipitation and average temperature as described below. Another condition for the inclusion of a station was that it has continuous data during the simulation period 1961–1990. The five selected climate stations are listed in Table 1 (Fig. 1a). They are ordered according to the annual precipitation ranging from 460 to 940 mm. The altitude of the stations ranges from 164 m a.m.s.l. in Artern to 567 m a.m.s.l. in Hof-Hohensaas. The higher altitudes in

the basin (up to 1100 m) were ignored, because most of the agricultural land is at lower altitudes. Namely, about 40% of agricultural land is located in areas lower than 200 m, 79% lower than 400 m and 96.4% lower than 600 m. In addition, five climate zones represented by the selected climate stations were defined for the Saale basin using the following five-step procedure:

1. two gridded maps were produced for the long-term average annual temperature and precipi-

2. after that both maps were normalised by converting the long-term average annual temperature and precipitation using the formulas:

$$P_{ij}^n = \frac{P_{ij} - \bar{P}}{S_P} \quad \text{and} \quad T_{ij}^n = \frac{T_{ij} - \bar{T}}{S_T},$$

where P_{ij} , T_{ij} are the long-term average annual precipitation and temperature for grid cell i ,

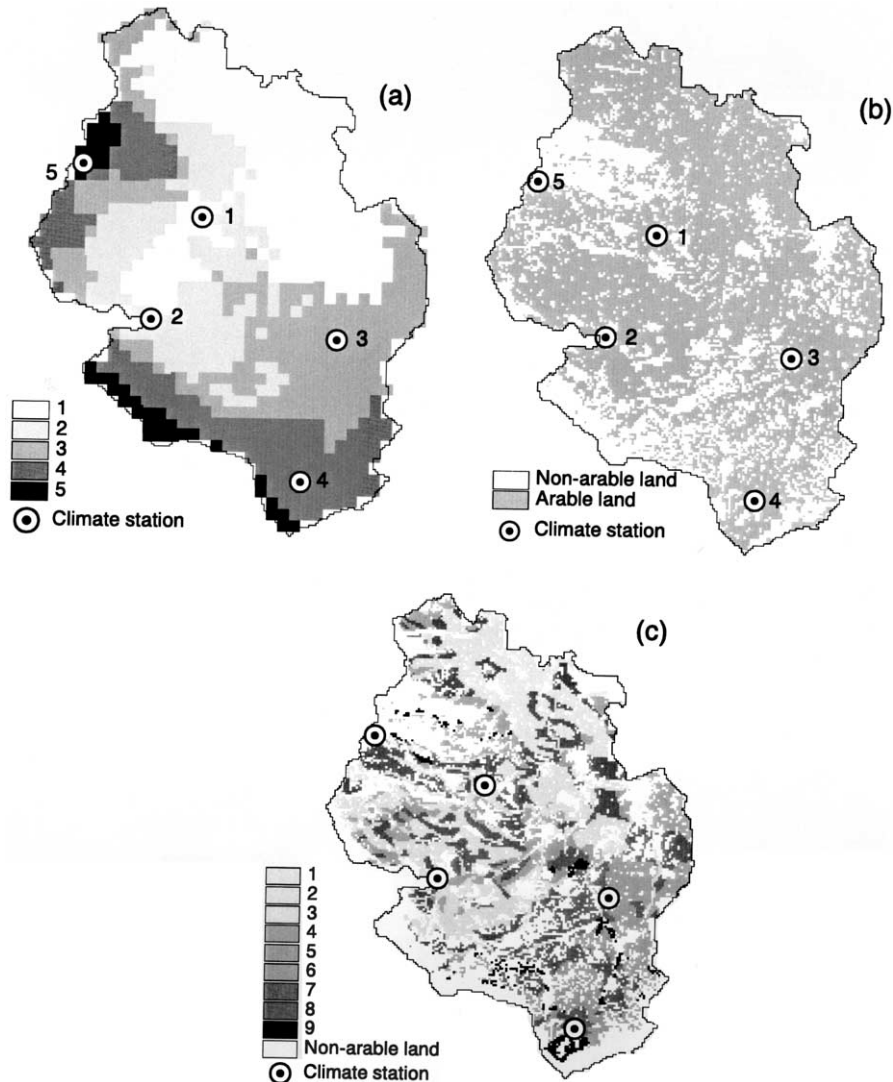


Fig. 1. Five climate zones represented by the climate stations (a), arable land (b) and nine soil classes in the arable land (c) for the Saale drainage basin.

j ; \bar{P} , \bar{T} are the long-term average annual precipitation and temperature for the whole basin; S_P , S_T are the standard deviation of the long-term average annual precipitation and temperature for the whole basin; and P_{ij}^n , T_{ij}^n are the normalised long-term average annual precipitation and temperature for grid cell i, j ;

- so-called ‘climatic distances’ were calculated between every pixel and five climate stations as

$$d_{ij}^k = |P_{ij}^n - P_{St(k)}^n| + |T_{ij}^n - T_{St(k)}^n|,$$

where $P_{St(k)}^n$, $T_{St(k)}^n$ are the normalised long-term average annual precipitation and temperature for climate station k ; d_{ij}^k is the ‘climatic distance’ between pixel i, j and climate station k ;

- for every pixel the minimum climate distance was defined $\min(d_{ij}^k)$ and then the climate zones were defined by assigning pixel i, j to the climate zone with the minimum climatic distance;
- the set of pixels belonging to climate station k created the corresponding climate zone.

Another option for the definition of climate zones could be to distinguish between the growing and non-growing season and to use the temperature and precipitation average values for the growing and non-growing seasons separately. However, as soon as we have many winter crops included in the rotations, and nitrogen leaching occurs also in winter, the long-term annual average values for temperature and precipitation were used for the definition of climate zones. The outlined climate zones allowed mapping of the obtained simulation results for the basin (see Section 4).

The arable land (Fig. 1b) includes 34 soil types (BÜK-1000, Hartwich et al., 1995), whereas 23 of them occupy 96.7% of the total cropland area. Loess soils or soils from loess mixed with weathering products are the dominant types, rocky soils occur mainly in the highland and mountain areas, where arable land is rare. The 23 soils were subsequently classified into nine soil classes (see Table 1 and Fig. 1c), primarily in accordance with their field capacity, saturated hydraulic conductivity and occurrence in arable land (Table 1). The nine soil classes represent a wide range of field capacities (32.3–49.8 vol.%) and two orders of magni-

tude of saturated hydraulic conductivity (0.4–41.1 mm h⁻¹).

Five elevation classes represented by topographic slope were considered: class 1 with the minimal slope of 0.2%, classes 2, 3 and 4 with the slopes of 2.5, 5 and 7.5%, respectively, and class 5 with the maximum slope of 10%. The maximum slope was chosen taking into account the real slope steepness in the cropland of the basin.

2.3. Choice of land management practices

Three rotation schemes, 10 years each, and three fertilisation schemes (Table 1) represent a range of agricultural management practices considered in the simulation experiments. The basic rotation and fertilisation schemes (scheme 1) were derived from the typical practices in the area (Krönert et al., 1999; Roth et al., 1998). Winter crops are indicated in Table 1 for the year when they are harvested. Two additional rotation schemes were applied; a more intensive rotation (scheme 2), which included two additional years of silage maize instead of 1 year of spring barley and 1 year of set-aside, and a less intensive rotation (scheme 3), which included two additional years of set-aside instead of 1 year of silage maize and 1 year of winter wheat.

For example, according to Krönert et al. (1999), cereals occupy 50.6–52.5% of arable land in the loess sub-region, which is comparable to 50–60% in our three rotation schemes. Winter wheat as a valuable crop occupies 20.2–28.7% of arable land in the loess sub-region and 20–30% in our three rotations. The real occurrence of maize (8–9.4%) is comparable to 10% in our basic rotation scheme 1, while it differs in rotations 2 and 3 (this was done on purpose to study the level of intensification). Intertillage row crops potatoes and sugar beet are reported as occupying 15.4–16.9% of arable land together, which is comparable to 20% of potatoes in the simulation experiments. The substitution is reasonable, because these two crops are similar regarding crop yield and N uptake.

