Plant and Soil **181**: 109–121, 1996.

Modeling of nitrogen transformations and translocations

Jörg Richter and Dinesh Kumar Benbi
*Institute of Geography and Geoecology, Technische Universität Carolo-Wilhelmina, Braunschweig, Germany**

Key words: microbial immobilization, net N-mineralization, nitrate leaching, plant N-uptake, simulation

Abstract

Different submodels within complex model packages on N regimes - for plant N-uptake, net N-mineralization, nitrate leaching and microbial N immobilization - are critically reviewed mainly with regard to their prediction ability on the basis of three comparative papers. Only for some of the processes adequate statistical evaluation of the models was possible. Compared to the other statistically evaluable process, nitrate leaching, modeling of plant N-uptake yields the better results. Most models for mineralization use arbitrary approaches rather than empirical ones. Although only approximate estimates of N mineralisation were at hand, the models generally behave expectedly poor. Only one model - DAISY - out of 16 involved in the comparison uses an explicit microbial biomass sub-model including microbial growth, decline and maintenance terms. So DAISY is the only model coupling C and N cycles. But what is true for an individual model describing the C and N transformation of a lab incubation experiment seems to be valid for most of the complex simulation work on the C and N regimes: this model was said to be overparameterized with respect to the available data.

Introduction

Thirty years ago, in Europe we used about one fourth of the mineral nitrogen fertilizer amounts of today. Since yields only doubled in this period we have surplus nitrogen problems in intensive farming leading to high amounts of vagabonding nitrogen in the plants, the atmosphere and the water bodies. Now, science is asked to solve the problems caused by misinterpretation of the role of nitrogen by its practioners.

Process simulation is believed to be a comprehensive and integrative tool not only for understanding but also for managing problems with nitrogen in the environment. To use process simulation effectively for research as well as for advisory purposes of nitrogen regimes, we should have a basic and quantitative understanding of all the essential processes involved in the respective situation. For the temperate climate of central Europe, our deterministic N-regime models for arable crops now usually comprise nitrogen uptake by plants, the processes of ammonification and nitrification of organic nitrogen, nitrate leaching and denitrification. For ammonification-nitrification, there is now a great body of basic knowledge from incubation experiments, which should be used in simulations of field situations. For root uptake, even approaches using simple root distribution patterns usually perform satisfactorily, although they can not simulate translocations within the plants or disappearance of surplus ammonia by evaporative processes. Also leaching is a process which may be simulated simply and quite correctly even in rather heterogeneous fields. Denitrification is thought to be of minor importance in well drained arable field soils in temperate climate.

To reach a generally higher degree of agreement between simulation and measurement, future development in modeling seems to concern essentially processes like denitrification, microbial immobilization, ammonia volatilization and ammonium exchange and fixation-defixation. A comprehensive picture of the nitrogen cycle in the soil is given in Figure 1. With regard to denitrification, we may be in a phase where it may still be worthwhile to compare different simulation approaches on the basis of their relative ability to represent experimental losses. Only recently we ourselves incorporated the description of ammonium exchange and fixation-defixation into our approaches. The majority of NH_4^+ ions may be withdrawn from soil solution by ion exchange if nitrification is slow.

* FAX No: + 495313918170

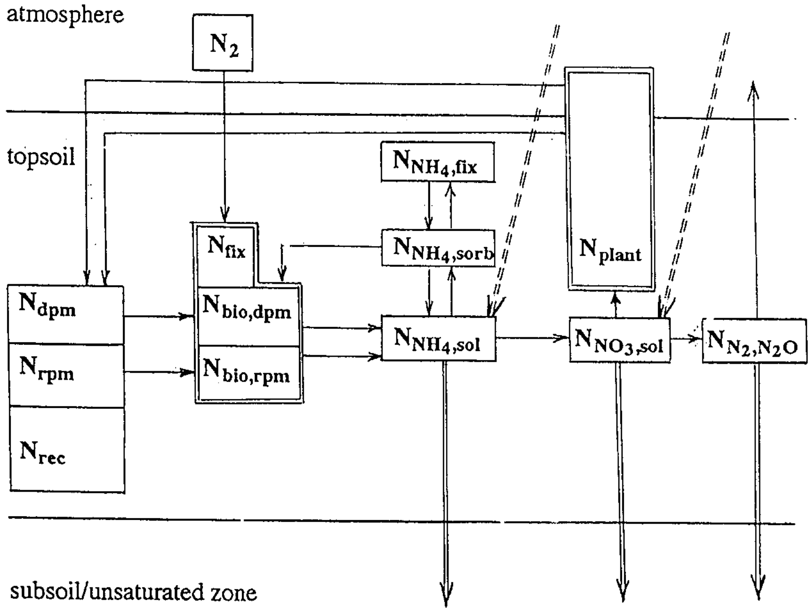

Figure 1. A presentation of the nitrogen cycle.

This ammonium may also be fixed within relatively short periods (days) and defixate within decades, when the ammonium concentration in the solution decreases again. Moreover, the microbial immobilization submodel may fill a gap, but till now we have only limited quantitative knowledge of the real processes. This is especially so because we are unable to treat the process separately from other processes, as we apparently can do for net N mineralization. Applying our model approach to understand nitrogen regimes in arid calcareous loess soils in China, ammonia loss has to be included in the model with special regard to the forms in which most nitrogen comes into the field, namely as urea and ammonium bicarbonate.

In this paper we will not demonstrate our newest approaches mentioned in the last paragraph since there is only limited experimental proof for them. Instead we would like to stick to the more easily described processes on which comprehensive work has already been done. Especially, we would like to confront some concepts with their use in related approaches of some well known model simulation packages. In two recent reports these different simulation packages have extensively been compared regarding their ability to describe N-regimes in part as well as in toto. - The reports are:

1. European Communities - Commission EUR 13501, 1991 - hereafter referred as report 1.
2. Groot J J R, de Willigen P and Verberne E L J, 1991 - hereafter referred as report 2.

Materials and methods

In report 1, Vereecken et al. (1991), selected 5 out of 9 complex models used to compare simulation results with measured or estimated output components of the water and nitrogen regimes: N-mineralization, denitrification, nitrate leaching, and crop N-uptake at harvest. Measurements or estimates were based on data sets for two to five years of three differently cropped sandy soils, two from Denmark and one from the Netherlands. Five statistical criteria were used to evaluate simulations (Table 1). The coefficient of determination-equivalent was regarded as an expression of the scattering of the simulated values relative to the scattering of the measurements. Negative modeling efficiencies indicate that the mean of the measured values is a better estimate than the mean of the simulated values. Correspondingly, positive coefficients of residual mass indicate a tendency of the simulations to underestimate the measured values, and vice versa. No comparison has been done based on measured time series of nitrate-N profiles. The models were originally created for different purposes but will not be characterized here besides their abilities evaluated below. The 5 models in the review of Vereecken et al. (1991), are ANIMO, DAISY, EPIC, RENLEM and SWATNIT.

