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Calculation of nitrogen mineralization and leaching in fallow soil using a simple dynamic model

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Summary

Simple models describing nitrogen processes are required both to estimate nitrogen mineralization in field conditions and to predict nitrate leaching at large scales. We have evaluated such a model called LIXIM, which allows calculation of nitrogen mineralization and leaching from bare soils, assuming that these are the dominant processes affecting N in bare soil. LIXIM is a layered, functional model, with a 1-day time step. Input data consist of frequent measurements of water and mineral N contents in soil cores, standard meteorological data and simple soil characteristics. The nitrate transport is simulated using the 'mixing-cells' approach. The variations in N mineralization with temperature and moisture are accounted for, providing calculation of the 'normalized time'. An optimization routine is used to estimate the actual evaporation and the N mineralization rates that provide the best fit between observed and simulated values of water and nitrate contents in all measured soil layers.

The model was evaluated in two field experiments (on loamy and chalky soils) including treatments, lasting 9–20 months. The water and nitrate contents in soil were satisfactorily simulated in both sites, and all treatments, including a ^{15}N tracer experiment performed in the loamy soil. In the chalky soil, the calculated water balance agreed well with drainage results obtained in lysimeters and independent estimates of evaporation. At both sites, N mineralization was reduced by the incorporation of crop residues (wheat or oilseed rape straw); the amounts of nitrogen immobilized varied between 20 and 35 kg N ha^{-1}. In the treatments without crop residues, the mineralization rate followed first-order kinetics (against normalized time) in the loamy soil, and zero-order kinetics in the chalky soil. In the latter soil, the mineralization kinetics calculated *in situ* were close to the kinetics measured in laboratory conditions when both were expressed against normalized time.

Introduction

Improving the prediction of nitrogen (N) mineralization in agricultural soil is recognized as crucial for improving fertilizer recommendations and reducing the risks of NO_3^- leaching. It is one objective of the integrated models simulating the N cycle in soil–plant systems, together with the knowledge of the various processes involved. Comparing several of these simulation models, de Willigen & Neeteson (1985) and de Willigen (1991) concluded that it was important to improve submodels of N mineralization and to test them more thoroughly. However, testing them requires the precise quantification of mineralization in field conditions, which is difficult because several processes are involved, and the spatial variation of inorganic N is so large in soils (Delphin & Gassmann, 1992). Studies on unfertilized, fallow soil are often preferred to cropped and fertilized soils because fewer processes need to be considered; for example, rhizodeposition and accumulation of N in roots, which are difficult to assess, can be avoided. Mineralization and leaching are usually the two dominant processes occurring in fallow soil.

Rees *et al.* (1994) indicated that incubation of undisturbed soil cores *in situ* is one possible way to measure net mineralization. Vinther (1994) used this technique and could calculate consistent mineralization rates every month. However, he pointed out that one disadvantage of the method was that different physical conditions prevailed inside and outside the incubated cores. The calculation model presented in this paper does not suffer this drawback. Its objective is to calculate simultaneously net mineralization and leaching of N in field conditions. It has several interests, as follows.

1 It uses easily measurable field data: measurements of water and mineral N profiles in bare soils at different dates.

2 It allows us to test the consistency of the field data relative to the model, and the validity of the underlying hypotheses: denitrification and preferential flow are negligible.

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3 It provides mineralization kinetics against normalized time which can easily be compared with laboratory data obtained at constant temperature and moisture conditions.

The model

As mentioned above, our model, LIXIM, is designed to estimate N mineralization and leaching in bare soil which can be sampled frequently by coring for measuring water and mineral N content at different depths. The conditions required for its application are: (i) the absence of plant cover or a slowly growing crop transpiring little water, shallow rooting and taking up little N; (ii) a rather rapid nitrification, and (iii) measurement of water and mineral N in several soil layers (minimum three layers).

Water and solute transport

Using the terminology defined by Addiscott & Wagenet (1985), the water and solute leaching submodel in LIXIM is a 'deterministic functional model with a layer approach'. It is derived from the approach proposed by Burns (1974) and the 'mixing-cells' concept developed by Van Ommen (1985) and Van der Ploeg *et al.* (1995) for nitrate movement. The soil is divided into multiple horizontal layers characterized by their maximum water-holding capacity, at field capacity, and a least amount of available water, at permanent wilting point. The time step of the model is the day.

Water moves in the soil either as upward flow (evaporation) or downward flow (drainage). The redistribution of the water is assumed to be complete at the end of each day. Drainage occurs from one layer i to layer $i+1$ when the sum of water contained in layer i and the daily amount of flowing water exceeds field capacity. By contrast, evaporation is simulated differently in LIXIM from that in Burns's model (1974). We suppose that evaporation affects simultaneously the upper layers up to a maximum depth, with the constraint that the moisture content of each layer cannot decrease to less than the water content at permanent wilting point. The relative contribution of each layer i to total evaporation is proportional to

$$\frac{E_{ai}}{E_a} \propto \left(1 - \frac{Z_i}{Z_e}\right)^{\alpha} K_i, \quad Z_i \le Z_e, \tag{1}$$

where E_{ai} is the actual evaporation of layer i (mm), E_a is the total actual evaporation (mm), Z_i is the depth of layer i (cm), Z_e is the maximum depth affected by evaporation (cm), α is a power coefficient, and K_i is an 'evaporative conductance' defined by

$$K_i = \frac{\theta - \theta_{wp}}{\theta_{fc} - \theta_{wp}}, \tag{2}$$

where θ is the actual water content of layer i, and θ_{fc} and θ_{wp} are its water contents at field capacity and wilting point, respectively (cm^3 cm^{-3}). Varying the parameters Z_e and α in this empirical formula allows us to account for the variations in hydraulic conductivity between soils.

The solute transport is simulated using the approach proposed by Terkeltoub & Babcock (1971) and Burns (1974). These authors suggested that the transfer of a non-interactive solute could be described by complete mixing of the flowing solute with the resident solute of each layer, followed by the drainage of the excess water and the leaching of associated solute. In steady-state drainage conditions, the fractional solute transfer of each layer to the next one is given by

$$f = \frac{q}{q + \theta\ \Delta z}, \tag{3}$$

where f is the fraction of solute leached from each layer, q is the daily water flow (mm), and Δz is the thickness of each layer (mm). This algorithm is used in our program.

Link with other solute transport models

We point out that this approach markedly differs from the one also developed by Burns (and therefore often referred to as 'Burns's model') in his second (Burns, 1975) and third papers (Burns, 1976). Burns integrated Equation (3) by depth to calculate the fraction of solute leached below a given depth z. For solute applied at the soil surface, he gave the following equation:

$$F = \left(\frac{I}{I + \theta\ \Delta z}\right)^{z/\Delta z}, \tag{4}$$

in which I is the cumulative water flow (mm):

$$I = \int q(t)\mathrm{d}t. \tag{5}$$

Towner (1983) showed that if Δz was small enough then this equation was equivalent to the simpler one:

$$F = \exp\left(-\frac{\theta z}{I}\right). \tag{6}$$

Scotter *et al.* (1993) have further analysed this equation and concluded that it was 'consistent with an independent flow tube soil leaching model, rather than the soil solution being well-mixed at each soil depth as Burns suggested'. This paradox is explained by the fact that Equation (4) considers a single drainage event with the water flow I instead of repeating Equation (3) for the sequence of elementary water flow events $q(t)$. This simplification can result in a strong dispersive behaviour when I is large (see Figure 3 in Scotter *et al.*, 1993), very far from the mixing assumption of the initial model.

In fact, Burns's model, Equation (3), used in LIXIM can be compared with the mechanistic convection–dispersion equation (CDE model). Towner (1983) has shown that Equation (3) can be written as

$$\frac{\Delta C_i}{\Delta t} = -\frac{q}{\theta}\frac{(C_i - C_{i-1})}{\Delta z}, \tag{7}$$

where C_i is the solute concentration in the layer i at time t. In comparison, the CDE can be written as (e.g. Addiscott & Wagenet, 1985)

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial z^2} - \frac{q}{\theta}\frac{\partial C}{\partial z}, \tag{8}$$

where D is the apparent dispersion coefficient (cm^2 day^{-1}).

As indicated by Towner, Equation (7) is one finite-difference solution of the CDE model in which the dispersion term is neglected. In fact, the finite-difference method results in a numerical dispersion which compensates for the omission of the physical dispersion term $D\frac{\partial^2 C}{\partial z^2}$ in Equation (8).

A similar approach is the 'mixing-cells' model proposed by Van Ommen (1985) and developed by others (e.g. Villermaux, 1987; Jauzein *et al.*, 1989). It was applied to nitrate by Van der Ploeg *et al.* (1995) who also derived Equation (7). Villermaux (1987) has shown that the mixing-cells theory gives results that are identical to the CDE model if the Peclet number is equal to $2(J-1)$ and if $J > 20$, J being the number of layers (or mixing cells). These two conditions are equivalent to the following ones:

$$\Delta z = 2\lambda, \tag{9}$$

and

$$\Delta z \leq \frac{z}{20}, \tag{10}$$

with

$$\lambda = \frac{\theta D}{q} \tag{11}$$

in which λ is the dispersivity length (cm). Therefore the equivalence between the functional (Burns or mixing-cells) and the mechanistic (CDE) models is true if the layer thickness and the soil dispersivity are small enough and in the ratio 2:1. Comparisons between the two models relative to NO_3^- leaching have been made by Van der Ploeg *et al.* (1995) who found good agreement between the two approaches when the dispersivity was less than 5 cm. In LIXIM, the layer thickness has been taken as $z = 1$ cm, which would correspond to the dispersivity $\lambda = 0.5$ cm. We checked that the transport submodel of LIXIM gave similar results to those published by Van der Ploeg *et al.* (1995) with this dispersivity.