The rates of fertilisation applied in the model experiments are crop-specific (Table 1). The cereals (winter wheat, winter barley, winter rye and spring barley) are fertilised by mineral N three times, including once in autumn for winter crops,

Table 1
Classification of natural conditions and agricultural land management in the Saale River basin used for the simulation experiments with the SWIM model

<i>I. Climate zones, represented by climate stations</i>						
No	Station name	Station number	Altitude, m a.m.s.l.	Average annual precipitation (mm)	Average annual temperature (°C)	
1	Artern	3402	164	460	8.4	
2	Erfurt	4200	316	503	8.0	
3	Gera-Leumnitz	4406	311	611	8.0	
4	Hof-Hohensaas	4027	567	732	6.5	
5	Bad Sachsa	3988	335	940	7.6	
<i>II. Soil classes, represented by soil types (BÜK-1000)</i>						
No	Name of the main soil belonging to the class	Main soil ID	Other soils ID	Occurrence in arable land (%)	Field capacity in root zone (vol. %)	Saturated conductivity in root zone (mm/h)
1	Floodplain soil from loamy-clay sediments	9	8, 49	7.0+4.4 ^a	39.3	5.0
2	Tschernosem from loess	36	–	13.8+0	39.7	9.9
3	Braunerde-Pelosol from weathering products	51	–	4.8+0	49.8	0.4
4	Braunerde from loess and weathering products	59	42	7.6+4.3	35.3	4.8
5	Tschernosem-Braun- nerde from loess	40	46, 11	5.1+4.5	36.9	17.5
6	Braunerde from loess and weathering products	56	48	6.4+5.7	37.5	9.0
7	Pseudogley-Tschern- osem from loess	38	37, 41, 61, 64	3.9+12.2	38.6	20.5
8	Parabraunerde-Pse- udogley from loess	43	44, 45, 53, 57	3.2+6.3	36.9	13.9
9	Braunerde from sour rocks	55	–	4.3+0	32.3	41.1

Table 1 (Continued)

III. Rotation schemes										
No	Crop sequence	2	3	4	5	6	7	8	9	10
1	po ^b	ww	sb	wr	set-aside	ww	wb	po	ww	ma
2	po	wb	ma	ww	wr	ww	ma	po	ww	ma
3	po	set-aside	sb	wr	set-aside	ww	wb	po	ww	set-aside

IV. Fertilisation schemes										
No	Winter wheat (fertilisation rate in kg ha ⁻¹)	Winter barley (fertilisation rate in kg ha ⁻¹)	Winter rye (fertilisation rate in kg ha ⁻¹)	Spring barley (fertilisation rate in kg ha ⁻¹)	Potatoes (fertilisation rate in kg ha ⁻¹)	Maize (fertilisation rate in kg ha ⁻¹)	Set-aside (fertilisation rate in kg ha ⁻¹)			
1	30+60+30 N ^c	20+60+20 N	20+60+20 N	60+20+20 N	140 N	180 N	0 N			
	30+30 org N ^d	30+30 org N	30+30 org N	30+30 org N	30+30 org N	30+30 org N	0 org N			
2	45+90+45 N	30+90+30 N	30+90+30 N	90+30+30 N	210 N	270 N	0 N			
	45+45 org N	45+45 org N	45+45 org N	45+45 org N	45+45 org N	45+45 org N	0 org N			
3	15+30+15 N	10+30+10 N	10+30+10 N	30+10+10 N	70 N	90 N	0 N			
	15+15 org N	15+15 org N	15+15 org N	15+15 org N	15+15 org N	15+15 org N	0 org N			

^a Occurrence of the main soil plus occurrence of other soils.

^b po—potatoes, ww—winter wheat, wb—winter barley, wr—winter rye, sb—spring barley, ma—silage maize.

^c Fertilisation by mineral N.

^d Fertilisation by organic N.

while for silage maize and potatoes the total annual amount is applied only once, during the sowing (Roth et al., 1998). In addition, organic fertiliser is applied using the following rules: for winter crops 30 kg ha⁻¹ of organic N is applied 23–43 days before sowing (depending on the previous crop) and 30 kg ha⁻¹ is applied at the beginning of March; and for summer crops 30 kg ha⁻¹ is applied at the end of October of the previous year and 30 kg ha⁻¹ is applied 6 weeks after sowing in the spring. Two other fertilisation schemes were used in the model by increasing (scheme 2) or decreasing (scheme 3) the fertilisation rates by 50% without changing the time of application.

The three rotation schemes and three fertilisation schemes were combined. It is worth mentioning that the same fertilisation scheme 1 combined with three different rotations assumes a different total amount of fertilisers applied in a 10-year period: a larger amount with rotation scheme 2 and a smaller amount with rotation scheme 3 compared to the amount with rotation scheme 1. This is due to a higher amount applied for the 3-year maize in rotation scheme 2 and no application for three years of set-aside in rotation scheme 3.

Simulation runs were performed for 30 years, 1961–1990, for all possible combinations of five climate zones, nine soil classes, three rotation schemes, three fertilisation schemes and five elevation zones, which produced $5 \times 9 \times 3 \times 3 \times 5 = 2025$ time series with daily time step.

3. Modelling system

The modelling system SWIM (Fig. 2) includes as its kernel a continuous-time spatially distributed model, which integrates hydrology, vegetation, nutrients (nitrogen, N and phosphorus, P) and sediment fluxes at the river basin scale. In addition, it includes an interface to the Geographic Information System GRASS (1993), which allows the extraction of spatially distributed parameters including elevation, land use, soil types and the routing structure for the model initialisation. The model can be applied for

mesoscale river basins (or regions) with an area up to 25 000 km², or, after validation in representative sub-basins, for regions of similar size.

The simulated hydrological system consists of four control volumes: the soil surface, the root zone, the shallow aquifer and the deep aquifer. The soil column is sub-divided into several layers in accordance with the soil database. The water balance for the soil column includes precipitation, surface runoff, evapotranspiration, percolation and subsurface runoff. The water balance for the shallow aquifer includes groundwater recharge, capillary rise to the soil profile, lateral flow and percolation to the deep aquifer.

The module representing crops and natural vegetation is an important interface between hydrology and nutrients. A simplified EPIC approach (Williams et al., 1984) is included in SWIM for simulating arable crops (like wheat, barley, rye, maize, potatoes) and aggregated vegetation types (like 'pasture', 'evergreen forest', 'mixed forest'), using specific parameter values for each crop/vegetation type. The model uses a concept of phenological crop/plant development based on:

- daily accumulated heat units;
- Monteith's approach (1977) for potential biomass;
- water, temperature and nutrient stress factors; and
- harvest index for yield partitioning.

The simplification in comparison with the field-scale model EPIC concerns mainly phenological processes and is aimed in enabling the parametrisation of the model at the regional scale. Vegetation in the model affects the hydrological cycle by the cover-specific retention coefficient, which influences runoff and indirectly the amount of evapotranspiration, which is simulated as a function of potential evapotranspiration and LAI.

The nitrogen and phosphorus modules include the following pools: nitrate nitrogen (N_m in Fig. 2), active and stable organic nitrogen (N_{oa} and N_{os} , respectively), organic nitrogen in the plant residue (N_{res}), labile phosphorus (P_{lab} in Fig. 2), active and stable mineral phosphorus (P_{mac} and P_{mst} , respectively), organic phosphorus (P_{org}) and phosphorus in the plant residue (P_{res}), and the flows: fertilisation, input with precipitation, min-

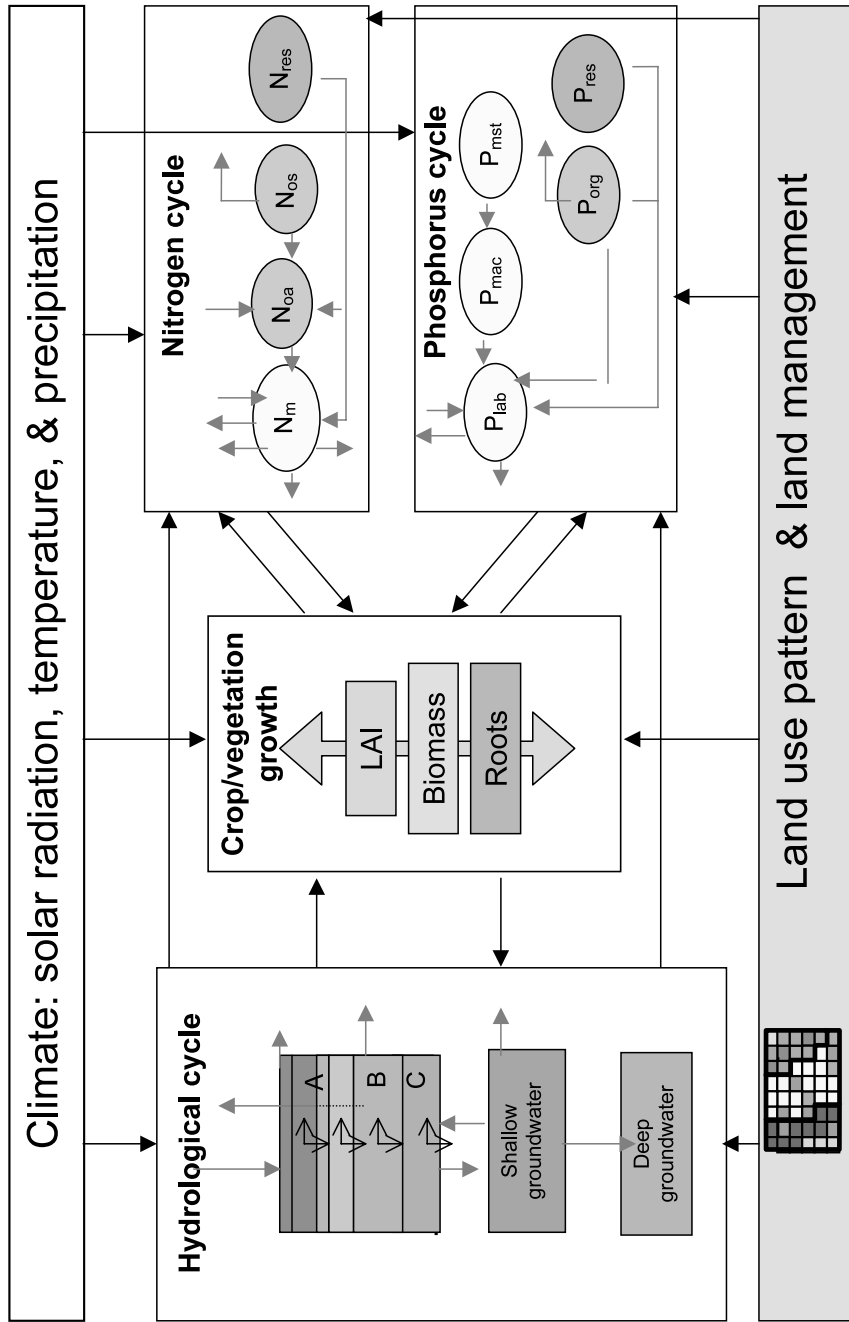


Fig. 2. A generalised flowchart of the SWIM model, coupling hydrological processes, vegetation growth and nutrient dynamics.