Table 1. (=Table 1 of Vereecken et al.) Statistical criteria for evaluation of the simulated results according to Loague et al. (1991)

Criterion	Symbol	Calculation formula[a]	Range	Optimum
Maximum error	ME	Max $\lvert P_i - O_i \rvert_{i=1}^{n}$	≥ 0	0
Root mean square error	RMSE	$(\sum_{i=1}^{n}(P_i - O_i)2/n)^{1/2} \cdot 100/\bar{O}$	≥ 0	0
Coefficient of determination	CD	$\sum_{i=1}^{n}(O_i - \bar{O})^2 / \sum_{i=1}^{n}(P_i - \bar{O})^2$	≥ 0	1
Modelling efficiency	EF	$(\sum_{i=1}^{n}(O_i - \bar{O})^2 - \sum_{i=1}^{n}(P_i - O_i)^2)/(\sum_{i=1}^{n}(O_i - \bar{O})^2)$	≤ 1	1
Coefficient of residual mass	CRM	$\sum_{i=1}^{n} O_i - \sum_{i=1}^{n} P_i)/(\sum_{i=1}^{n} O_i)$	≤ 1	0

[a] P_i = predicted value i, O_i = observed value i, $\bar{O}$ = mean of the observed values, n = number of data pairs,

In report 2, de Willigen (1991) compared 14 models with regard to the submodels involved and their descriptions of the different processes. The results of simulations based on data sets from the Netherlands given to all the modellers were also included. In addition to other models, ANIMO, DAISY and SWATNIT also participated in this comparison. In the same report, Otter-Nacke and Kuhlmann (1991) compared three out of the same 14 models with respect to their ability to predict N_{min}-contents in early spring under farmers field conditions. The models were run between harvest and spring of the following year for two different winter periods for at least 70 farmers field plots. The model performance was evaluated according to the number of cases in which prediction was within $\pm$ 20 kg N_{min} ha^{-1} of the measured profile contents. This is the observed average difference between two measurements repeated on the same field plot for the relatively homogeneous loess field soils if sampling is done with great care (Richter et al., 1984). Neither ANIMO, DAISY nor SWATNIT were included in the latter comparison.

Results and discussion

Beginning with the paper of Otter-Nacke and Kuhlmann (1991), results may simply be presented by showing i) the worst case of the first year, where no initial conditions were at hand, and ii) the results of the second year using measured data on N_{min} in soil after harvest of the preceding crop as initial condition (Fig. 2). There was an agreement of around 66% for the first and around 75% cases for the second year. The latter improvement is essentially due to the fact, that initial values were at hand for this year. Detailed information on the results are contained in Table 2. According to the authors, the Mean Bias Error (MBE) indicates if the model gives well balanced results. Only model B yielded well balanced simulations, while model C overestimated measured values by 6 to 7 kg N ha^{-1} for both years. If such an increase in agreement of roughly 10% for the relatively simple winter models marks an essential progress - can we expect a similar progress by extending the simulation period to the whole season, with the much more complex situations and processes? It should be clearly stated that these authors proved the suitability of models for advisory purposes.

On the basis of the other review papers of the two reports, a more detailed picture on the modeling approaches and a rough evaluation of the abilities to predict the different processes such as **nitrogen uptake by plants, net-N mineralization, nitrate leaching** and **microbial immobilisation** may be given. Time series of N_{min} profiles and sums could also help to qualify an approach. However, as in the paper of Otter-Nacke and Kuhlmann (1991) where no measured N_{min} time series were at hand, both review papers (de Willigen, 1991; Vereecken et al., 1991) use time series only scarcely. The following evaluation will essentially follow these original reviews.

N plant uptake: the soil process modelers can do best

According to Vereecken et al. (1991), the modeling efficiency (Fig. 3 and Table 3) for plant N-uptake is high in comparison to nitrate leaching, and is small only for the Jyndevad site with the poor sand. Considering the substantial variation of measured N uptake the performance of the relevant submodels seems to be good. One would expect that even relatively small variation in simulated N-uptake may have relatively large effects on the simulation quality of the other processes, e.g. leaching. However, for the Jyndevad site the modeling efficiency for nitrate leaching is highest.

Also de Willigen (1991) concluded, that above ground variables had been simulated more accurately than below ground ones. Some of the compared models calculated dry matter production and N-uptake in an independent way, i.e. without parameter fitting.

Table 2. Statistical parameters for the comparison of the N_{min}-profile content in spring of three selected models in Otter-Nacke and Kuhlmann (1991)

Year	Model	n	Differences <10(kg(N)ha^{-1})		>20(kg(N)ha^{-1}		ME[a]	MBE	MAE
			no.	(%)	no.	(%)			
1988	A	114	50	43.9	39	34.2	76	-11.03	18.0
	B	126	50	39.7	37	29.4	95	-1.60	17.0
	C	84	25	29.8	32	38.1	65	0.02[b]	18.9
1989	A	68	19	27.9	21	30.9	71	-1.17	19.2
	B	69	32	47.1	12	17.6	68	1.37	14.3
	C	53	29	54.7	17	32.1	47	6.25	13.7

[a]ME – Maximal Error, MBE – Mean Bias Error, MAE – Mean Absolute Error.
[b]Probably misprinted in Otter–Naoke and Kuhlmann (1991); should read 6.02.