Nitrogen transformations

The submodel of LIXIM that represents the transformations of N considers mainly net mineralization (transformation of organic N into NH_4^+) and nitrification. Denitrification is normally treated as negligible, although it can be accounted for in the simulations if necessary. The volatilization of NH_3 is also neglected. In order to fulfil these two assumptions, it is advisable not to use the model in soils in which the nitrification is slow relative to ammonification (and which therefore contain large amounts of NH_4^+-N) or which received large quantities of chemical N fertilizers or organic fertilizers rich in NH_4^+-N (e.g. pig slurry) during or immediately before the experiment.

Mineralization, nitrification and denitrification are assumed to occur only in the topsoil, i.e. to a fixed depth Z_m which is at least equal to the ploughing depth. Mineralization, nitrification and denitrification rates can be treated as constant over each time interval. This hypothesis appears to be good enough in experiments carried out with short time intervals (2–3 weeks for example), since the rates vary from one interval to the other. It may be insufficient with longer time intervals. In this case, the mineralization rate is allowed to vary with soil temperature and moisture. During each day j, the mineralization rate is then calculated as

$$V_m(j) = V_p \sum_{i=1}^{N_m} f(T_{ij}) g(\theta_{ij}), \tag{12}$$

in which $V_m(j)$ is the actual mineralization rate (kg N ha^{-1} day^{-1}), V_p is the potential mineralization rate (kg N ha^{-1} day^{-1}) at a given reference temperature, T_{ref}, and at optimal water content, θ_{opt}, T_{ij} and θ_{ij} are the mean daily temperature and water content of layer i on day j, N_m is the number of layers contributing to N mineralization, and $f(T)$ and $g(\theta)$ are the temperature and moisture functions, respectively. Water content throughout the profile is simulated, so that θ_{ij} is known. To simplify the model and the inputs, the soil temperature profile is not calculated, and only one temperature is considered (soil at –10 cm or air at +2 m) as a standard meteorological input. Equation (12) is then simplified as

$$V_m(j) = V_p f(T_j) \sum_{i=1}^{N_m} g(\theta_{ij}), \tag{13}$$

where T_j is the mean daily temperature measured in the soil or the air. The cumulative N mineralized (kg N ha^{-1}) over each measurement interval Δt (days) is

$$M = \sum_{j=1}^{\Delta t} V_m(j). \tag{14}$$

The temperature and moisture functions were chosen on the basis of the review made by Rodrigo *et al.* (1997). The Van't

Table 1 Input variables and fixed and fitted parameters used in the LIXIM model

	Input variables	
Weather	Daily rainfall, potential evapotranspiration (Penman), air temperature (2 m)	
Soil	Water content, NH_4^+ and NO_3^- contents (for each layer, at each measurement date)	
D_a	Bulk density (for each layer)	
θ_{fc}	Water content at field capacity (for each layer)	
θ_{wp}	Water content at wilting point (for each layer)	
	Fixed parameters	Value
Z_e	Maximum soil depth contributing to water evaporation	60 cm
α	Coefficient of reduction of evaporation through depth	3 (Expt 1) or 2 (Expt 2)
Z_m	Maximum soil depth contributing to N mineralization	32 cm
K	Temperature coefficient (Van't Hoff) for N mineralization	0.115 K^{-1}
c	Relative N mineralization rate at wilting point	0.20
C_r	Mineral N concentration in rain	2.0 mg N l^{-1}
	Fitted parameters	
R	Actual to potential evapotranspiration ratio (E_a/E_p)	
V_p	Potential mineralization rate at reference temperature and optimal water content	

Hoff function was adopted to describe the effect of temperature:

$$f(T) = \exp[K(T - T_{ref})] = Q_{10}{}^{\left(\frac{T-T_{ref}}{10}\right)}, \qquad (15)$$

where T_{ref} is the reference temperature (in this paper T_{ref} = 15°C), K is the temperature coefficient, and Q_{10} is the Van't Hoff coefficient. We used the temperature coefficient previously established by Balesdent & Recous (1997) for humified organic matter decomposition, namely $K = 0.115\ K^{-1}$ (corresponding to $Q_{10} = 3.17$).

The moisture function adopted is

$$g(\theta) = (1 - c)\frac{\theta - \theta_{wp}}{\theta_{fc} - \theta_{wp}} + c, \qquad (16)$$

where c is the mineralization rate at wilting point, θ_{wp}, relative to the maximum mineralization rate, which is supposed to occur at field capacity, θ_{fc}.

The calculation of these temperature and moisture functions is also essential to calculate the 'normalized time' as suggested by Andrén & Paustian (1987). The 'normalized time', which is the equivalent of the 'hydrothermal time' used in crop physiology (Gummerson, 1986), is calculated as

$$t_n = \sum_{j=1}^{\Delta t} f(T_j) \sum_{i=1}^{N_m} g(\theta_{ij}). \qquad (17)$$

It is expressed in 'normalized days' (ndays). Equation (14) can be written as

$$M = V_p t_n. \qquad (18)$$

In the absence of NH_3 volatilization and denitrification, the variation of nitrate N due to biological activity during each time interval is

$$\Delta N = M - \Delta A, \qquad (19)$$

where ΔA is the variation of the ammonium N content during the time interval Δt. This equation yields the simulated nitrate content, N, which is the fitted variable of the nitrogen submodel.

Model simulations

The input variables and the fixed and fitted parameters used by LIXIM, are summarized in Table 1. The full model combines a simulation model for predicting water content, and nitrate content, N, in the soil profile against time, which derives from the submodels described above, and an optimization routine that can calculate two parameters of the model: the ratio of actual to potential evapotranspiration, E_a/E_p, and the potential rate of mineralization V_p. The potential evapotranspiration is calculated from Penman's (1949) equation, on the assumption that the ratio E_a/E_p varies between 0 and 1 in fallow soil.

The model can be run either in simulation mode when these two parameters are fixed or in fitting mode (model inversion) to estimate the two parameters. In the latter case, which we use in this paper, the optimization is made for each time interval k by fitting the observed and simulated water and nitrate contents in each layer at the end of this time interval. The program minimizes the criterion

$$RR = RRMSE(\theta, k) + RRMSE(N, k), \qquad (20)$$

where $RRMSE(Y, k)$ is the relative root mean square error for the Y variable:

$$RRMSE(Y,k) = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(\frac{Y_{ik} - \hat{Y}_{ik}}{\bar{Y}_k}\right)^2}, \tag{21}$$

where n is the number of measured layers, Y_{ik} and $\hat{Y}_{ik}$ are the observed and simulated Y values (water or nitrate content), and $\bar{Y}_k$ is the mean of the observed values at the end of interval k. One advantage of using the relative root mean square error (*RRMSE*) instead of the absolute RMSE is that it 'normalizes' the two fitting variables (water and nitrate content) which can then be summed up in a common criterion (*RR*).

The statistical criteria used to evaluate the model are (Smith *et al.*, 1996)

- the mean difference

$$MD(Y) = \frac{1}{mn}\sum_{k=1}^{m}\sum_{i=1}^{n}(Y_{ik} - \hat{Y}_{ik}), \tag{22}$$

- the absolute root mean square error

$$RMSE(Y) = \sqrt{\frac{1}{mn}\sum_{k=1}^{m}\sum_{i=1}^{n}(Y_{ik} - \hat{Y}_{ik})^2}, \tag{23}$$

- and the modelling efficiency

$$EF(Y) = 1 - \frac{\sum_{k=1}^{m}\sum_{i=1}^{n}(Y_{ik} - \hat{Y}_{ik})^2}{\sum_{k=1}^{m}\sum_{i=1}^{n}(Y_{ik} - \bar{Y}_{ik})^2}, \tag{24}$$

in which Y represents either the soil water content, or the nitrate content, N, and m is the number of measured time intervals.

Field experiments

Experiment 1 (Mons 1991–92)

This experiment was carried out in 1991–92 at Mons-en-Chaussée in northern France (49°80′N, 3°60′E). Full details of the experiment can be found in Darwis (1993). The soil is a deep loamy soil (Orthic Luvisol) the characteristics of which are given in Table 2. The experiment started in August 1991 in an agricultural field after the harvest of a winter wheat crop. Eighteen adjacent plots (2 m × 8 m) were taken within the field, corresponding to six treatments with three replicates. The six treatments consisted of three tillage operations × two rates of wheat straw addition:

- D0: disc ploughing; no straw returned;
- R0: rotavator tillage; no straw returned;
- M0: no tillage ('mulch'); no straw returned;
- DS: disc ploughing; straw incorporated;
- RS: rotavator tillage; straw incorporated;
- MS: no tillage ('mulch'); straw left on the soil surface.

After harvest, wheat straw (stubble, chaff and straw) was completely removed from all the experimental plots. In the three treatments with returned straw, applied at the rate of 3590 kg C ha^{-1}, the amount of straw needed per m^2 (800 g) was weighed and spread on the corresponding soil surface on 30 August 1991. The soil was immediately tilled by disc ploughing (depth ≈ 10 cm) or rotavator (depth ≈ 18 cm). Disc ploughing was repeated on 10 October, whereas rotavating was done once only. The soil was not tilled in the M0 and MS treatments, except on 3 March 1992, when the soil was ploughed at the same time as in the other treatments. The weeds and volunteers were destroyed by several herbicide applications in all treatments.

To test the leaching model, ^{15}N tracer was applied on day 2 (1 September 1991) in the treatments without straw (D0, R0 and M0). A small amount of labelled K^{15}NO$_3$ (4.5 kg N ha^{-1}, atom% excess = 2.01%) was added in solution by hand spraying.