eralisation, denitrification, plant uptake, leaching to groundwater, losses with surface runoff, interflow and erosion.

The nitrogen mineralisation model is a modification of the PAPRAN mineralisation model (Seligman and van Keulen, 1991). The model considers two sources of mineralisation: fresh organic N pool, associated with crop residue and the active organic N pool, associated with the soil humus. The stable organic N pool is not subjected to mineralisation. Organic N flow between the active and stable pools is described with an equilibrium equation, assuming that the active pool fraction at equilibrium is 0.15. The decomposition rate of residue is a function of C:N ratio, C:P ratio, temperature and water content in soil. The mineralisation from the active organic N is a function of temperature and water content in soil.

Denitrification causes $\text{NO}_3\text{-N}$ to be volatilised from soil. The denitrification occurs only under the conditions of oxygen deficit, which usually is associated with high water content in soil. Besides, as one of the microbial processes, denitrification is a function of soil temperature and carbon content. The soil water factor considers total soil water and is represented by an exponential function, which reaches 0.5 at 0.7 of field capacity and approaches 1.0 close to field capacity.

Nitrogen uptake by crop is estimated using a supply and demand approach. The daily crop N demand is calculated as a function of the optimal N concentration in the crop biomass and already accumulated N in biomass. Three parameters are specified for every crop in the crop database, which describe: normal fraction of nitrogen in plant biomass at emergence, at half-maturity and at maturity. Then the optimal crop N concentration is calculated as a function of growth stage. The crop is allowed to take nitrogen from any soil layer that has roots. Uptake starts at the upper layer and proceeds downwards until the daily demand is met or until all N has been depleted.

The total amount of water lost from the soil layer is the sum of surface runoff, lateral subsurface flow (or interflow) and percolation from this layer. The amount of nitrate nitrogen lost with water is the product of $\text{NO}_3\text{-N}$ concentration and

water loss. The amount of $\text{NO}_3\text{-N}$ left in the layer is adjusted daily. Then the $\text{NO}_3\text{-N}$ concentration is estimated by dividing the weight of $\text{NO}_3\text{-N}$ by the water storage in the layer. Amounts of $\text{NO}_3\text{-N}$ contained in surface runoff, lateral subsurface flow and percolation to groundwater are estimated as the products of the volume of water and the concentration.

Regarding the lateral transport, the wash-off is more important for nitrogen than for phosphorus. The latter is mainly transported with erosion. The interaction between nutrient supply and vegetation is modelled by the plant consumption of nutrients and using nitrogen and phosphorus stress functions, which affect the plant growth. The model SWIM is described in detail in Krysanova et al. (2000).

4. Analysis of simulation results

4.1. Model validation

Prior to this study SWIM was tested and validated sequentially for hydrology (in more than ten mesoscale sub-basins of the Elbe), for nitrogen dynamics, crop growth and erosion. The validation of nitrogen dynamics was performed for two mesoscale sub-basins of the Elbe: the Stepenitz (drainage area 575 km²) and the Zschopau (drainage area 1574 km²) (Krysanova and Becker 1999; Krysanova et al., 1999).

In addition, a hydrological validation for the whole Saale basin (gauge Calbe-Grizehne, 23 687 km²) was done. A comparison of the simulated and observed river discharge is shown in Fig. 3. The upper graph shows the comparison of the observed and simulated river discharge with the *daily time step* (though only years and months are indicated on the *x*-axis) at Calbe-Grizehne in 1985–1988. The Nash and Sutcliffe (1979) efficiency for this period is 0.82 and the difference in water balance is equal to -1% . The lower graph in Fig. 3 shows the comparison of the observed and simulated river discharge aggregated to the *monthly values* for 11 years period 1981–1991 (though only years are indicated on the *x*-axis). The coefficient of correlation is high: $r = 0.94$.

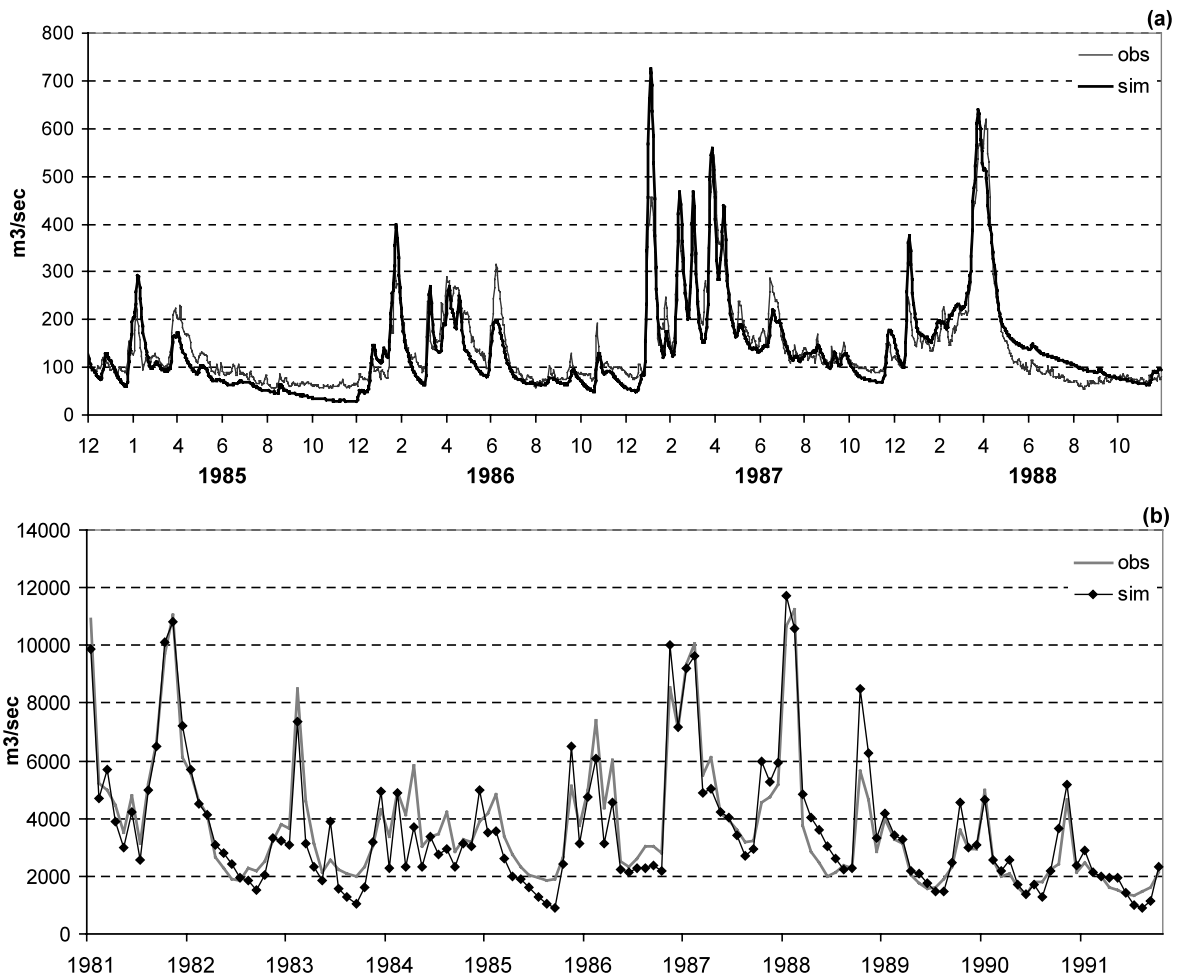


Fig. 3. Comparison of the daily (a) and monthly (b) dynamics of the observed and simulated river discharges for the Saale River, gauge Calbe-Grizelne.