Table 3. (= Table 6 of Vereecken et al., 1991) Statistical criteria for the performance of the different models on simulation of crop N-uptake (kg N ha^{-1} a^{-1}) for the different sites

Site	Model	n[a]	ME[b]	RMSE[c]	CD[d]	EF[e]	CRM[p]
Askov	ANIMO	6	31.6	25.9	0.60	0.70	0.10
	DAISY	5	23.2	16.5	0.66	0.89	-0.10
	EPIC	6	38.0	21.3	0.64	0.65	0.08
	SWATNIT	6	24.7	21.1	0.54	0.77	-0.09
Jyndevad	ANIMO	12	43.5	27.5	0.54	0.30	0.03
	DAISY	12	47.3	27.8	0.48	0.30	-0.17
	EPIC	12	106.0	33.8	0.28	-0.45	-0.10
	SWATNIT	12	56.3	32.1	0.39	0.04	-0.10
Ruurlo	ANIMO	25	172.2	16.5	1.31	0.86	0.04
	DAISY	12	60.0	11.4	0.91	0.97	-0.06
	EPIC	25	191.0	19.7	0.82	0.80	0.01
	SWATNIT	20	120.9	14.1	1.36	0.90	-0.05
All[g]	ANIMO	44	172.2	19.4	1.17	0.94	0.04
	DAISY	29	60.0	15.2	0.92	0.97	-0.08
	EPIC	44	191.0	22.9	0.92	0.90	0.00
	SWATNIT	39	120.9	17.0	1.06	0.95	-0.05

[a]n: number of observations.
[b]ME: maximum error.
[c]RMSE: root mean squared error.
[d]CD: coefficient of determination.
[e]EF: modeling efficiency.
[p]CRM: coefficient of residual mass.
[g] Including Pittem, Belgium.

The problem with fertilizer recommendations of today is, however, much more related to below ground processes like leaching.

Net N mineralization: "arbitrary" vs. empirical modeling

Table 4 (adopted from Vereecken et al., 1991) contains a description of the different organic matter pools used

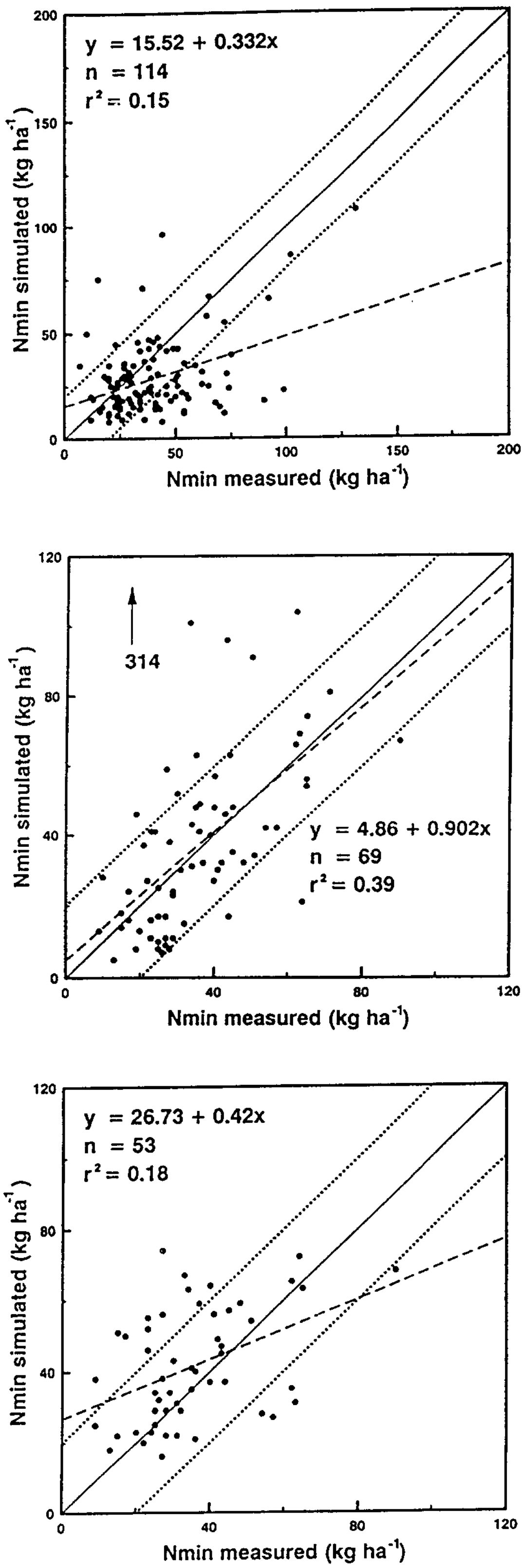

Figure 2. The worst case (model A) of the first year, where no initial conditions were at hand (top), compared with results of the second year using data after harvest of the preceding crop as initial condition (model B and C), after Otter-Nacke and Kuhlmann (1991).

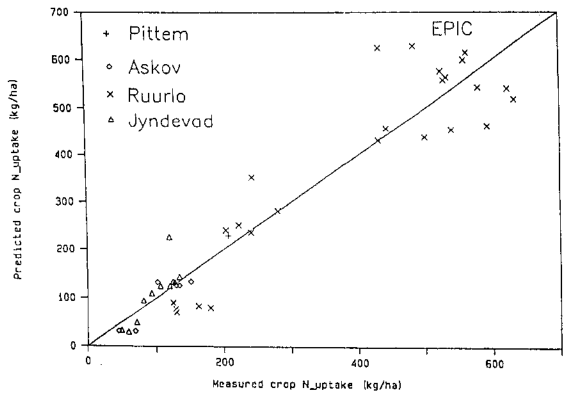

Figure 3. Comparison of measured with simulated N uptake by crops with EPIC.

in the different models of report 1 with respect to C/N ratio,% of organic C and half-life times of the usually first order mineralization of the organic material. RENLEM is not mentioned in Table 4, since RENLEM cannot treat short term mineralization. In this model the mineralization of newly added organic matter is assumed to be complete within one year and no change in the organic N content of the soil occurs. The pools of the different models vary greatly by number, N- and C- content and half-life times. Therefore, it is not amazing that the simulated mineralization figures in Table 5 are so different. The question arises what may be the reasons for the chosen pool numbers, sizes and time behaviour and how the submodels have been parameterized by the authors or users.

Although perhaps decisive for the judgement of simulation quality it was not possible to obtain the answers from the report. This is quit clear with regard to the summarizing report of Vereecken et al. (1991). But also from the more detailed model descriptions in the individual reports only very little can be drawn. Given pool names and attributed half-life times are presented almost always without reference to the scientific basis. For ANIMO it is merely stated that "a historical run of the program is performed" prior to any actual simulation in order to get a realistic initial condition. EPIC uses a modification of the mineralization model of Seligman et al. (1981) originally developed for pastures. Although this paper appeared before all publications suggesting two N-pools and reviving the incubation technique of Stanford and Smith (1972), the model already uses a two pool approach. Even the kinetic parameters used are very close to the estimates we ourselves regard as reliable. Inter alia, ANIMO seems to be the four compartment model instead of

Table 4. (= Table 3 of Vereecken et al., 1991) Characteristics of the different organic matter pools distinguished in the four dynamic models for the Jyndevad site, Danmark

Model	Pool	C/N ratio	% of organic C[a]	Half life time
SWATNIT	Litter	8	8-1	693 d
	Manure	10	±1	693 d
	Humus	12	92-99	189 y
EPIC	Stable humus	-[b]	-	-
	Fresh organic N	-	-	23 d
	Active organic N	-	-	2500 d
DAISY	Biomass pool 1	6	0.28	693 d
	Biomass pool 2	10	0.04	49.5 d
	Soil organic pool 1	11	±80	515 y
	Soil organic pool 2	11	±20	10 y
AMINO	Humus	16	99.2	50 y
	Fraction 2	12	<0.5	77 d
	Fraction 3	58	<0.5	3 y
	Fraction 4	76	0.5	130 d
	Fraction 5	76	<0.5	37 d
	Fraction 6	24	<0.5	65 d
	Fraction 7	24	<0.5	590 d

[a]Figures are approximative.
[b]No information given.