Soil cores were taken every 3–4 weeks until 7 July 1992 with a hydraulic coring device (auger diameter = 1.7 cm). Each core was split into seven layers (0–10, 10–20, 20–30, 30–60, 60–90, 90–120 and 120–150 cm). Each soil sample was obtained by mixing seven cores. The samples were frozen until extraction and subsequent analysis of water content (gravimetry), NH_4^+ and NO_3^- concentrations (colorimetry) and ^{15}N atom% excess (mass spectrometry). Recous *et al.* (1988) give details of the extraction and analysis procedures.

Experiment 2 (Rafidin 1994–96)

The second experiment was done in 1994–96 at Rafidin, near Châlons-en-Champagne (eastern France; 48°50′N, 2°15′E). Details of the experiment are given by Leviel *et al.* (1998) and Justes *et al.* (1999). The soil (Calcareous Rendosol) is a white rendzina overlying a chalk layer altered by cryoturbation (28–90 cm) and undisturbed chalk substratum (below 90 cm). Its characteristics are given in Table 2. The experimental site was close to the undisturbed lysimeter site at Châlons-en-Champagne (Ballif *et al.*, 1996). This allowed us to make comparisons of drained water between LIXIM outputs and lysimeter measurements.

The experiment started in September 1994 after harvest of a previous winter barley crop. The barley straw was exported but the stubble and chaff remained. The soil was kept either fallow or cropped with oilseed rape. In the latter case, the crop received either no nitrogen or 270 kg N ha^{-1} fertilizer. In July 1995, after harvest, the soil was kept fallow until the end of April 1996, except for one treatment where rapeseed volunteers were favoured and destroyed in November 1995. Four sets of data relative to bare soils are considered here:

- B00: fallow soil without oilseed rape residues, studied between September 1994 and April 1996;

Table 2 Particle-size distribution and chemical characteristics of the soils (in g kg^{-1} soil)

	Mons (Experiment 1)			Rafidin (Experiment 2)		
	Ap 0–28 cm	Bt 28–70 cm	Bt/C 70–140 cm	Ap 0–28 cm	C 28–90 cm	Chalk 90–120 cm
Clay ($<2\,\mu$m)[a]	199	324	265	99	37	35
Silt (2–50 μm)[a]	720	633	666	110	19	21
Sand (50–2000 μm)[a]	78	43	69	8	2	2
$CaCO_3$	3	0	0	783	942	942
Organic C	10.5	3.7	2.2	22.0	2.1	2.1
Organic N	0.97	0.5	0.3	1.98	–	–
pH (water)	7.8	7.8	7.9	8.3	8.7	8.8

[a] After removal of carbonate.

- BR0: fallow soil with oilseed rape residues from the crop without fertilizer-N, studied between July 1995 and April 1996;
- BR270: fallow soil with oilseed rape residues from the crop receiving 270 kg ha^{-1} fertilizer-N, studied between July 1995 and April 1996;
- VR270: fallow soil with oilseed rape and volunteers residues from the crop receiving 270 kg ha^{-1} fertilizer-N, studied between November 1995 and April 1996.

The weeds were destroyed chemically in the first three treatments. Soil cores were taken every 2 weeks with the hydraulic coring device. Each core was split into four layers (0–28, 28–60, 60–90 and 90–120 cm). Each soil sample was obtained by mixing eight cores. The samples were frozen until extraction and subsequent analysis of water content (gravimetry), and NH_4^+ and NO_3^- concentrations (colorimetry). As for Experiment 1, details of the extraction and analysis procedures are given in Recous *et al.* (1988).

A laboratory incubation was done on the soil sampled at the beginning of the experiment. Soil samples were taken in the ploughed layer (0–28 cm) on 30 August 1994. They were first passed through a 5-mm sieve to remove most of the plant residues (mainly straw and roots from barley). Then the plant residues, isolated on other soil samples by sieving under water (C:N ratio = 45), were added back to the soil in the proportion found in the field (30 mg dry matter to 32 g fresh soil, corresponding to 1.8 t dry matter ha^{-1}). Small amounts of deionized water were added to increase the moisture content to 240 g water kg^{-1} soil (corresponding to about –300 kPa matrix potential). The soil samples were placed in 50-ml vials inserted into 2-l glass jars, each of them containing a beaker with 30 ml M NaOH to trap the CO_2 evolved. The soils were incubated for 52 weeks at 28 ± 0.5°C, with four replicates. The vials were periodically aerated, the soil moisture was restored at 240 g kg^{-1} and the CO_2 traps changed. Soil inorganic N was extracted with 100 ml M KCl per vial. The inorganic N was determined as previously described. Since the incubation was made at a temperature and moisture content different from the reference values, the Equations (15) to (17) were used to calculate the normalized time in incubation, in a similar way to the field experiments.

In both experiments, bulk densities were measured with a gamma densimeter attenuation probe. Water content at permanent wilting point was measured on soil aggregates using the Richards pressure plate at –1.6 MPa water potential. Water content at field capacity was estimated from water measurements obtained in field conditions. It was calculated as the mean of the greatest water content values recorded, after excluding the largest two values. The normalized time was calculated from air temperature data in Experiment 1 and from soil temperature data (–10 cm) in Experiment 2.

Results

Experiment 1

Simulation of water and nitrate contents. The distribution of the water content within the soil profile and its evolution in time was similar in the six treatments studied, whereas significant differences appeared in the distribution and evolution of the nitrate contents, as expected. The observed and simulated gravimetric water contents in each of the five layers of the treatment R0 are shown in Figure 1. The soil was relatively dry at the beginning of the experiment (31 August 1991), since the previous winter wheat crop had taken up water at least to 120 cm depth. The autumn and winter were drier than usual (269 mm rainfall from 1 September 1991 to 31 March 1992, corresponding to 60% of the 30-year mean), and so the layers came back slowly and successively to their maximum water content, which was taken as field capacity. The delay between each layer for reaching θ_{fc} was about 1 month. By contrast, the spring of 1992 was wetter than usual (235 mm from 1 April to 30 June), so that the soil water content remained close to field capacity, even in the first layer.

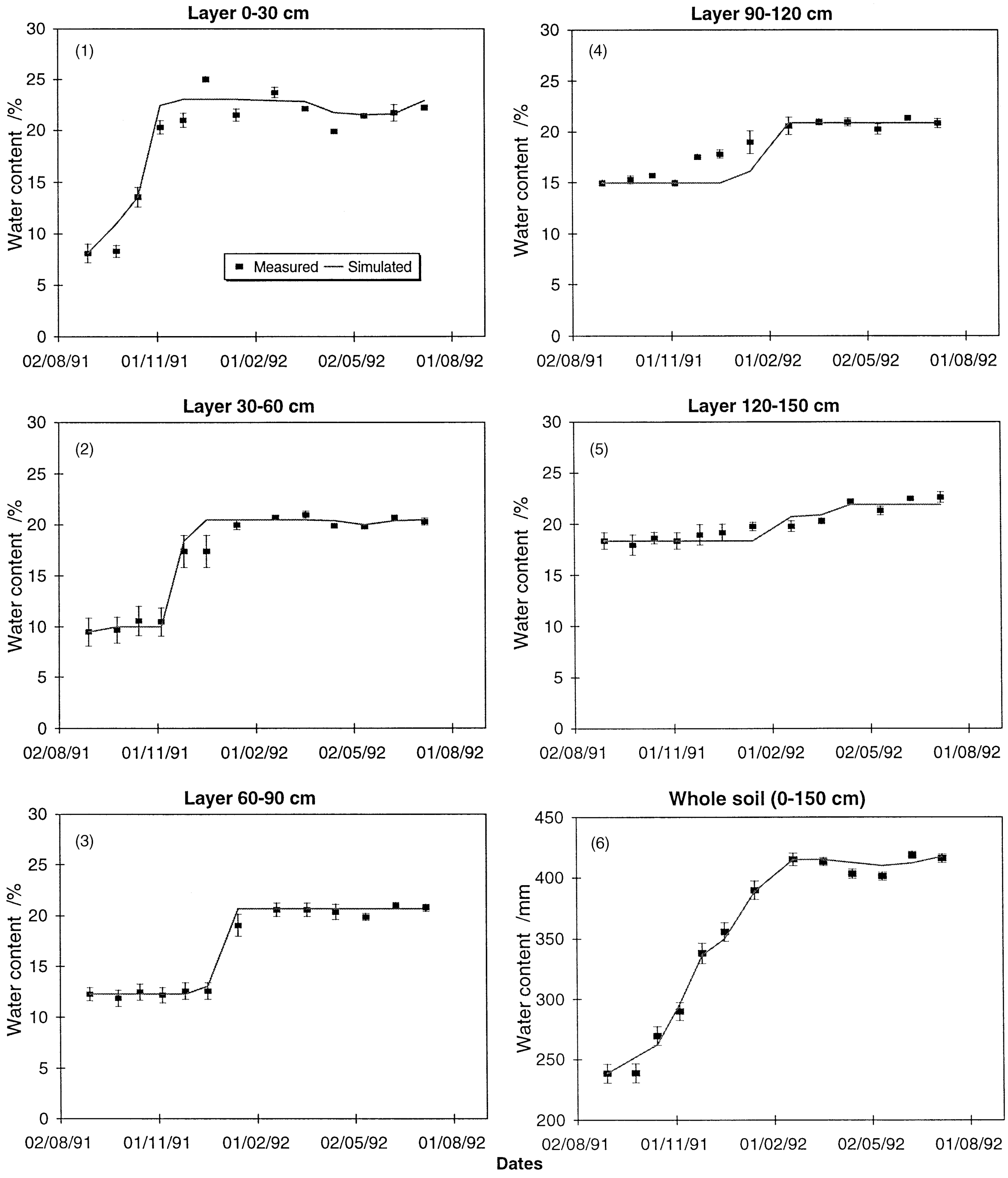

Figure 1 Evolution of observed and simulated water contents in Experiment 1 (Mons 1991–92) in the R0 treatment. Graphs 1–5 show the gravimetric water content (% of dry soil) in each of the five layers and graph 6 the water content of the whole soil (mm). Vertical bars represent standard errors.