4.2. Combined effect of climate, soil and elevation on N leaching

Modelled daily water fluxes (direct runoff, interflow, groundwater recharge and evapotranspiration) and daily N fluxes (N wash-off with direct runoff and interflow, N leaching to groundwater, N uptake by plants, N denitrification and N mineralisation) for all 2025 variants were aggregated to monthly, annual and average annual values and then analysed with respect to different natural conditions and management practices. In this paper only the monthly and long-term average annual fluxes are discussed.

The combined effects of climate, soil and elevation on N losses with water, considering direct runoff, interflow and leaching to groundwater, are depicted in Fig. 4. The three graphs include long-term average annual N losses for three slopes: the minimum slope of 0.2% (upper graph), the average slope of 5% (middle) and the maximum slope of 10% (lower graph). In this example, only the basic rotation and fertilisation schemes were considered. N losses with water for all soils increase with increasing precipitation from climate zone 1 to climate zone 5. Some soil classes (1–4) have low N leaching, which increases only slightly under wetter conditions (climate zone 5). N wash-off

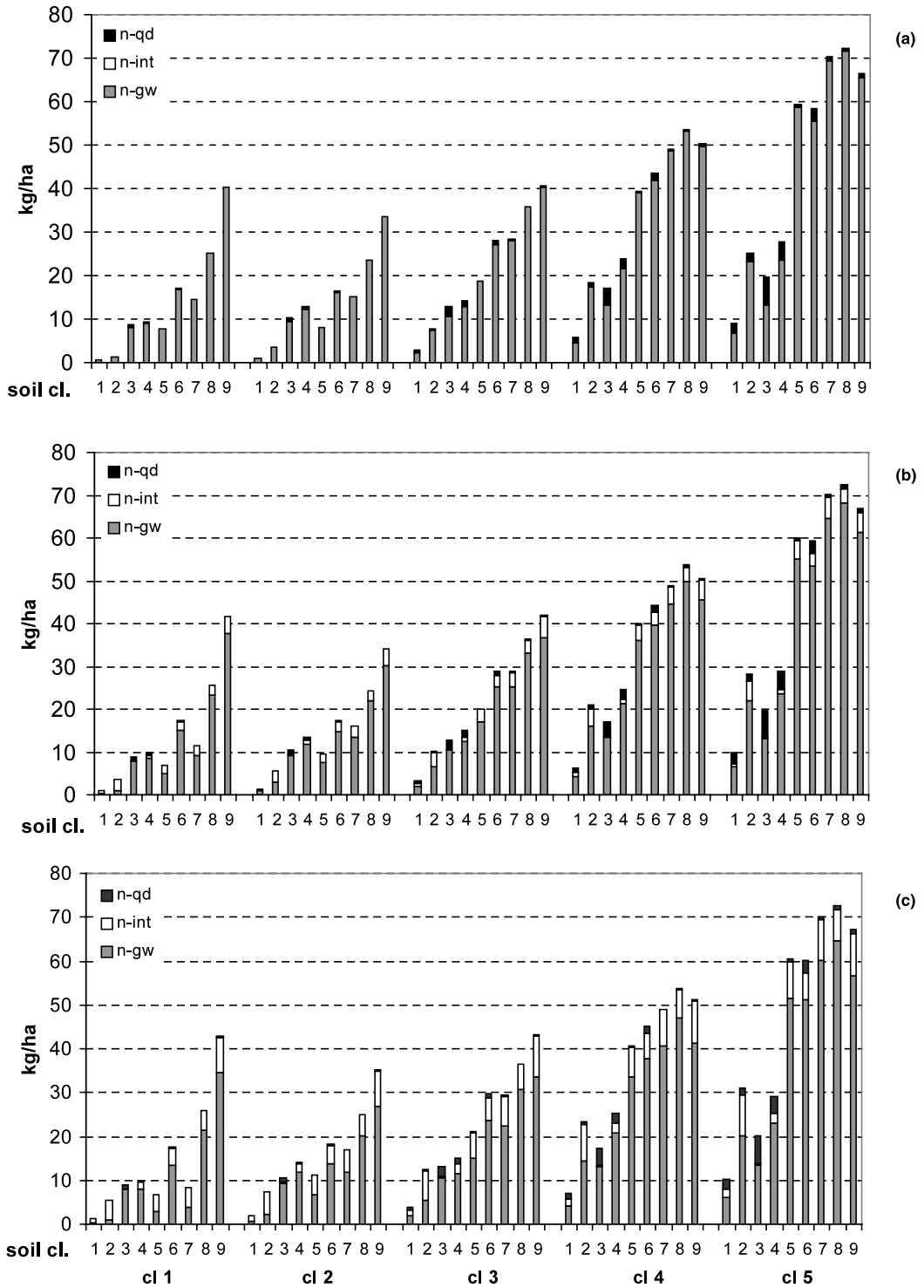


Fig. 4. Combined effects of climate (cl1, ..., cl5), soil classes (1, ..., 9) and elevation (a -SS = 0.002, b -SS = 0.05, c -SS = 0.10, where SS is the topographic slope) on the modelled long-term average annual N losses with water, considering fluxes in direct runoff (n-qd), interflow (n-inter) and to groundwater (n-gw).

with direct runoff is rather small, it is notable only for the less permeable soil classes 3 and 4 under wetter conditions.

As one can see in Fig. 4, total N losses with water fluxes are practically independent of elevation, however, the elevation affects the redistribution of fluxes: N losses in interflow increase at higher elevation and leaching to groundwater decreases, while the total amount remains practically the same. Consequently, the higher slopes were excluded from further analysis and as input for the metamodel. Under the minimum slope assumption (0.2%) the groundwater recharge and N leaching to groundwater for sandy soils increase only slightly and more significantly for loess soils in comparison with the average slope conditions, while the total N losses with water remain practically the same. This provides a sort of maximum estimate of N leaching to groundwater for all soils.

4.3. Effect of climate on monthly and seasonal dynamics of N fluxes

Fig. 5 shows the effect of climate on the monthly (three upper graphs) and annual (lower graph) N losses with water (marked *leach* +) and denitrification (marked *denit*) for soil class 5, considering the whole simulation period of 30 years and climate zones 2–4. Denitrification is added to N losses with water in these area-shaded graphs. The following observation can be made regarding N losses with water and to the atmosphere in dryer climate conditions (climate zone 2): N leaching is very low and does not exceed $1 \text{ kg ha}^{-1} \text{ year}^{-1}$ in more than half of the years in the simulation period and denitrification does not exceed $1 \text{ kg ha}^{-1} \text{ year}^{-1}$ in 8 years from 30 in the period. There are two relatively dry years 3 and 4 in the simulation period, when N leaching is practically zero in all three climate zones and N denitrification is almost zero in climate zones 2 and 3. In most cases, denitrification occurs simultaneously with N leaching, following water saturation in wet periods. The monthly sum of losses with water and to the atmosphere does not exceed 40 kg N ha^{-1} for this soil class in the considered

climate zones. In general, the increasing trend for N leaching in wetter conditions is evident: when precipitation increases from 503 through 611 to 732 mm on average, nitrogen losses from soil with water fluxes increase as well. For denitrification this trend is much less distinct (see Fig. 5d).

Fig. 6 shows seasonal dynamics of precipitation, water flows and N losses with water for soil class 6 in climate zones 1–4. Every monthly value was obtained by averaging the corresponding monthly values for the 30-year simulation period. Precipitation peaks occur in June and August and they increase from climate zone 1 to 4. Higher summer precipitation peaks and higher levels in winter are visible for climate zones 3 and 4. Water fluxes follow the precipitation trend increasing from climate zone 1 to 4. They are very low in summer in all cases and for climate zones 1 and 2 throughout the season (less than 10 mm/month). Nitrogen leaching also follows the increasing trend from climate zone 1 to 4. It is low in July–September/October and high in November–March.