Table 5. Comparison of the estimated with the simulated net N-mineralization (in kg N ha^{-1} a^{-1}) for four models and three sites in the comparison of Vereecken et al. (1991)

	Askov	Jyndevad	Ruurlo
Experimental estimates	75-49	82-97	85-126
EPIC	24-45	24-45	72-92
SWATNIT	77-78	102-103	110-230
ANIMO	40-60	60-90	200
DAISY	40-60	60-90	105

DAISY. For DAISY's subpool of soil organic matter it is stated qualitatively that the rate coefficients depend on the clay content of the soil. For SWATNIT the choice of the three compartments - a fast cycling soil litter pool, a slow cycling soil humus pool and a manure pool - is based on the referenced paper of Johnsson et al. (1987) which by the way may answer the above questions.

Although only approximative estimates for net N-mineralization are at hand (Table 5) the comparison with the simulated figures tells how well the different models reflect the figures of the different field experiments. Only SWATNIT seems to be able to predict the level of expected amounts, though only for the Danish experiments. For the Dutch experiments over 5 years, some of the SWATNIT simulations greatly overestimate net mineralization. This inability was judged by Vereecken et al. (1991) with the statement that "the organic N system in the SWATNIT simulation is clearly not yet in equilibrium." However, according to our own experience, the estimated figures for the Ruurlo plots after five years of continuous grazing and changing back to arable cropping with high mineral fertilizer N inputs, seem to be too small. EPIC strongly underestimated net mineralization in all experiments, while this error is less pronounced for ANIMO and DAISY.

Table 6. (= Table 2 of de Willigen, 1991) Soil biological processes considered in different models

Model	(a1)[a]	(a2)[b]	(a3)[c]	(b)[d]	(c)[e]
[A]	1	1	-	+	-
[B]	1	0	-	+	+
[C]	2	1	-	+	+
[D]	4	1	+	+	+
[E]	6	1	+	+	+
[F]	1	1	-	+	-
[G]	2	1	-	+	+
[H]	7	1	+	+	+
[I]	2	1	+	-	-
[J]	2	1	-	-	-
[K]	4	1	+	-	-
[L]	1	0	-	-	-
[M]	1	0	-	-	-
[N]	2	1	-	+	+

[a](a1): Number of pools in mineralization/immobilization reacion.
[b](a2): Order of the rate equations.
[c](a3): +One or more pools of biomass; - no biomass.
[d](b): +Nitrification considered.
[e](c): +Dentrification considered.

For the Dutch experiment, only DAISY predicted the estimated mineralization by a relatively constant value. Which parameterization renders such a success of a 7 pool mineralization model?

Also the models compared in report 2 used quite different pool numbers for mineralization (Table 6): only 5 out of 14 use two compartments, 5 only one compartment and the residual 4 use between 4 and 7 pools: Model [D] is ANIMO, here with only four mineralizable N pools, model [H] is DAISY with 7 pools. Within the five models using two compartments there is SWATNIT (model [G]), which in the comparison of Vereecken et al. (1991) was said to use three compartments. Infact, the kinetic coefficients of two pools are identical (Table 4), so it is justified to speak of only two pools. Two of the other models use the submodel of Bergström the pools of which are characterized as litter and faeces. The remaining two models also use similar pool designs, namely crop residues and soil organic matter. However, for one of them the same reference as SWATNIT, Johnsson et al. (1987) is cited.

The obviously arbitrary choice of number, size and kinetic coefficients of organic pools - for nitrogen at least - is puzzling all the more because for the description of net mineralization safe progress has been made during the last decade by an empirical approach. Since the often cited trial of van Veen (1977) to evaluate the extent and decomposability of the N-pools according to their chemical composition, the renewed interest in Stanford and Smith's (1972) incubation technique brought a real step forward in the evaluation of pool numbers, sizes and kinetics. Initially, there were two independent papers asserting that in incubation experiments with field moist soils mineralization is best described by superposing two first order decomposition curves whose coefficients differ roughly by one order of magnitude (Molina et al., 1980; Nuske and Richter, 1981). Now it seems to be well justified to describe N mineralization by superposing the decay of two fractions or pools often referred to as decomposable (dpm) and resistant plant material (rpm; for a review see e.g., Benbi and Richter, 1994). The kinetic description used is the first order degeneration for small substrate concentrations of the more general Michaelis-Menten approach. The kinetic coefficient is essentially dependent on temperature, moisture and pH. Typical half-life times at 10 °C average soil temperature are around 0.35 years ($\approx$ 130 days) for the fast decomposing dpm and about 4.5 years ($\approx$ 1650 days) for the slow rpm pool. Pool sizes of the dpm fraction are, depending on the type of crop, between 1/2 to 2/3 of the N of the plant residues left on the field after harvest. The size of the rpm N-pool depends primarily on organic matter and clay content of the soil. It ranges from 500 to 800 kg N ha^{-1} $topsoil^{-1}$ for luvisols (Nordmeyer and Richter, 1985; Richter et al., 1994). The pool itself is replenished essentially by the other 1/3 to 1/2 of residual N in crop residues which is not dpm N and may vary also according to management conditions. Only very little - around 1% of the organic residues - is directed via this pool to more recalcitrant pools, the decomposition of which is extremely slow and which are, therefore, neglected in simulation. The two-pool-estimates have been derived independently from incubation experiments and show little resemblance to the pool numbers, sizes and kinetic coefficients in Table 3. A similar approach exists for organic carbon (Jenkinson and Rayner, 1977).