We obtained a good agreement between observed and simulated values in this treatment (Figure 1) as well as in the other treatments, since the mean difference (MD) on water content was close to 0, and the root mean square error (RMSE) was slightly less than the standard deviations on measurements (Table 3). The modelling efficiency was high (EF ≈ 0.93).

The corresponding observed and simulated NO_3^--N contents in each of the five layers of the treatment R0 are shown in Figure 2. In this treatment and in the others, the amounts of NH_4^+-N were always small (less than 3 kg N ha^{-1} per layer) and are not shown here. The model could simulate reasonably well the measured nitrate content

Table 3 Statistical criteria for evaluating the model relative to data obtained in Experiments 1 and 2

		Water content				Mineral N content			
	N_f[a]	EF	MD	RMSE /g kg^{-1}	SD	EF	MD	RMSE /kg ha^{-1}	SD
Mons 1991–92									
D0	60	0.92	–1	10	11	0.87	–1.1	5.3	8.9
R0	60	0.92	–1	11	12	0.84	–0.9	5.3	7.1
M0	60	0.92	0	10	11	0.88	–1.2	4.7	8.5
DS	60	0.94	–1	9	13	0.87	–0.6	4.0	9.9
RS	60	0.93	–1	11	13	0.71	+0.2	4.4	6.7
MS	60	0.93	–1	9	12	0.65	–2.0	5.0	5.2
^{15}N[b]	60	0.92	–1	11	11	0.80	–0.7	7.8	9.6
Rafidin 1994–96									
B00	160	0.76	–4	13	11	0.93	–1.0	5.6	4.9
BR0	80	0.69	–6	16	21	0.97	–0.1	2.4	3.5
BR270	80	0.84	–5	13	12	0.90	+0.6	5.7	4.4
VR270	44	0.88	–1	11	19	0.85	–1.0	3.1	2.0

EF, modelling efficiency; MD, mean difference; RMSE, root mean square error; SD, standard deviation.

[a] N_f = number of fitted data (number of layers $n \times$ number of sampling dates N).

[b] Tracer experiment carried out in treatments D0, R0 and M0 (mineral N results in g ^{15}N ha^{-1}).

in the five layers with time. The greatest variations occurred in the first three layers because of leaching and mineralization, whereas the amount of nitrate in the deepest layer hardly changed as a result of the slow drainage. Similar results were obtained for the five other treatments (curves not shown). However, the agreement between observed and simulated values of nitrate was poorer than for water, as indicated by the statistical criteria (Table 3). The modelling efficiency for nitrate ranged between 0.65 and 0.88 and was around 0.93 for water. On the other hand, the spatial variation in nitrate content was greater than the variation in water content, and the RMSEs were always smaller than the experimental standard deviations. The MD was often slightly negative, indicating that the model somewhat overestimated the amounts of nitrate. The largest discrepancy occurred with the MS treatment in which the mean MD was –2 kg N ha^{-1}: the total amount of nitrate in the whole profile (0–150 cm) was then overestimated by 9 kg N ha^{-1}, i.e. 10% of the amount of nitrate.

^{15}N tracing experiment. The observed and simulated $^{15}NO_3^-$ contents in each of the five layers of the tracer experiment (mean of treatments D0, R0 and M0) are shown in Figure 3. Testing the model was hampered by two difficulties as follows.

1 There was a large variation in the $^{15}NO_3^-$ measurements. The mean standard deviation was 9.6 g ^{15}N ha^{-1}, corresponding to a mean coefficient of variation of 64%, while the mean coefficient of variation of the native, unlabelled nitrate was 31%.

2 Recovery of tracer was incomplete. The ^{15}N recovered in the soil as mineral N was less than the amount applied, 91 g ^{15}N ha^{-1}. The ^{15}N deficit was probably due to N immobilization soon after the application, as this is frequently observed (e.g. Recous *et al.*, 1988). This process was fortunately limited by the fact that the soil was left fallow and without fresh organic matter (no straw). The recovery of ^{15}N at the first three measurements (when all the ^{15}N was in the first layer) was not statistically different, and its mean, 72 g ^{15}N ha^{-1}, was taken as the initial effective $^{15}NO_3^-$ input.

Simulations by LIXIM were then run by imposing the mineralization rate of the ^{15}N tracer at 0, so that the transport part of the model could be tested. The measured ^{15}N contents in the different layers were correctly simulated by the transport model (Figure 3). The dates of appearance of the tracer in each layer were well predicted. The RMSEs, 7.8 g ^{15}N ha^{-1}, were smaller than the experimental standard deviations, 9.6 g ^{15}N ha^{-1}. The MD was slightly negative, mainly because the model seemed to overestimate the $^{15}NO_3^-$ content in the 90–120 cm layer at the end of the experiment.

Water and N fluxes. The water and N balances in the six treatments are summarized in Table 4. The model simulated that water drainage below 150 cm occurred only in spring 1992. At the end of the experiment (7 July 1992), the predicted amount of water drained was 131 ± 24 mm. The calculated evaporation was 202 ± 26 mm, corresponding to an evapotranspiration ratio E_a/E_p of 0.54 ± 0.07.

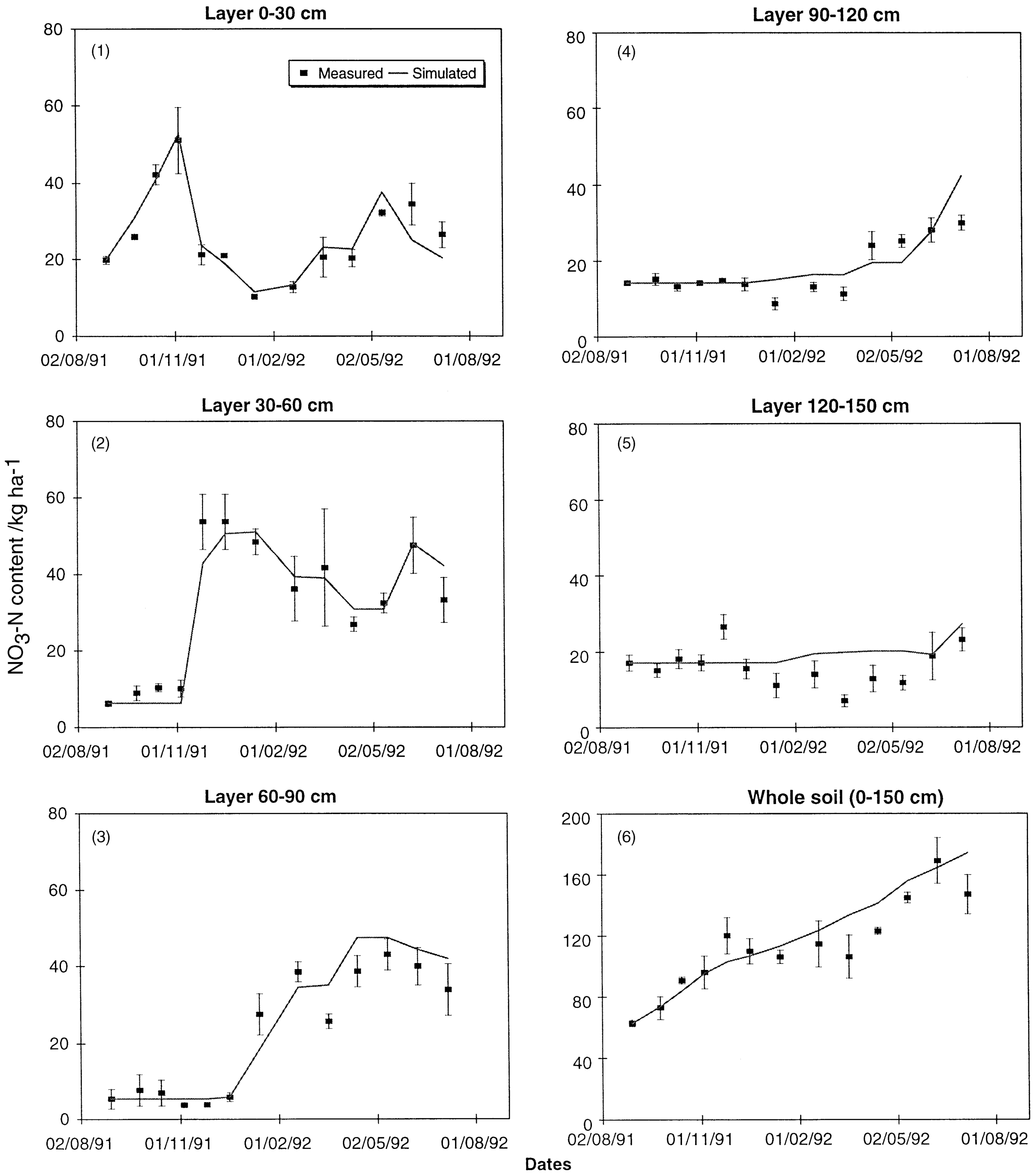

Figure 2 Evolution of observed and simulated nitrate contents in Experiment 1 (Mons 1991–92) in the R0 treatment. Graphs 1–5 show the nitrate content (kg N ha^{-1}) in each of the five layers and graph 6 the nitrate content of the whole soil (kg N ha^{-1}). Vertical bars represent standard errors.