4.4. Effect of land management on N fluxes

The effect of land management represented by rotation and fertilisation schemes on N uptake by plants, N denitrification and N losses with water is shown in Fig. 7 for four soil classes 1, 3, 6 and 8. The values presented in this figure are averaged over five climate zones. Fertilisation rates by mineral N (including N deposition with precipitation) and mineralisation of organic N are depicted as positive values on the graphs, while N uptake, N denitrification and N leaching are shown as negative values. The effect of higher fertilisation rates is obvious: both losses and uptake are higher when fertilisation scheme 2 is applied, and lower when fertilisation scheme 3 is applied, but the effect is non-linear: 50% increase/decrease in fertilisation does not lead to the same extent of change in uptake, denitrification or mineralisation. Also, changes in crop rotation affect N plant uptake and N losses: both are highest for rotation scheme 2 and lowest for rotation scheme 3. This figure also demonstrates that the balance of ni-

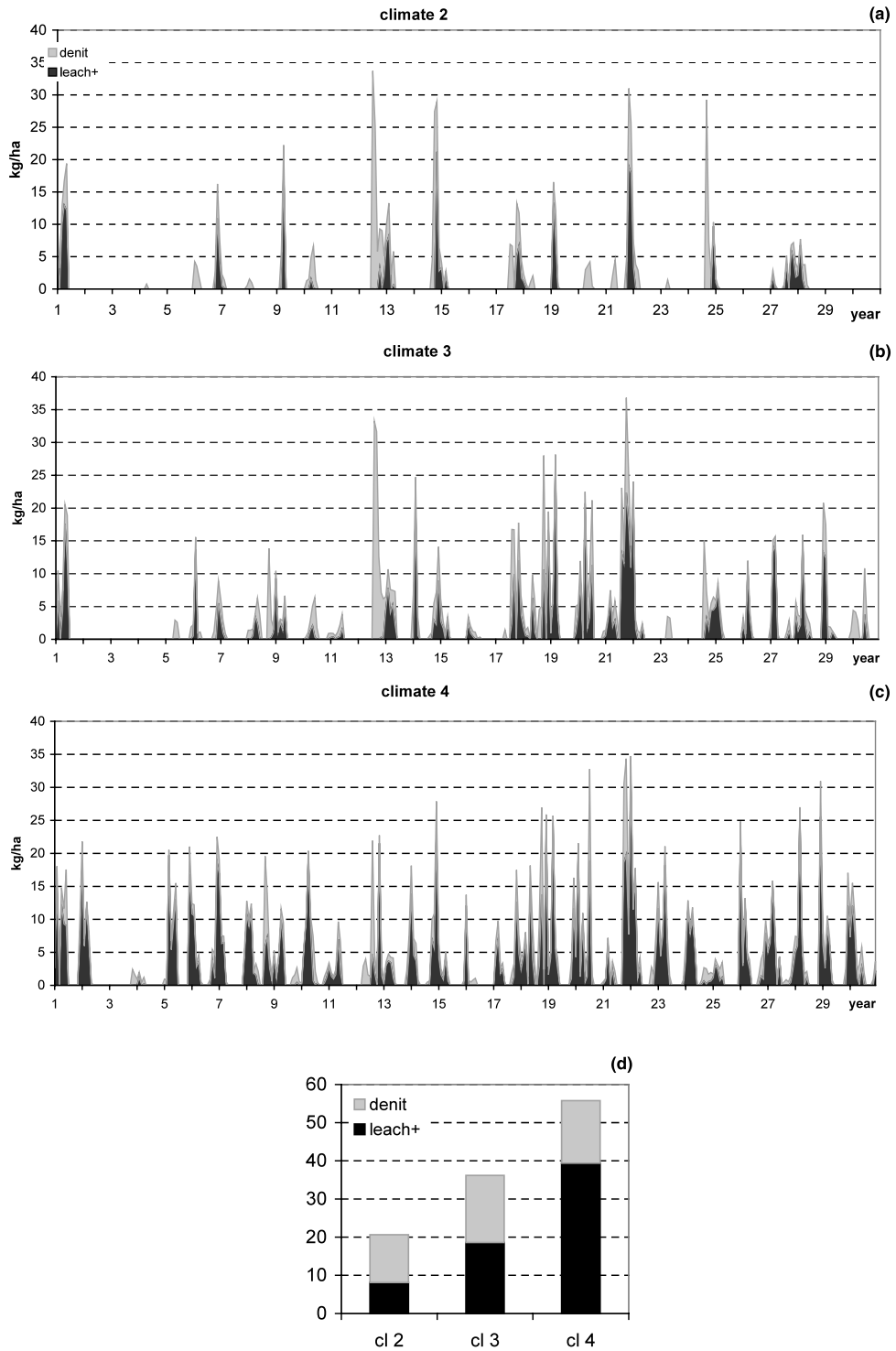


Fig. 5. The effect of climate on the monthly N losses with water (leach +) and denitrification (denit) for soil class 5 and climate zones 2 (a), 3 (b) and 4 (c), considering the whole simulation period of 30 years; and comparison of average annual N losses with water and to atmosphere for these three climate zones (d).

trate nitrogen is kept: differences between the input and output flows reflect changes in $\text{NO}_3\text{-N}$ content in soil, which do not exceed 4 kg ha^{-1} in all cases.

The analysis of results also shows that gaseous N losses are relatively high and leaching to groundwater is relatively low in soil classes 1–4 (see examples for soil classes 1 and 3 in Fig. 7). This pattern is attributed to a high field capacity and low saturated hydraulic conductivity, which enhances denitrification in these soils and assures their low permeability for water and associated fluxes. Very high denitrification in soil class 1 is caused by equally high fertilisation rates by mineral and organic fertilisers, applied to all soils in our simulations. In reality, lower rates of mineral

fertiliser and no organic fertiliser would be applied for soils with high organic matter content and low permeability, like soil class 1.

In contrast, leaching to groundwater is much higher and denitrification is zero in soil classes 7–9 (see e.g. soil class 8 in Fig. 7). This is mainly due to larger proportion of sand and higher saturated hydraulic conductivity of these soils. Soil classes 5 and 6 are intermediate in this respect: both denitrification and N leaching occur in these soils (see Figs. 5 and 7).

4.5. Spatial patterns

Modelling results for the long-term average annual N leaching, N denitrification, N mineralisa-

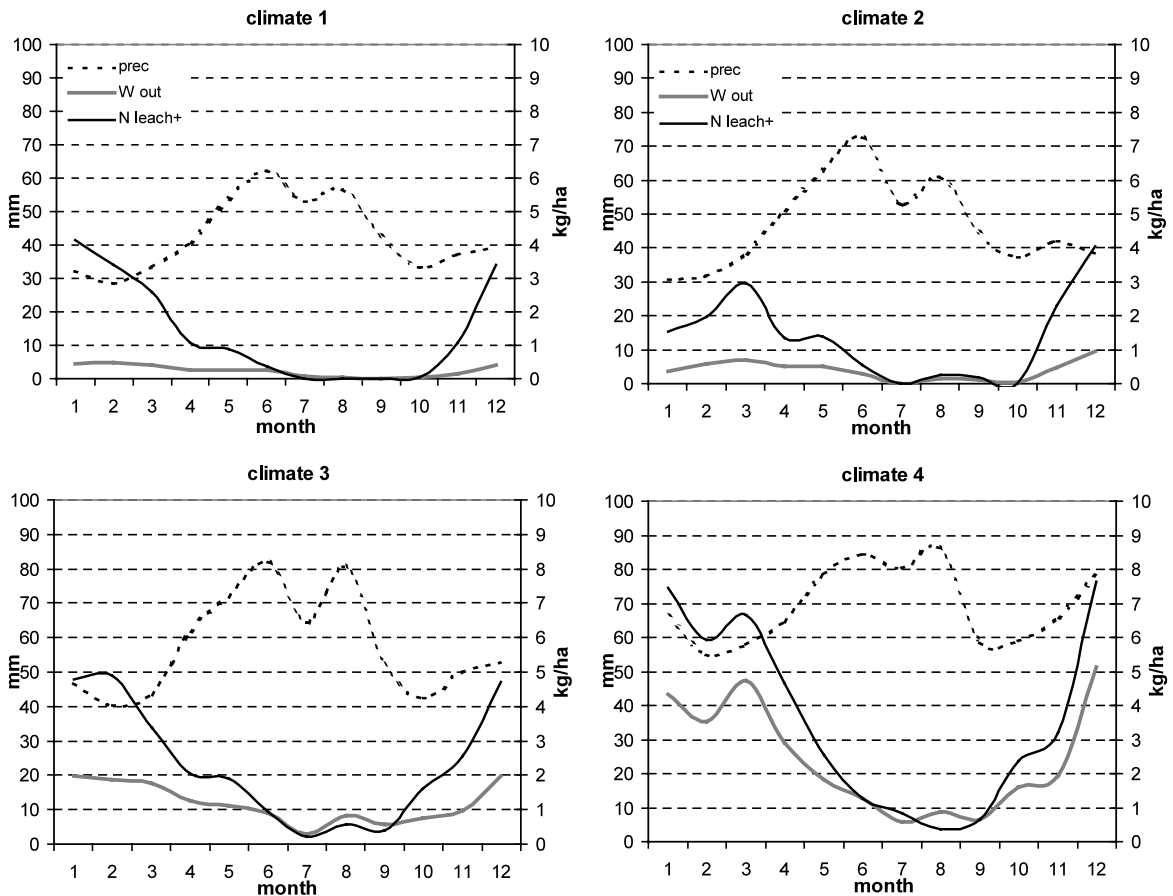


Fig. 6. Seasonal dynamics of precipitation (prec), water flows (W out: the sum of direct runoff, interflow and percolation to groundwater) and N losses with water (N leach+) for soil class 6 in climate zones 1–4.