Nitrate leaching: "mechanistic" vs. "phenomenological" modeling of the water movement

Nitrate leaching essentially seems to "balance" the surplus N fertilization in humid climates. It depends primarily on drainage rates (or vice versa, on evapotranspiration), soil texture and fertilization rates and distribution. Correct simulation depends, therefore, first on the quality of estimates of evapotranspiration ET and to a much smaller extent on the quality and method of modeling the water movement. There are principally two ways of modeling water movement: the so-called "mechanistic" approach, (which is not well described by this term and binds us to the mechanistic Newton paradigma) and the capacity approach (for a review see Addiscott and Wagenet, 1985). The mechanistic approach uses the well-known Richards equation and needs a complete data set of parameters, $\psi(\theta,z)$ and $K(\theta,z)$. Since these are not at hand in normal field situations, these parameter functions have to be calculated from easy-to-obtain characteristics by co-called pedotransfer-functions. Instead, capacity models use a more rigorous approach: they avoid the use of conductivities and make only use of information on the possible limits of the water storage. - What is to be expected from these different approaches?

In the comparison of Vereecken et al. (1991), it is stated that actual ET varied greatly from one model to the other. But the reviewers felt unable to judge the quality of the ET parts of the models by the measured moisture profiles. Regarding the water movement and storage, however, the models showed, for the Danish experimental sites, systematic differences between the capacity type model (EPIC) and the "mechanistic" models (ANIMO, DAISY, SWATNIT). The mechanistic models, all using the same hydraulic model SWATRE, predicted substantial changes in water storages for the two years, whereas storage was not much changed in EPICs capacity model. Unfortunately, there were no measurements at the beginning and the end of the simulated periods to judge these results.

At the Dutch experimental site considerable capillary rise can be expected from the shallow and varying water table. EPICs capacity type model is expected (Vereecken et al., 1991) not to be able to reflect this situation, but instead it does. Perhaps the explanation for this is simply that the reviewers may have disregarded the "presence" of the groundwaters in the upper equilibrium limit - similar to field capacity - which, therefore, exerts a tendency to pull water upwards according to ET.

In report 2, 14 models are compared. In two of them a water transport model is not included but instead an external water transport calculation scheme is used. This is perhaps true for others apart from these two, because a similar explanation holds for ANIMO. Anyhow, of the remaining 12 models, 6 use mechanistic models for water transport, the other 6 rely on capacity models. According to the reviewers, the evaluation with regard to the water movement on this basis reveal a slight superiority of the capacity based models above the mechanistic approaches. As an example, the comparison of the two model performances done for the

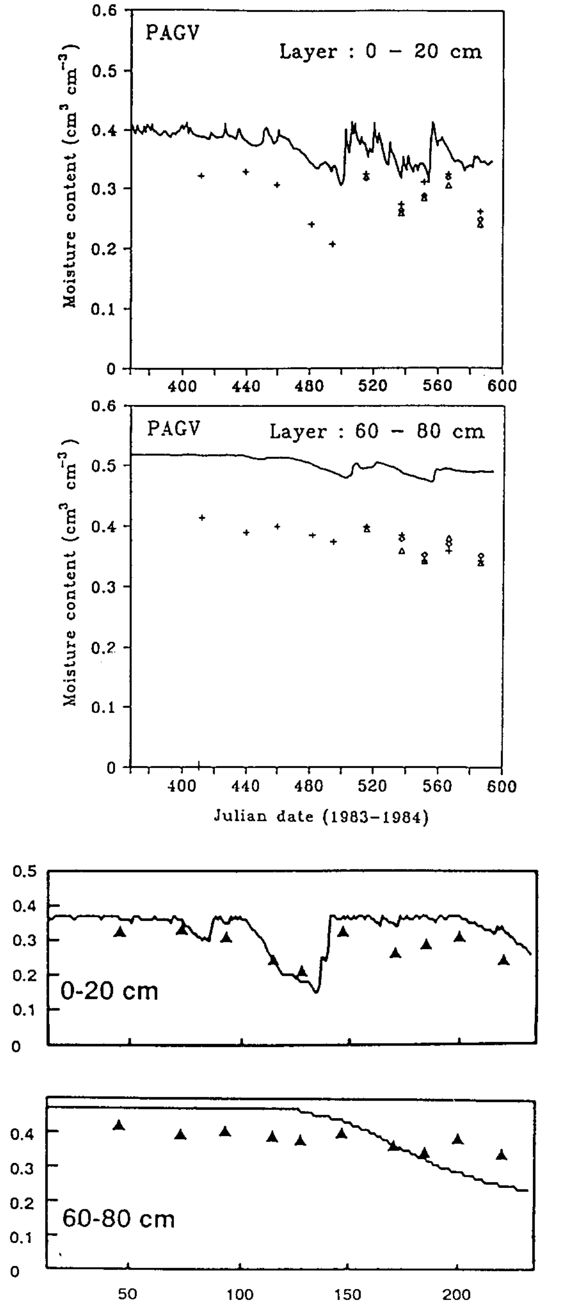

Figure 4. A comparison between measurements and simulations of soil moisture content in two layers with a "mechanistic" (model [G], above) and a capacity based submodel (model [I]) of water transport for the PAGV-site for 1984, given in Groot et al. (1990).

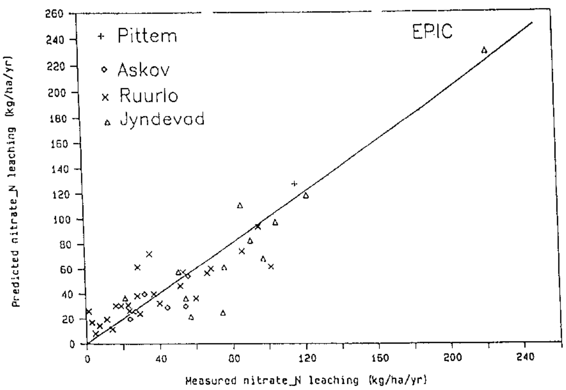

Figure 5. Annual nitrate leaching: comparison of the simulated (EPIC) with the measured field observations (Fig. 3a of Vereecken et al., 1991).

PAGV-site for two layers, 0 to 20 and 60 to 80 cm depth is shown in Figure 4.

Despite the different approaches for N-mineralization and water movement a comparison with measured nitrate leaching in report 1 reveals (Table 7), that ANIMO, DAISY and EPIC are similar in quality. DAISY seems to be a little superior in behaviour, because it explains 89% (EF) of the measured variability with a RMSE of only 27%, but it does so on a reduced sample of only 29 data sets out of 43. RENLEM showed a tendency to overestimate leaching. SWATNIT did the opposite. EPIC (Fig. 5) overestimated by about 40 kg ha^{-1}.