The amounts of N leached below 150 cm calculated by LIXIM were not significantly different between the treatments, the mean being 28 ± 6 kg N ha^{-1} (Table 4). We attribute the absence of difference to there being little drainage. The mean nitrate concentration of drained water, calculated as the ratio between leached N and drained water, was very stable among treatments: 92 ± 3 mg NO_3^- l^{-1}.

The N mineralization kinetics calculated by LIXIM are plotted in Figure 4(a). The kinetics differ between the treatments with and without straw. The net N mineraliza-

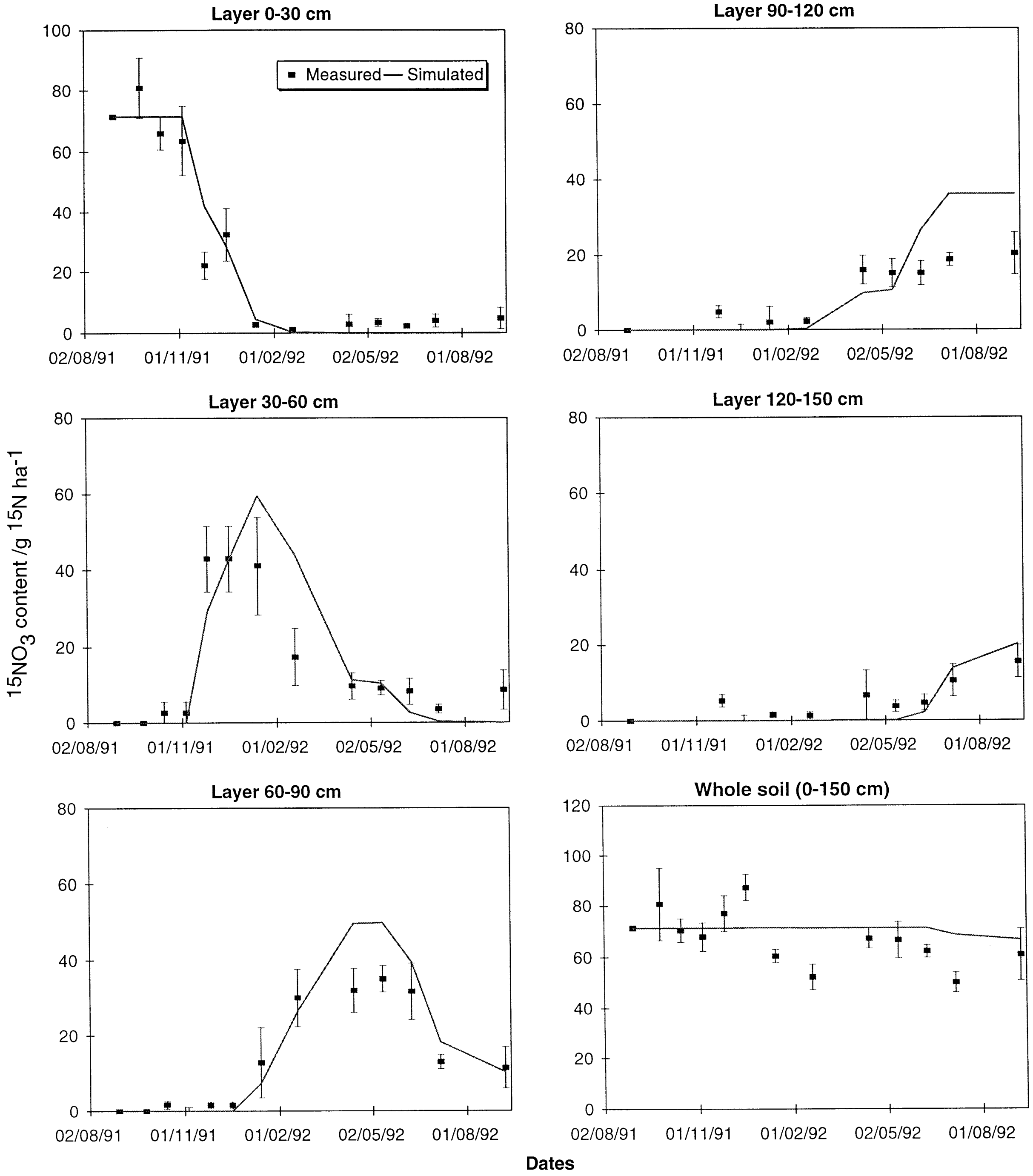

Figure 3 Evolution of observed and simulated $^{15}NO_3^-$ content in each of the five soil layers and total soil $^{15}NO_3^-$ content (g ^{15}N ha^{-1}) in Experiment 1 (Mons 1991–92). Values are the mean of D0, R0 and M0 treatments. Vertical bars represent standard errors.

tion was less in the soils that received wheat straw, showing that decomposing straw resulted in net N immobilization (which can be calculated by difference between the treatments without and with straw). Immobilization of N was initially faster in treatment R, i.e. in the soil tilled with a rotavator and where the straw was incorporated to the greatest depth. The least immobilization in autumn and winter was found in treatment M (no-tilled soil). In this treatment, immobilization increased rapidly in March after ploughing. We attribute this to the mixing of the soil and straw which enhanced decomposition and rendered mineral nitrogen accessible to straw decomposers. The maximum amount of N immobilized was 26, 33 and 31 kg N ha^{-1} in the treatments R, D and M,

Table 4 Simulated cumulative values: actual to potential evapotranspiration ratio (E_a/E_p), drained water, mineralized N, leached N and mean concentration of nitrate in drained water in Experiments 1 and 2

	Period	E_a/E_p	Drained water /mm	Mineralized N /kg ha^{-1}	Leached N /kg ha^{-1}	Concentration /mg NO$_3^-$ l^{-1}
Mons						
D0	Aug 91 – July 92	0.60	109	129	23	95
R0	Aug 91 – July 92	0.46	159	135	39	95
M0	Aug 91 – July 92	0.59	117	133	25	93
DS	Aug 91 – July 92	0.62	106	96	22	93
RS	Aug 91 – July 92	0.48	156	112	31	90
MS	Aug 91 – July 92	0.62	141	102	29	90
Rafidin						
B00	Sept 94 – April 96	0.57	405	149	92	100
BR0	July 95 – April 96	0.49	112	87	2	8
BR270	July 95 – April 96	0.45	116	99	8	30
VR270	Nov 95 – April 96	0.61	60	51	4	29

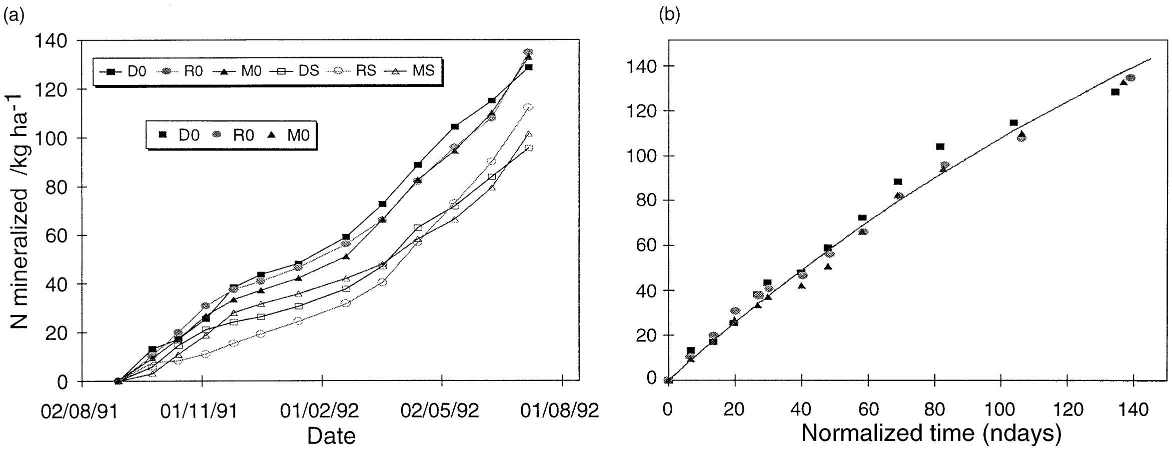

Figure 4 Cumulative net N mineralized calculated by LIXIM in Experiment 1: (a) N mineralized against real time in the six treatments; (b) N mineralized against 'normalized time' in the three treatments without wheat straw.

respectively. It was obtained in mid-February in treatment R and at the end of the experiment (7 July 1992) in the other two treatments.

The amounts of N mineralized calculated in the treatments without straw are plotted against normalized time in Figure 4(b). No significant difference appeared between treatments, indicating that tillage of the soil without fresh organic residues had little or no influence on the mineralization rate. Furthermore, the cumulative N mineralized was close to that for a first-order kinetic reaction, and the data could be fitted to a classical exponential curve:

$$N = N_0\,[1 - \exp(-kt)], \tag{25}$$

where N_0 is the 'N mineralization potential' (Stanford & Smith, 1972), and k is the rate constant. In our experiment, the best fit (least squares method) gave the following values: $N_0 = 302\,\mathrm{kg\,ha^{-1}}$ and $k = 0.0044\ \mathrm{nday^{-1}}$ (at the optimum water content and 15°C temperature). The potential mineralization rate V_p therefore decreased from $1.32\,\mathrm{kg\,N\,ha^{-1}\ nday^{-1}}$ at time 0 to $0.79\,\mathrm{kg\,N\,ha^{-1}\ nday^{-1}}$ at the end of the experiment (342 days corresponding to about 136 ndays).