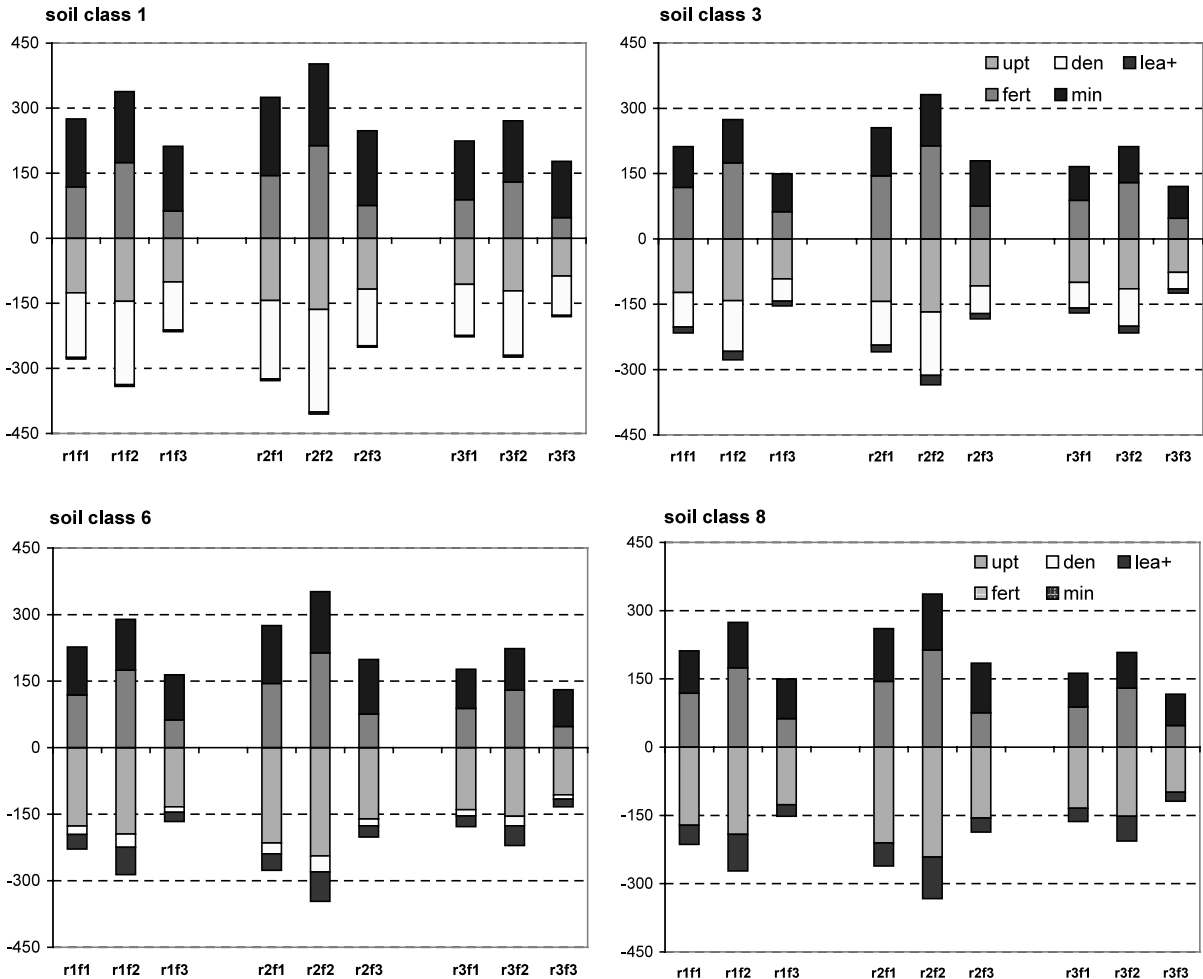


Fig. 7. Effect of rotation and fertilisation schemes (r1f1, ..., r3f3) on simulated long-term average annual N fluxes: N mineralisation (min.), N uptake by plants (upt), gaseous losses (den) and N losses with water (lea+) (in kg ha⁻¹ year⁻¹).

tion and N uptake for the basic rotation and fertilisation schemes are mapped for the Saale River basin on 1 × 1 km raster grid (Fig. 8). The same differences between soil types as shown in Figs. 4 and 7 and the climate gradient are visible. Average annual N leaching ranges from 1 to 15 kg ha⁻¹ in less permeable loess soils (classes 1–5) in climate zones 1–3 to 50–72 kg ha⁻¹ in more sandy soils (classes 7–9) in climate zones 4 and 5. In contrast, the highest denitrification (up to 160 kg ha⁻¹ year⁻¹) occurs on the floodplain close to river courses (soil class 1, which has the lowest leaching). The high denitrification is associated

with the high field capacity and low saturated hydraulic conductivity, which leads to the oxygen deficit. Nitrogen uptake is highest for the soil classes 2, 5 and 7 (all of the Tschernosem-type) in climate zones 1–3 and mineralisation is the highest for soil class 1 (floodplain soil with high organic matter content). Despite of a high mineralisation, this soil has the largest denitrification losses, but not the highest productivity.

4.6. Validation

An indirect validation of N balance for the

Saale River basin was performed using regional data on nitrogen fluxes collected from literature (DVWK, 1985; Scheffer and Schachtschabel,

1984; Blume, 1992). Table 2 contains regionally specific ranges for the validation of the simulated N balance.

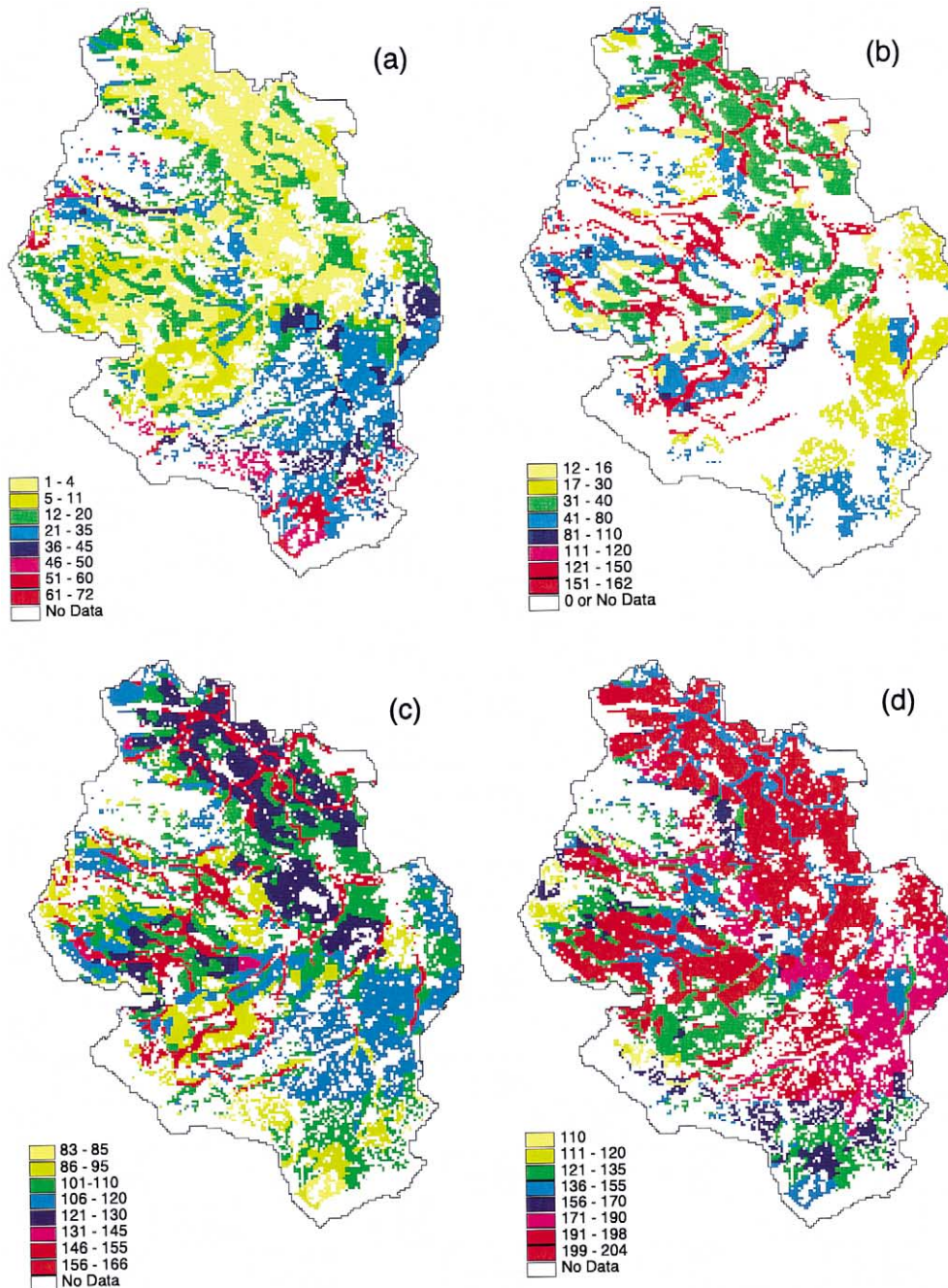


Fig. 8. Spatial distribution of the simulated long-term average annual N leaching (a), N denitrification (b), N mineralisation (c) and N plant uptake (d) (in $\text{kg ha}^{-1} \text{ year}^{-1}$) in the Saale River basin for the basic rotation and fertilisation schemes.