In report 2, evaluation of the models regarding leaching has been done on the basis of comparisons with the mineral N contents or depth profiles in a much less exhaustive way as in the first report. Reflecting the combined result of all N processes, no clear distinction can be made regarding the way of modeling N-mineralization or water movement. This may be seen as supporting the conclusions drawn by the first reviewers (Vereecken et al., 1991) that there is obviously no difference in simulation quality in the different approaches.

Following this conclusion the question may arise whether the quality of estimates by simulation of nitrate leaching has really improved in comparison e.g. to the empirical graphical estimates of Kolenbrander (1981) (Fig. 6). Or, in other words, is all the simulation work on nitrogen processes really justified, at least with regard to leaching? Although we can not give an adequate answer, the application of Kolenbrander's approach to data gathered more recently by Walther et al. (1985) shows that it is still a valuable approach. Therefore, we may doubt great progress in the field of simulation of nitrate leaching.

Microbial N-immobilisation: the neglected process may be most essential

Based on a general comparison of the results from 14 models, de Willigen (1991) draw conclusions similar to the ones in an earlier report in 1985 based on only 6 participants and their models. He stated that the essential error may stem from the lack of simulating the soil microbial processes. None of the models could account for the apparent mineral nitrogen loss observed shortly after application of fertilizers in late spring or early summer.

Microbial immobilization in soils will not play a role in long term approaches except where changes of land use or management take place. But regarding short term and seasonal changes only one - DAISY - out of originally 9 models in the review of the report 1 (Vereecken et al., 1991) and, at a first look, four out of 14 models in report 2 (de Willigen, 1991) take explicitely into account one (or more) soil microbial biomass pools. However, also in report 2 only one - again DAISY - model is making efforts in using two separate biomass pools describing biomass turnover by growth and decline rates as well as by maintenance. The others do not really model growth and maintenance of microbial biomass explicitly, but instead regard microbes as consumers of substrates only. One other modeler seems to make use of Jenkinson's approach, but it was not possible to get a clear picture of how this has really been done. None of these four models, however, showed especially good agreement with measured soil nitrate profiles or contents despite their special efforts.

Our own comparisons between measured and simulated soil nitrate profiles show short term discrepancies after soil frost and after manuring and tillage procedures as well as long term deviations during the vegetation season. Based on such discrepancies we have realised since a long time ago the lack of a microbial pool and submodel (Kersebaum and Richter, 1991; Richter et al., 1987). Besides possible explanations of seasonal variation of soil mineral N on the basis of changing the relative extent of ammonification and nitrification, together with a change of NH_4^+-sorption or fixation, seasonal variation of microbial biomass and/or N seems to be of major importance. In order to get a sound basis for simulations, expensive measurements are necessary to follow microbial biomass N

Table 7. (=Table 4 of Vereecken et al., 1991) Statistical criteria of the performance of the five different models on simulation of nitrate leaching (kg N ha^{-1} a^{-1}) for the three different sites

Site	Model	n[a]	ME[b]	RMSE[c]	CD[d]	EF[e]	CRM[f]
Askov	ANIMO	6	13.4	20.2	1.29	0.60	-0.15
	DAISY	5	24.5	30.0	0.95	0.28	0.10
	EPIC	6	20.4	24.4	0.69	.42	-0.13
	RENLEM	6	55.4	64.9	0.20	-3.09	-0.18
	SWATNIT	6	16.0	32.9	6.38	-0.05	-0.07
Jyndevad	ANIMO	12	41.3	23.0	1.02	0.82	-0.10
	DAISY	12	26.5	19.4	1.25	0.87	0.01
	EPIC	12	49.6	28.0	0.72	0.74	0.17
	RENLEM	12	45.2	35.5	0.68	0.58	0.17
	SWATNIT	12	54.1	28.9	0.82	0.72	-0.07
Ruurlo	ANIMO	24	61.8	56.5	1.87	0.44	0.17
	DAISY	12	39.7	47.1	1.29	0.68	0.15
	EPIC	24	53.7	52.0	1.46	0.53	-0.13
	RENLEM	24	55.4	76.1	1.15	-0.01	0.52
	SWATNIT	19	85.7	86.6	0.33	-0.31	-0.45
ALL[g]	ANIMO	43	61.8[h]	36.2	0.96	0.78	0.00
	DAISY	29	39.7	27.2	1.09	0.89	0.05
	EPIC	43	53.7	37.1	1.17	0.77	0.01
	RENLEM	43	55.4	53.4	0.83	0.52	0.27
	SWATNIT	38	85.7	52.6	0.63	0.53	-0.27

[a] n : Number of observations.
[b] ME : Maximum error.
[c] RMSE : Root mean squared error.
[d] CD : Coefficient of determination.
[e] EF : Modelling efficiency.
[f] CRM : Coefficient of residual mass.
[g] Including Pittem, Belgium.
[h] This column repeats erroneously the previous one in Vereecken et al. (1991).

changes accurately at field scale (Lindloff et al., 1994; Widmer, 1993).

Modeling a system showing different activities with changing environmental conditions seems to be quite a difficult task. Following the original idea of Vinogradsky (1949), microbial biomass needs to be split into 2 pools, a fast responding zymogeneous and a rather indolent autochthoneous one. Further, also two metabolic states may be distinguished, an active and a dormant one. According to this line, a Pirt type model (Pirt, 1975) may be developed in different ways: one perhaps according to Kersebaum and Richter (1994), another one according to Yevdokimov et al. (1993) in order to see, which one gives better response to the few data over the season, directly measured or indirectly estimated as stated in Kersebaum and Richter (1991). The Kersebaum and Richter (1994) approach uses two different biomass pools, but up to now only one state of activity. Furthermore it uses two organic pools differing in size and decomposability, according to our experience with mineralisation experiments. Differences to usual biomass growth approaches reside in the use of a nonlinear death or decline rate evolving essentially logistic growth on both biomass pools. Blagodatsky's approach (used in Yevdokimov et al., 1993) differs in using only one organic pool but two different states, an active and an inactive one. Furthermore, according to the experience of soil microbiologists, a purely soluble organic matter pool is used. Figure 7 shows the pool and flux diagram of that model.