Experiment 2

Simulation of water and nitrate contents. The observed and simulated gravimetric water contents in each of the four layers of the treatment B00 are shown in Figure 5. The measured water content varied mainly in the ploughed layer (0–28 cm) and little in the deepest layers (28–60, 60–90 and 90–120 cm). Water content was generally well simulated, particularly in the first two layers. The modelling efficiency for all layers was

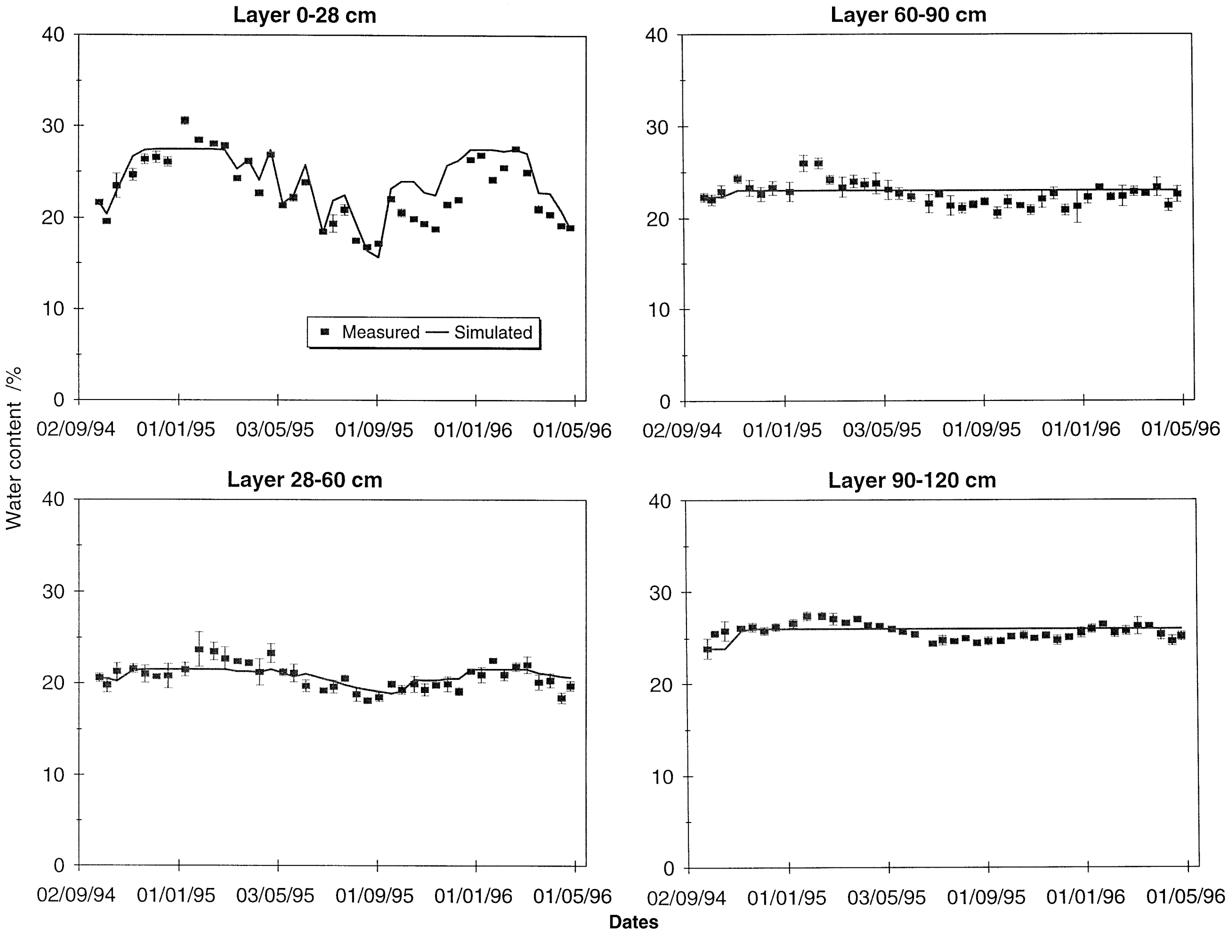

Figure 5 Evolution of observed and simulated gravimetric water contents (% of dry soil) in each of the four measured layers in Experiment 2 (Rafidin 1994–96, B00 treatment). Vertical bars represent standard errors.

0.76; the mean RMSE was similar to the mean standard deviation (Table 3). However, the model simulated no change in water content in the deepest two layers after November 1994, whereas a slight decrease was observed during the summer of 1995 followed by an increase at the end of the year. The simulated value was constant (at field capacity) since the evaporative depth (Z_e) was taken at 60 cm, as in the first experiment. Simulations with a greater Z_e value (90 or 120 cm) indicated that water content could be better simulated in the deeper layers but resulted in a much poorer fit in the second layer (the water content being greatly underestimated). This parametrization was therefore not retained. On the other side, the water content in the ploughed layer was slightly overestimated (mean MD = –10 g kg^{-1}), particularly in autumn 1995. Consequently, the normalized time calculated by LIXIM was also overestimated, by about 3%.

The observed and simulated nitrate contents in each of the four layers of the treatment B00 are shown in Figure 6. The succession of predominant leaching and mineralization phases is revealed by the evolution of the mineral N in the first layer. Good agreement was found between observed and simulated values. The modelling efficiency was 0.93, and the mean RMSE almost equal to the mean standard deviation (Table 3), although the variation of mineral N measurements was small in this experiment (mean coefficient of variation = 11%). A noticeable discrepancy was found in the 60–90 cm layer: the appearance of the second peak of nitrate was postponed by the model. Another lack of fit concerns the fourth layer: the amounts of nitrate decreased slightly at the end of the winter while the model predicted a constant value. However, the observed decrease was not statistically significant.

The model was also able to give a good prediction of the water and nitrate evolution in the other three treatments (BR0, BR270 and VR270). The modelling efficiency varied between 0.69 and 0.88 for water and from 0.85 to 0.97 for nitrate (Table 3). No substantial bias was found.

Water and N fluxes. The water and N balance in the four treatments are summarized in Table 4. The ratio of actual to potential evapotranspiration E_a/E_p calculated by LIXIM was less in spring and summer than in autumn and winter, when it was close to 1. Its mean value for the whole duration of each

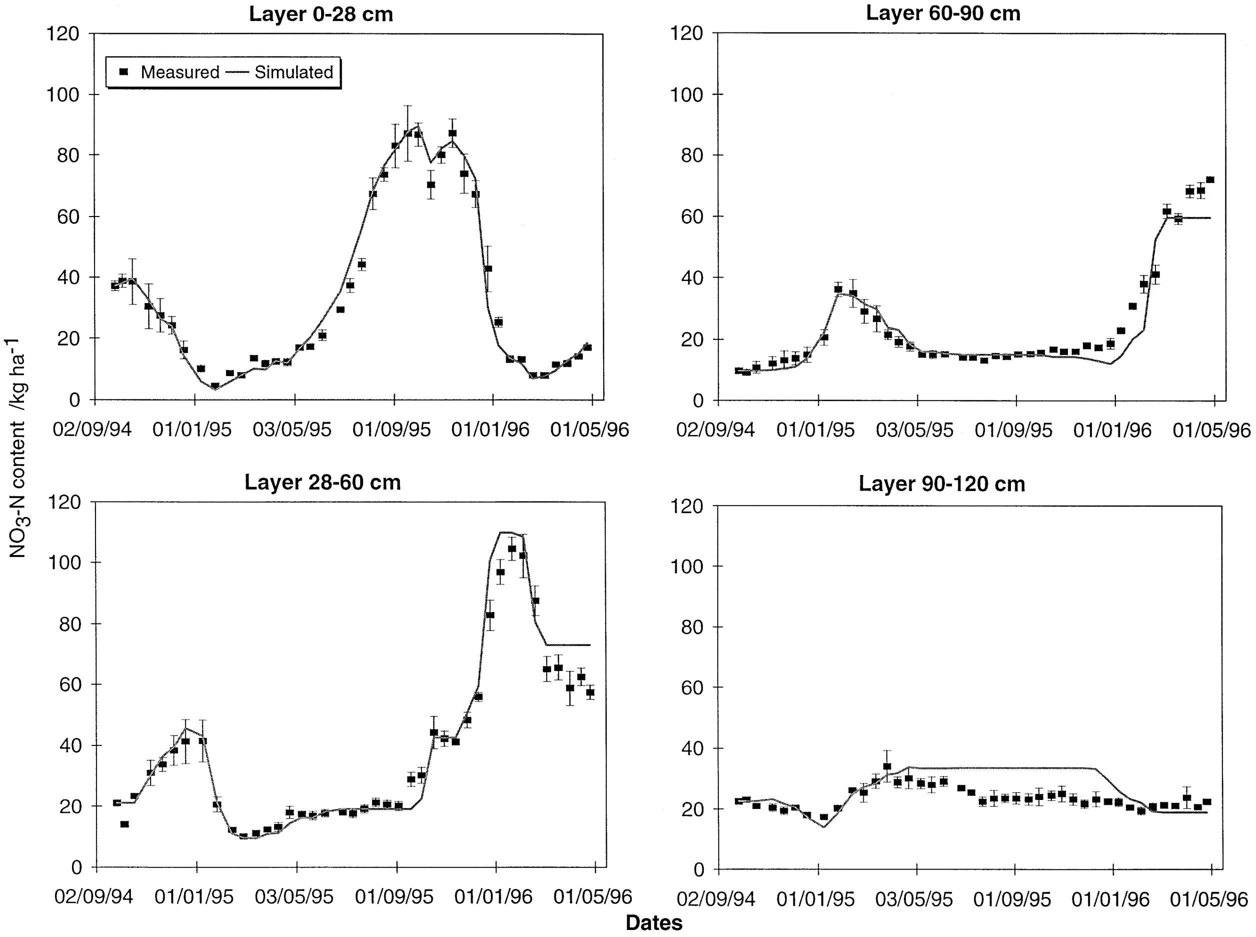

Figure 6 Evolution of observed and simulated nitrate N contents (kg N ha^{-1}) in each of the four measured layers in Experiment 2 (Rafidin 1994–96, B00 treatment). Vertical bars represent standard errors.

treatment varied from 0.45 (BR270) to 0.61 (VR270). The water drainage calculated by LIXIM in the longest experiment B00 could be compared with the lysimeter results obtained in a very similar Rendzina by Ballif *et al.* (1996). Since there was no lysimeter the history of which was exactly identical to the B00 treatment, we took the average of two sets of lysimeters: the one that was permanently fallow, and those that were fallow for 10 months during the winter wheat–sugarbeet succession. The comparison is shown in Figure 7. Good agreement was found, the differences being smaller than the repeatability of the lysimeters. This validated the water balance calculated by LIXIM.