Table 2

Regionally specific ranges for nitrogen flows in arable land in northern Germany

Flow of nitrogen	Conditions	Range (kg ha ⁻¹ year ⁻¹)	Reference, year; page
Mineralisation	Arable land in general	40–180	DVWK, 1985; 37
	Sand with 0.13% of N content	120	DVWK, 1985; 37
	Parabraunerde (loess) with 0.1% N	90	DVWK, 1985; 37
	Braunerde (loess) with 0.155% N	136	DVWK, 1985; 37
	Schwarzerde with 0.25% N	220	DVWK, 1985; 37
	Kalkmarsch with 0.4% N	352	DVWK, 1985; 37
Denitrification	Arable land in general	20–60	DVWK, 1985; 50
	Arable land, maximum	About 100	DVWK, 1985; 50
Plant uptake	In general	50–150	Blume, 1992; 83
	Grains, maize	100–200	DVWK, 1985; 50
	Grass, sugar beet	200–250	DVWK, 1985; 50
N losses with water	Arable land, average fertilisation	0–100, depending on crop, soil and fertilisation	DVWK, 1985; 119
	Arable land in general	2.1–79.6	Ryding and Rast, 1989
	Sandy soils	27–113 (mean = 55)	Scheffer and Schachtschabel, 1984; 232
	Clay-rich soils	9–66 (mean = 24)	Scheffer and Schachtschabel, 1984; 232

Nitrogen mineralisation varies from 83 to 166 kg ha⁻¹ year⁻¹ for the basic rotation and fertilisation schemes in our simulation experiments (Fig. 8), which corresponds to the range from 40 to 180 kg ha⁻¹ year⁻¹ in Table 2. It is higher for soil classes 1 and 2 with higher organic matter content. Denitrification is in the range from 0 to 84 kg ha⁻¹ year⁻¹ for soil classes 2–9 and it is higher than 100 kg ha⁻¹ year⁻¹ (up to 162 kg ha⁻¹ year⁻¹) only for soil class 1 in our study. Rather high denitrification in soil class 1 is caused by high fertilisation rates (including organic fertiliser), which were applied in our simulation experiments for all soil classes irrespectively of their organic matter content. Nitrogen uptake varies between 110 and 204 kg ha⁻¹ year⁻¹ and is the highest for soil classes 2, 5 and 7 in climate zones 1–3. The range is comparable to that indicated in Table 2. Nitrogen losses with water are in the range from 1 to 72 kg ha⁻¹ year⁻¹, which is in a good correspondence with the range 2.1–79.6 kg ha⁻¹ year⁻¹

for arable land in general and the range 9–66 kg ha⁻¹ year⁻¹ for clay-rich soils in Table 2. In general, the modelling results including those presented in Figs. 4–8 are comparable to the ranges indicated in Table 2 and the differences between climate zones and soils are plausible.

In addition, the results of a regression analysis between the long-term average N leaching and N denitrification for nine soil classes, on one hand, and average saturated hydraulic conductivity for these soils, on the other, are shown in Fig. 9. The non-linear regression analysis was based on the equation

$$y = ax^b$$

The coefficients of determination are $R^2 = 0.57$ for the N leaching case and $R^2 = 0.41$ for the N denitrification case. The coefficients of determination are not high. In our view, this is quite understandable and confirms the fact that nitrogen dynamics in soil results from the interrelation of many non-linear processes, which cannot be

substituted by simple linear regression-type models. However, the non-linear trend in the case of N losses with water is similar to that in Hoffmann and Johnsson (1999), where the dependence between N leaching and clay content in soil was investigated.

4.7. Final assessment of factors influencing N leaching

Finally, the assessment of sensitivity of the modelled potential N leaching to groundwater to variations in natural and anthropogenic conditions was done using the full set of simulated long-term average values. The average N leaching for the specific case was related to the global average N leaching over all variants. The variation between different soil classes is the highest among all influencing factors (Fig. 10) and shows more than one order of magnitude difference between classes 1 and 9. Secondly, climate conditions and fertilisation schemes produce the next largest variations ($\pm 65\%$). The sensitivity to crop rotations is the smallest ($\pm 20\text{--}25\%$). Consequently, the relative importance of natural and anthropogenic factors affecting N leaching in the Saale River basin is the following: (1) soil, (2) climate, (3) fertilisation rate and (4) crop rotation.

5. Conclusions

The analysis of factors influencing N fluxes in soils leads to the following conclusions. Total N losses with water fluxes are practically independent of elevation, however, the elevation affects redistribution of fluxes: N losses in interflow increase at higher elevation and leaching to groundwater decreases. N losses with water increase with increasing precipitation from climate zone 1 to climate zone 5 for all soils. For denitrification this trend is much less distinct. In most cases, denitrification occurs simultaneously with N leaching, following water saturation in wet periods, excluding the soil classes with zero denitrification. Less permeable soil classes 1–4 have low N leaching, which increases only slightly under wetter conditions and they have rather high gaseous losses. In contrast, leaching to groundwater is much higher and denitrification is zero in soil classes 7–9. Soil classes 5 and 6 are intermediate in this respect: both denitrification and N leaching occur in these soils. The effect of changing fertilisation rates is the following: both N leaching and N uptake are higher/lower, when fertilisation rates are higher/lower, but the effect is rather non-linear.

In general, the modelling results including those presented in Figs. 4–8 are comparable to the regional ranges indicated in Table 2 and the dif-

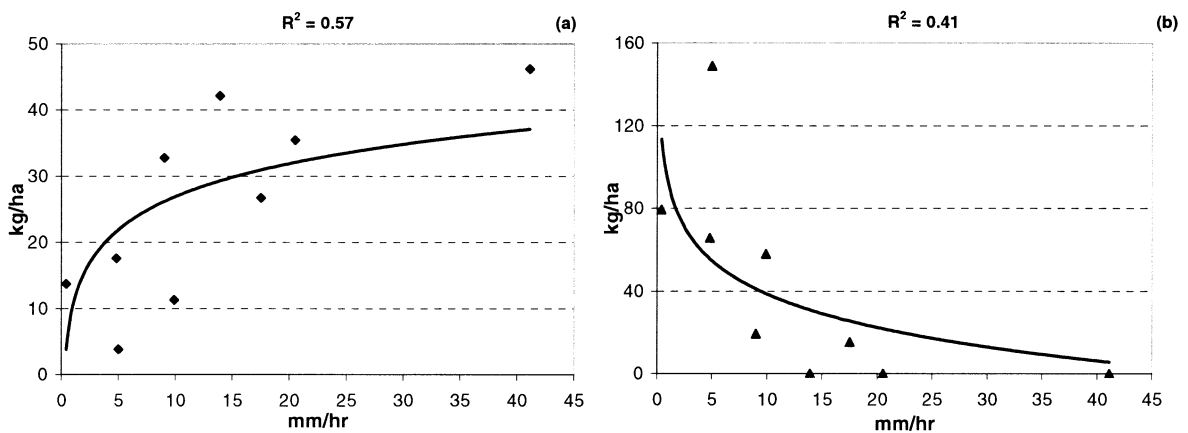


Fig. 9. Non-linear regression curves ($y = ax^b$) between the long-term average nitrogen leaching and saturated hydraulic conductivity (a) and between the long-term average nitrogen denitrification and saturated hydraulic conductivity (b), considering nine investigated soil classes.