Parameterization of such a model, even for laboratory experiments, is a laborious task. Figure 8 shows

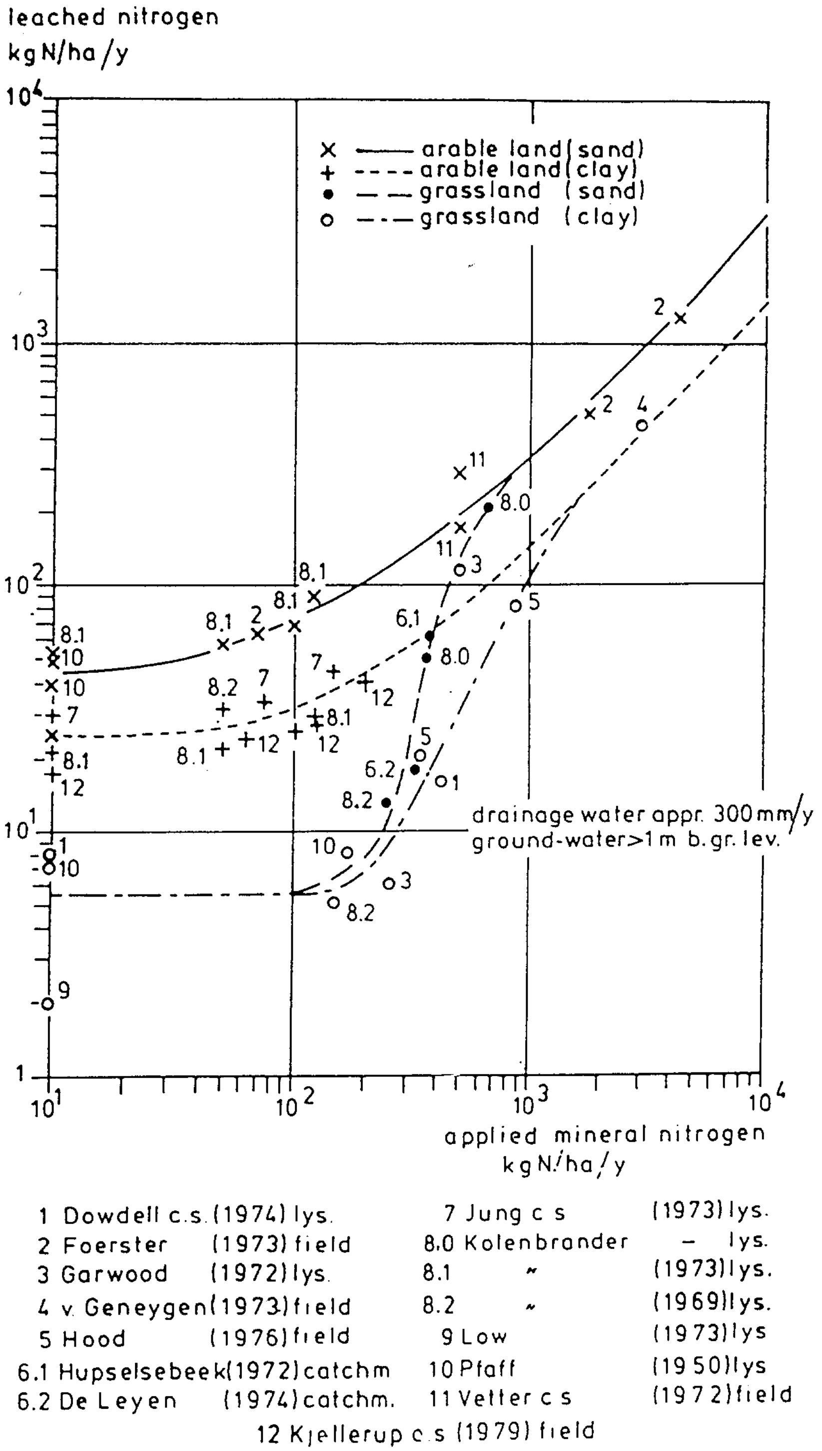

Figure 6. Annual nitrate leaching rates in arable and grassland, depending on applied fertilizer nitrogen and drainage, according to Kolenbrander (1981).

the simulation with fitted parameters using modern parameter estimation techniques (here embedded in the statistical program package BMDP) of a steady state incubation experiment of Smith et al. (1986), according to Kersebaum and Richter (1994). The essential task of the experiment of Smith et al. (1986), was to

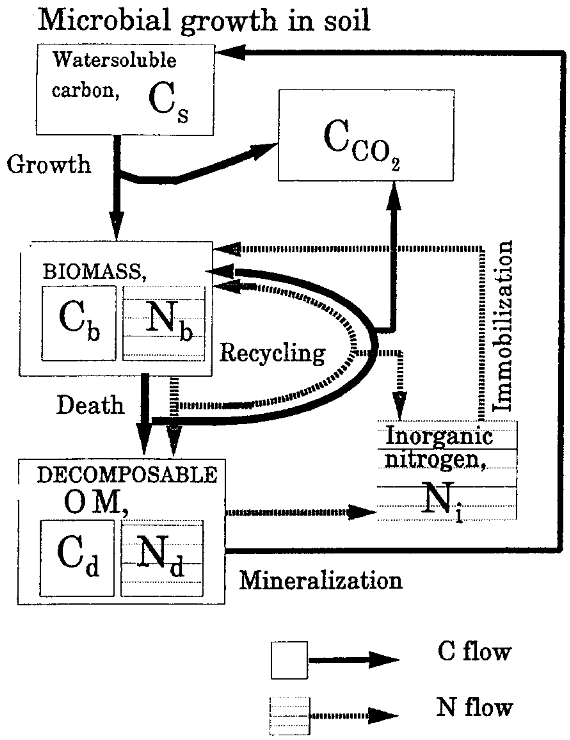

Figure 7. A sketch of the model of Blagodatsky according to Yevdokimov et al. (1993).

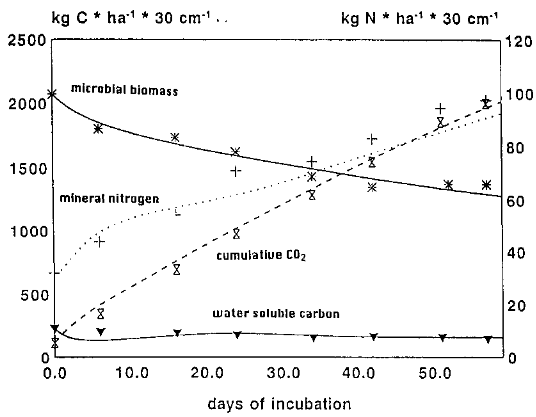

Figure 8. Simulation with fitted parameters using modern parameter estimation techniques, according to Kersebaum and Richter (1994).

estimate maintenance parameters. We would be happy to have similar results of field observations, where we have additional difficulties with the changing environmental conditions. But since this example also shows that the model was overparameterized with respect to available experimental data, the situation is usually worse for conventional field experiment designs. In the terminology of mathematicians, the design decides whether the involved mathematical problem is "well posed" or "ill conditioned" (Kersebaum and Richter, 1994).