Our results agreed well with the independent calculations made by Leviel *et al.* (1998) on the same experiment during the first year: they calculated an evaporation of 276 mm and a drainage of 341 mm from 27 September 1994 to 28 June 1995. The corresponding values calculated by LIXIM were 293 and 295 mm, respectively.

The N balance in the treatments with oilseed rape residues (BR0 and BR270) is summarized in Table 4. Outputs from LIXIM indicated that net mineralization was less in these treatments than in the soil without residues (B00) in summer and autumn 1995. The decomposition of these residues resulted in net immobilization of approximately 20 kg N ha^{-1} in both treatments during the 4 months following incorporation in 1995 and partial remineralization during the year 1996, in agreement with laboratory incubations (see details in Justes *et al.*, 1999).

The cumulative N mineralization calculated by LIXIM in the soil permanently bare and without crop residues (B00) is plotted against time in Figure 8(a) and against normalized time in Figure 8(b). The kinetics against time show a curvilinear shape with an increased mineralization rate in spring and summer. When expressed against normalized time, the mineralization becomes linear. More precisely, the kinetics are bilinear. During the first phase, between 0 and 52 ndays (normalized days), the mineralization rate was small: $V_p = 0.26$ kg N ha^{-1} nday^{-1} ($r = 0.997$, $n = 9$). During the second phase, 52–274 ndays, the mineralization rate was larger: $V_p = 0.60$ kg N ha^{-1} nday^{-1} ($r = 0.998$, $n = 33$). The first phase with reduced N mineralization is attributed to N immobilization associated with decomposition of the barley crop residues.

The second phase would correspond to decomposition of humified organic matter. We verified that the simulation obtained by imposing these V_p values gave as good results as the previous one.

These field results were then compared with the laboratory incubation data (Figure 8b). Four of the points of the incubation experiment were not statistically different from the field experiment; only on the second date was there any difference. The possibility of extrapolating incubation results to field conditions is therefore demonstrated, as long as the moisture and temperature conditions are well accounted for.

Sensitivity analysis

A sensitivity analysis was done on Experiment 2 (treatment B00) by varying the value of the main parameters (Table 1) within a reasonable range. Five parameters in particular were considered: θ_{fc}, θ_{wp}, Z_e, α and Z_m. The impact of their variation on modelling efficiency is shown in Figure 9(a,b), and the impact on three important variables (drainage, nitrate concentration, mineralization) is represented in Figure 9(c–e).

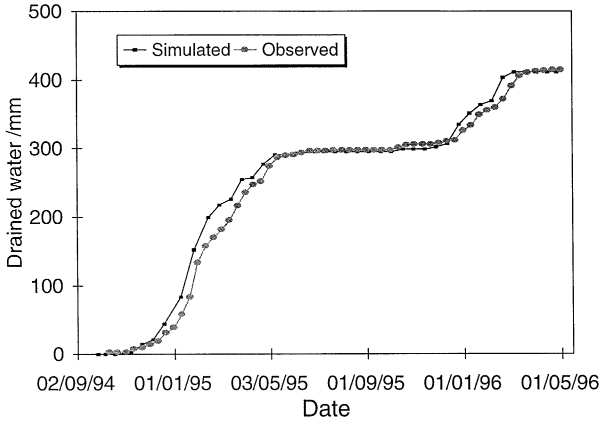

Figure 7 Cumulative amount of drained water against time in Experiment 2 (Rafidin 1994–96, B00 treatment): comparison of values calculated by LIXIM with lysimeter measurements.

The parameter that had the greatest effect on modelling efficiency is θ_{fc}, the water content at field capacity. A 10% reduction in θ_{fc} relative to the nominal value chosen resulted in a bad fit for water content, since modelling efficiency decreased from 0.76 to 0.32. Conversely, a 5% increase reduced the efficiency to 0.47. This parameter exerted a smaller effect on modelling efficiency for nitrogen, but it had the greatest impact on the output variables: drained water, N leached and N mineralized.

The evaporation parameters Z_e and α significantly influenced the modelling efficiency. Their effect was somehow contradictory on the simulation of water and nitrate contents. Increasing the contribution of deep layers to evaporation (by increasing Z_e or reducing α) reduced the quality of fit for water and nitrate, whereas decreasing it improved the simulation of nitrate and worsened the simulation of water. Changing the nominal values had a moderate effect on predicted drained water simulation (Figure 9c) and a very small effect on nitrate concentration and N mineralized (Figure 9d,e).

The parameter Z_m, maximum depth contributing to N mineralization, had a very small effect on water but a significant effect on nitrate simulation. The chosen value (32 cm) was calculated as the ploughing depth increased by about 20% to account for possible mineralization in the deeper layer which contains significant amounts of organic N (Table 2). In fact, reducing Z_m by 20% improved the fit between observed and simulated nitrate contents. A similar result was obtained for Experiment 1 (results not shown). This suggests that only the ploughed layer would contribute to total N mineralization, even though organic N is present below this depth. However, variations in Z_m had little effect on the prediction of drainage, NO_3^- concentration and mineralization.

The parameter θ_{wp}, moisture content at wilting point, had little influence on modelling efficiency, N or water balance. It

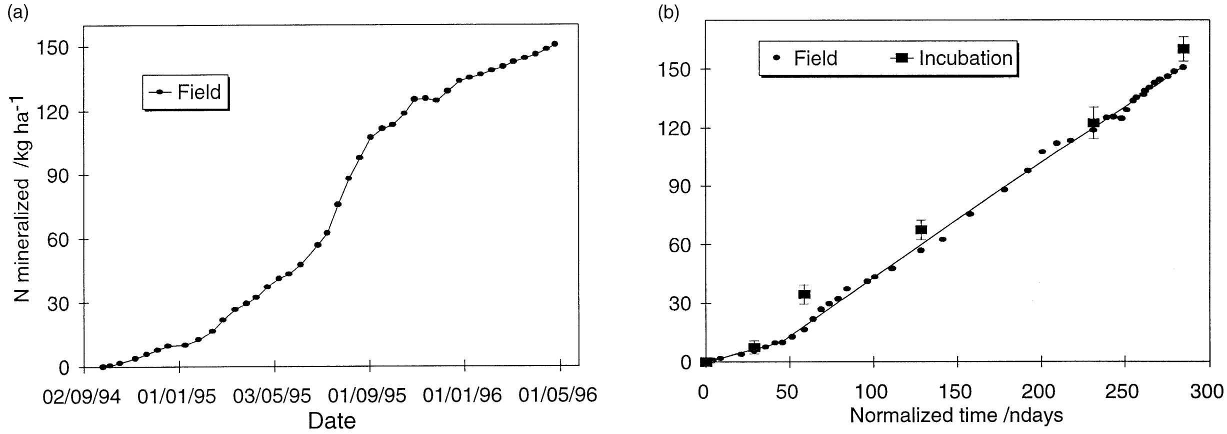

Figure 8 Cumulative amount of N mineralized calculated by LIXIM in Experiment 2 (Rafidin 1994–96, B00 treatment): (a) N mineralized against time; (b) N mineralized against 'normalized time' compared with laboratory incubation data.

also had a very limited effect on the calculation of normalized time: changing θ_{wp} from –20% to +20% would have modified the ndays from +2% to –3%. The parameter c, relative N mineralization rate at wilting point, also affects the calculation of normalized time. The value chosen, 0.20, may be criticized (Rodrigo *et al.*, 1997), but a 50% variation of this parameter results in only a 4% variation in the normalized time.

Discussion

This simple, functional model could simulate correctly the water and nitrate contents within the soil profiles in the two experiments over rather long periods of time. No systematic bias was observed. This result does not necessarily mean that the model is valid. Indeed, compensations could be possible between water evaporation and drainage, or between N