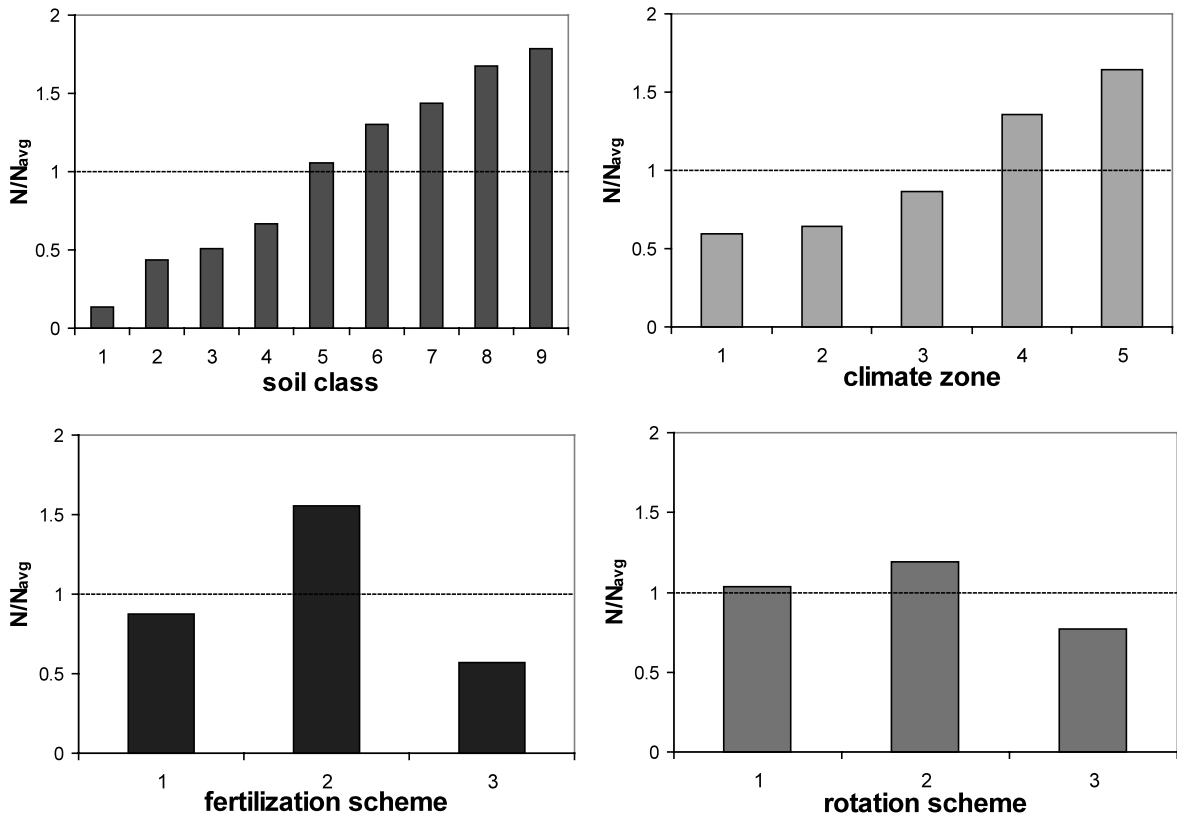


Fig. 10. Sensitivity of the simulated potential N leaching to groundwater depending on soil type, climate, fertilisation and rotation, estimated as ratios between the average N leaching for specific cases and the global average N leaching.

ferences between climate zones and soils are plausible. The relative importance of natural and anthropogenic factors affecting N leaching in the Saale River basin in the framework of studied ranges was established as follows: (1) soil, (2) climate, (3) fertilisation rate and (4) crop rotation. The simulation results provide a basis for the fuzzy-rule based metamodel approach, which is described in the second paper (Haberlandt et al., 2002). They can be also used as database for regionalisation in larger regions using other methods.

Acknowledgements

The authors are grateful to all agencies which provided data for this study; to PhD students

Fred Hattermann and Bernhard Ströbl for data preparation and to Theresia Petrow for drawing Figs. 1 and 8 in ARC/VIEW. Thanks to two anonymous reviewers for their comments.

References

- Arheimer, B., Brandt, M., 2000. Watershed modelling of non-point nitrogen pollution from arable land to the Swedish coast in 1985 and 1994. *Ecological Engineering* 14, 389–404.
- Arhonditsis, G., Tsirtsis, G., Angelidis, M.O., Karydis, M., 2000. Quantification of the effects of nonpoint nutrient sources to coastal marine eutrophication: applications to a semi-enclosed gulf in the Mediterranean Sea. *Ecological Modelling* 129, 209–227.
- Arnold, J.G., Williams, J.R., Srinivasan, R., King, K.W., Griggs, R.H., 1994. SWAT, Soil and Water Assessment Tool. USDA, Agriculture Research Service, Grassland, Soil and Water Research Laboratory, Temple, TX 76502.

- Beaujouan, V., Durand, P., Ruiz, L., 2001. Modelling the effects of the spatial distribution of agricultural practices on nitrogen fluxes in rural catchments. *Ecological Modelling* 137, 93–105.
- Blume, H.P., 1992. *Handbuch des Bodenschutzes*, 2nd ed., ECOMED publisher.
- Børgesen, C.D., Djurhuus, Kyllingsbaek, A., 2001. Estimating the effect of legislation on nitrogen leaching by upscaling field simulations. *Ecological Modelling* 136, 31–48.
- DVWK: Bodennutzung und Nitrataustrag-Literaturoberwertung über die Situation bis 1984 in der Bundesrepublik Deutschland, 1985, Deutscher Verband für Wasserwirtschaft und Kulturbau e.V., Hamburg, Berlin, Germany.
- GRASS4.1 Reference Manual, 1993. US Army Corps of Engineers. Construction Engineering Research Laboratories, Champaign, IL.
- Grimvall, A., Stålnacke, P., 1996. Statistical methods for source apportionment of riverine loads of pollutants. *Environmetrics* 7, 201–213.
- Hartwich, R., Behrens, J., Eckelmann, W., Haase, G., Richter, A., Roeschmann, G., Schmidt, R., 1995. *Bodenübersichtskarte der Bundesrepublik Deutschland 1:1000000*, Hannover, Germany.
- Haberlandt, U., Krysanova, V., Bardossy, A., 2002. Assessment of nitrogen leaching from arable land in large river basins. Part II. Regionalisation using fuzzy rule based modelling. *Ecological Modelling* 150 (3), 277–294.
- Hansen, S., Jensen, H.E., Nielsen, N.E., Svendsen, H., 1991. Simulating of nitrogen dynamics and biomass production in winter wheat using the Danish simulation model DAISY. *Fertilizer Research* 27, 245–259.
- van Herpe, Y., Troch, P.A., Callewier, L., Quinn, P.E., 1998. Application of a conceptual catchment scale nitrate transport model on two rural river basins. *Environmental Pollution* 102 (S1), 569–577.
- Hoffmann, M., Johnsson, H., 1999. A method for assessing generalised nitrogen leaching estimates for agricultural land. *Environmental Modelling and Assessment* 4, 35–44.
- Johnsson, H., Bergström, L., Jansson, P.E., Paustian, K., 1987. *Agricultural Ecosystems and Environment* 18, 333–356.
- Krönert, R., Franko, U., Haferkorn, U., Hülsbergen, K.-J., Abraham, J., Biermann, S., Hirt, U., Mellenthin, U., Ramsbeck-Ullmann, M., Steinhardt, U., 1999. *Gebiets-wasserhaushalt und Stoffhaushalt in der Lößregion des Elbegebietes als Grundlage für die Durchsetzung einer nachhaltigen Landnutzung*, UFZ Leipzig-Halle GmbH, Leipzig, Germany.
- Krysanova, V., Becker, A., 1999. Integrated modelling of hydrological processes and nutrient dynamics at the river basins scale. *Hydrobiologia* 410, 131–138.
- Krysanova, V., Müller-Wohlfeil, D.I., Becker, A., 1998. Development and test of a spatially distributed hydrological/water quality model for mesoscale watersheds. *Ecological Modelling* 106, 261–289.
- Krysanova, V., Gerten, D., Klöcking, B., Becker, A., 1999. Factors affecting nitrogen export from diffuse sources: a modelling study in the Elbe basin. In: Heathwaite, L. (Ed.), *Impact of Land-Use Change on Nutrient Loads from Diffuse Sources*, IAHS Publ. No. 257, pp. 201–212.
- Krysanova, V., Wechsung, F., Arnold, J., Srinivasan, R., Williams, J., 2000. SWIM, Soil and Water Integrated Model. User Manual. PIK, Potsdam, 239 p.
- Monteith, J.L., 1977. Climate and the efficiency of crop production in Britain. *Philosophical Transactions of the Royal Society of London Series B* 281, 277–329.
- Nash, J.E., Sutcliffe, J.V., 1979. River flow forecasting through conceptual models, 1. A discussion of principles. *Journal of Hydrology* 10, 282–290.
- Scheffer, F., Schachtschabel, P., 1984. *Lehrbuch der Bodenkunde*, 11th ed., Enke, Stuttgart, Germany.
- Seligman, N.G., van Keulen, H., 1991. PAPERAN A simulation model of annual pasture production limited by rainfall and nitrogen. In: Frissel, M.J., van Veen, J.A. (Eds.), *Simulation of Nitrogen Behaviour of Soil–Plant Systems*, Proc. Workshop, Wageningen, January–February 1980, pp. 192–221.
- Refsgaard, J.C., 1997. Parametrisation, calibration and validation of distributed hydrological models. *Journal of Hydrology* 198, 69–97.
- Roth, D., Knoblauch, S., Pflieger, I., Herold, L., 1998. *Nitratgehalte im Sickerwasser und N-Austrag aus unterschiedlichen Agrarstandorten Thüringens*, Thüringer Landesamt für Landwirtschaft, Jena, Germany.
- Ryding, S.O., Rast, W. (Eds.), 1989. *The control of eutrophication of lakes and reservoirs*, Man and the Biosphere Series, vol. 1, Paris.
- Wegehenkel, M., 2000. Test of a modelling system for simulating water balances and plant growth using different complex approaches. *Ecological Modelling* 129, 39–64.
- Williams, J.R., Renard, K.G., Dyke, P.T., 1984. EPIC—a new model for assessing erosion's effect on soil productivity. *Journal of Soil and Water Conservation* 38 (5), 381–383.
- de Wit, M., 1999. *Nutrient fluxes in the Rhine and Elbe basins*, Universitat Utrecht.