Concluding remarks

All the above evaluations were done without special regard to the spatial variability of the investigated fields, either structured or non-structured ones. Heterogeneity of the soil properties as well as of the inputs like precipitation, nitrogen or management practices may have a strong influence on the quality of the results. This explains the large scattering of individual measurements. This should not discourage us from trying to get a more quantitative understanding using process simulation. We should, however, remain aware of the fact that modeling does not necessarily entail the accurate quantitative description of all involved processes - but rather requests to find the essential ones.

References

Addiscott T M and Wagenet R J 1985 Concepts of solute leaching in soils: a review of modeling approaches. J. Soil Sci. 36, 411–424.

Benbi D K and Richter J 1994 Concepts of nitrogen mineralization kinetics and potentially mineralizable nitrogen in soils: A review of the modeling approaches. Soil Biol. Biochem. (*Submitted*).

de Willigen P 1991 Nitrogen turnover in the soil-crop system: comparison of fourteen simulation models. Fert. Res. 27, 141–149.

European Communities 1991 Commission EUR13501. Soil and ground-water res. report II - Nitrate in soils, Luxembourg 1991, 544 p.

Groot J J R, de Willigen P and Verberne E L J 1991 Nitrogen turnover in the soil-crop system - Modelling of biological transformations, transport of nitrogen and nitrogen use efficiency. Proceedings of a workshop held at the Institute for Soil Research, Haren, The Netherlands, 5–6 June 1990. Fert. Res. 27, 141–383.

Jenkinson D S and Rayner J H 1977 The turnover of soil organic matter in some of the Rothamsted classical experiments. Soil Sci. 123, 298–305.

Johnsson H, Bergström L, Jansson P E and Paustian K 1987 Simulated nitrogen dynamics and losses in a layered agricultural soil. Agric. Ecosyst. Environ. 18, 333–356.

Kersebaum K C and Richter J 1991 Modelling nitrogen dynamics in a plant-soil system with a simple model for advisory purposes. Fert. Res. 27, 272–281.

Kersebaum K C and Richter O 1994 A model approach to simulate C and N transformations through microbial biomass. *In* Nitrogen Mineralization in Agricultural Soils. Eds. J J Neeteson and J Hassink. pp 221–229. AB-DLO Thema's, Wageningen, the Netherlands.

Kolenbrander G J 1981 Leaching of Nitrogen in Agriculture. *In* Nitrogen Losses and Surface Run-Off. Ed. J C Brogan. pp 199–216. Den Haag, the Netherlands.

Lindloff A, Nieder R and Richter J 1994 Temporary microbial immobilisation of nitrogen in an arable loess soil. *In* Nitrogen Mineralization in Agricultural Soils. Eds. J J Neeteson and J Hassink. pp 221–229. AB-DLO Thema's, Wageningen, the Netherlands.

Molina J A E, Clapp C E and Larson W E 1980 Potentially mineralizable nitrogen in soil: the simple exponential model does not apply for the first 12 weeks of incubation. Soil Sci. Soc. Am. J. 44, 442–444.

Nordmeyer H and Richter J 1985 Incubation experiments on nitrogen mineralization in loess and sandy soils. Plant and Soil 83, 433–455.

Nuske A and Richter J 1981 N mineralization in loess-parabrownearthes: incubation experiments. Plant and Soil 59, 237–247.

Otter-Nacke S and Kuhlmann H 1991 A comparison of the performance of N simulation models in the prediction of Nmin on farmers' fields in the spring. Fert. Res. 27, 341–347.

Pirt S J 1975 Principles of Microbe and Cell Cultivation. Blackwell, Oxford, UK.

Richter J, Nordmeyer H and Kersebaum K C 1984 Zur Aussagesicherheit der N_{min}-Methode. Z. Acker- Pflanzenbau 153, 285–296.

Richter J, Kersebaum K C and Utermann J 1988 Modelling of the Nitrogen Regime of Arable Field Soils for Consultation Purposes. *In* Nitrogen Efficiency in Agricultural Soils. Eds. D S Jenkinson and K S Smith. pp 371–383. Elsevier, Amsterdam, the Netherlands.

Richter G M, Widmer P and Richter J 1994 Biological relevance of easily extractable organic nitrogen (EUF-N_{org}) for the estimation of nitrogen mineralization. Eur. J. Agron. 3, 281–289.

Seligman N G and van Keulen H 1981 PAPRAN: A simulation model of annual pasture production limited by rainfall and nitrogen. *In* Simulation of Nitrogen Behaviour of Soil-Plant Systems. Eds. M J Frissel and J A van Veen. pp 192–221. Pudoc, Wageningen, the Netherlands.

Smith J L, McNeal B L, Cheng H H and Campbell G S 1986 Calculation of microbial maintenance rates and net nitrogen mineralisation in soil at steady state. Soil Sci. Soc. Am. J. 50, 332–338.

Stanford G and Smith S J 1972 Nitrogen mineralization potentials of soils. Soil Sci. Soc. Am. Proc. 36, 465–472.

Van Veen J A 1977 The behaviour of nitrogen in soil. Doctoral thesis, Amsterdam, the Netherlands.

Vereecken H, Jansen E J, Hack-ten Brooke M J D, Swerts M, Engelke R, Fabrewitz S and Hansen S 1991 Comparison of simulation results of five nitrogen models using different datasets. *In* European Communities - Commission EUR13501: Soil and groundwater res. Report II - Nitrate in soils, Luxembourg 1991. pp 321–338. See reference European Communities, 1991.

Vinogradsky S 1949 Microbiologie du Sol: Problemes et Methods. Masson et Cie, Paris, France.

Walther W, Scheffer B and Teichgräber B 1985 Ergebnisse langjähriger Lysimeter-, Drän- und Saugkerzenversuche zur Stickstoffauswaschung bei landbaulich genutzten Böden und ihre Bedeutung für die Belastung des Grundwassers. Veröff. Inst. Stadtbauwesen TU Braunschweig, 40. 340 p.

Widmer P 1993 Zeitliche und räumliche Variabilität der mikrobiellen Biomasse in niedersächsischen Böden. Doctoral thesis, Hannover, Germany.

Yevdokimov I V, Blagodatski S A and Kudeyarov V N 1993 Microbiological immobilization, remineralization and plants uptake of fertilizer nitrogen. Eurasian Soil Sci. 25, 64–72.

Section editor: R Merckx