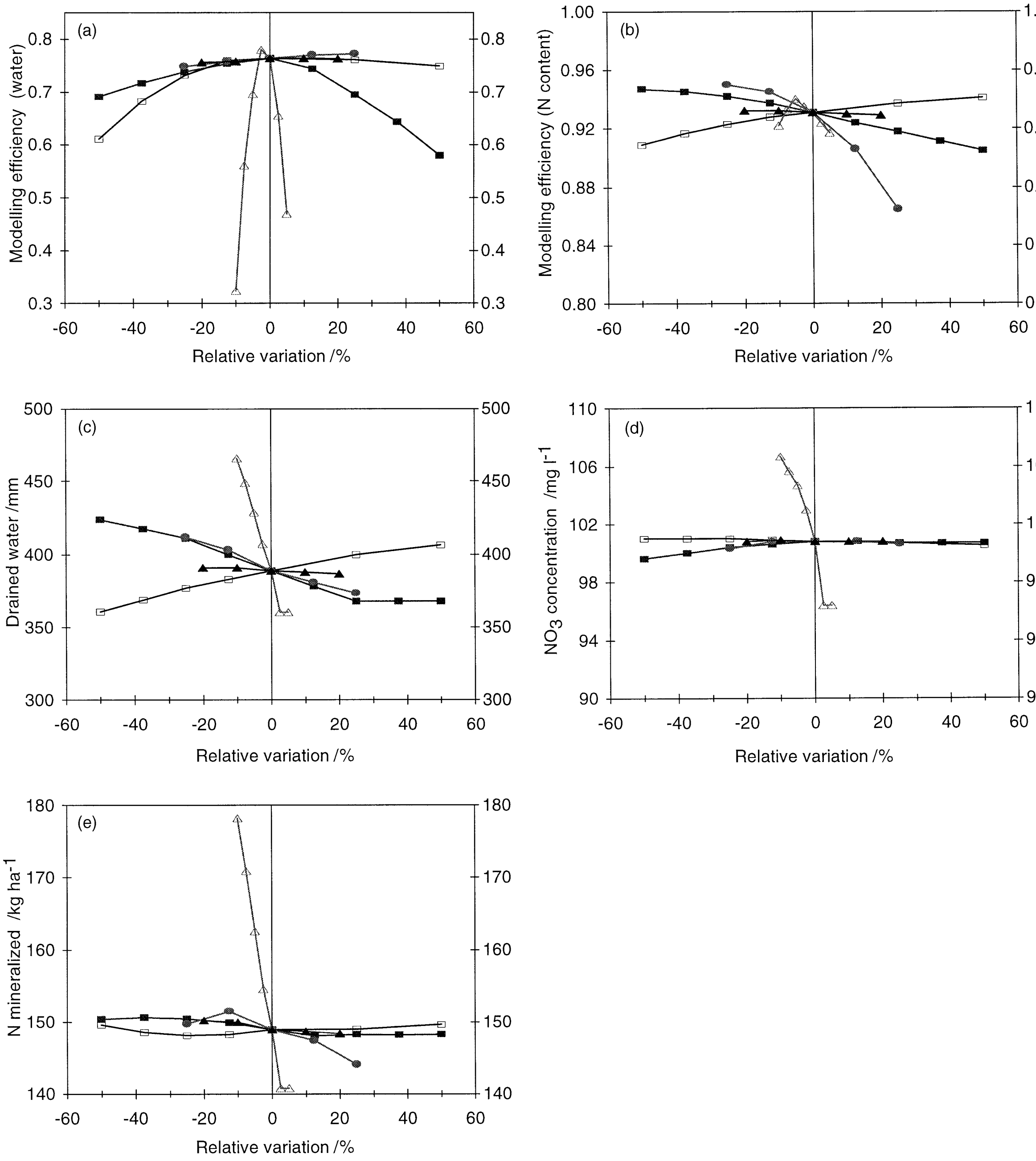

Figure 9 Sensitivity analysis applied to Experiment 2 (Rafidin 1994–96, B00 treatment). Effect of parameter variation on: (a) modelling efficiency for water content, (b) modelling efficiency for mineral N content, (c) total amount of drained water, (d) average nitrate concentration of drained water, and (e) total amount of N mineralized. Symbols: ■, Z_e, thickness of layer contributing to evaporation; □, α, evaporation coefficient; ●, Z_m, thickness of layer contributing to mineralization; △, θ_{fc}, water content at field capacity; ▲, θ_{wp}, water content at wilting point.

mineralization and leaching. However, the simulated evaporation and drainage fluxes were found to agree well with the independent measurements made in Experiment 2. In Experiment 1 the movement of the $^{15}NO_3^-$ tracer was correctly simulated on average, even though the variation of the measurements showed the heterogeneity of solute transport at a local scale. Khanif *et al.* (1984) also found that Burns's model (1974) gave a reasonably good prediction of nitrate profiles in soils during winter.

Concerning solute transport, mechanistic models such as CDE, CLT (convective lognormal transfer model), MIM (mobile–immobile model) or MDM (multiple domain model) can account for physically based phenomena: homogeneous solute dispersion, heterogeneous solute dispersion, anion exclusion volume or by-pass flow, respectively (e.g. Vanderborght *et al.*, 1997). The absence of bias in our simulations suggests that these phenomena were of little importance in our experiments, at least at our field scale. In fact, the outputs from LIXIM are similar to those from the CDE model with a 0.5 cm dispersivity length, since we used a mixing-cell depth of 1 cm in our simulations.

This rather small dispersivity is plausible. Vanderborght *et al.* (1997) found that the dispersivity calculated on undisturbed soil monoliths increased with the water flow rate and varied between 0.6 and 2.7 cm for their smallest flow (5 mm day^{-1}). Ellsworth *et al.* (1996) studied solute transport in field experiments in unsaturated conditions (mean flow rate = 10 mm day^{-1}). They found that the dispersivity varied between 0.4 and 1.0 cm. These flow rates are similar to ours, since the mean flow rate was 4 mm day^{-1} during the days when positive efficient rainfall was recorded in both experiments. In these conditions, the CDE model and the mixing-cells model are equivalent, as shown by Van der Ploeg *et al.* (1995). Slightly larger dispersivities, but less than 5 cm, would not alter the predictions much. Other studies confirmed that mixing-cells models could give a good prediction of solute transport in soil (Van Ommen, 1985; Schoen, 1995).

Mechanistic models are attractive because they can describe all physical processes. Conversely, they are difficult to parameterize and therefore hard to validate (Vachaud *et al.*, 1993). They are useful mainly as research tools. The functional model described here (Burns or mixing cells) is easier to parameterize and could predict the evolution of nitrate within the profile rather well.

The sensitivity analysis indicated that water content at field capacity θ_{fc} was the most important parameter to be tuned. Our method of calculation, i.e. taking the mean of the largest measurements after removing the extreme values, appeared satisfactory since it gave the greatest modelling efficiency for water. The high sensitivity of modelling efficiency to θ_{fc} is a chance to find rapidly the optimal value in a given experiment. However, an independent method for determining this parameter would be preferable. In their review, Cassel & Nielsen (1986) indicated that 'there is no good alternative for measuring θ_{fc} other than the *in situ* field method'. But they also stated that 'measurements made on disturbed soil samples subjected to a given soil water pressure correlate with *in situ* field capacity measurements'. Several authors have suggested using a –5 to –10 kPa water potential for coarser-textured, –33 kPa for medium-textured and –50 kPa for finer-textured soils, though in many soils the water pressure at *in situ* field capacity is near the –10 kPa value, and this is what we have found. In the loamy soil (Experiment 1), θ_{fc} was 0.322 cm^3 cm^{-3}, and a similar matrix potential (–8 to –15 kPa) could be calculated from the retention curves established on a nearby field. In the Rendzina (Experiment 2), θ_{fc} had been estimated at 0.345 cm^3 cm^{-3}. Tensiometric measurements made in the field showed that this corresponded exactly to –10 kPa water potential (Leviel *et al.*, 1998).

The other parameters (Z_m, Z_e and α) have much less influence on the efficiency and the outputs of the model (Figure 9) and therefore do not require to be tuned very precisely. Once all these parameters have been fixed, one must examine the quality of fit between observed and simulated values of water and nitrate contents in the soil profile. If no satisfactory agreement is found then the model must be rejected: this can result either from the poor quality of N measurements or their large variation, or to the inadequacy of the model itself. The latter case may reflect problems in simulating water flow (evaporation), solute transport (e.g. preferential flow), or unaccounted processes (e.g. denitrification).

If a good agreement is found, as in our experiments, then one can trust the mineralization and leaching estimates of the model. We obtained consistent mineralization results showing immobilization of N associated with crop residues decomposition and regular, monotonic mineralization kinetics in soil without crop residues. The two types of kinetics found in field conditions are also encountered in laboratory incubations: for example, linear kinetics were reported by Addiscott (1983), whereas first-order kinetics were found by Stanford & Smith (1972). The difference could result from the fact that linear kinetics approximate the first order if the cumulative amount of mineralized N is small. Indeed a smaller proportion of the total organic nitrogen (N_{org}) was mineralized in the chalky than in the loamy soil at the end of the experiments: the respective amounts were 2.15% and 3.77%, although the normalized time was the reverse: 278 and 137 ndays, respectively. In fact, comparing the two kinetics until the same amount of N is mineralized (2.15%) shows that they do not differ significantly from linearity (Figure 10). The regression line can be written as

$$\frac{M}{N_{org}} = at_n, \tag{26}$$

or, using Equation (18),

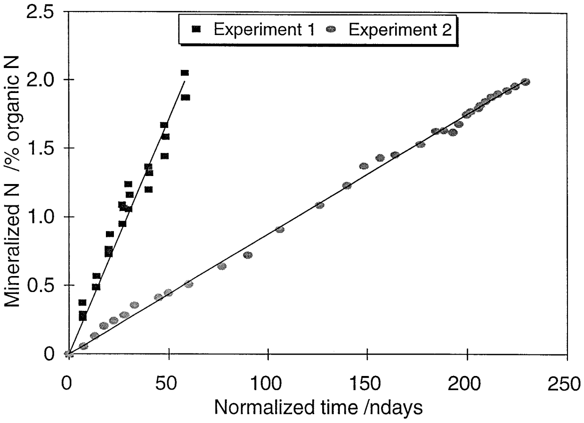

Figure 10 N mineralized in proportion of total soil organic N against normalized time in the two soils (treatments where crop residues were removed). Experiment 1: treatments D0, R0 and M0. Experiment 2: treatment B00. The immobilization phase found in Experiment 2 has been removed (0–52 ndays). The values of Experiment 1 have been limited to the maximum value found in Experiment 2, i.e. $M/N_{\mathrm{org}} = 2.2\%$.

$$V_{\mathrm{p}} = aN_{\mathrm{org}}. \tag{27}$$

The slope a is the specific mineralization rate. Its value differed greatly between the two soils: 0.87×10^{-4} nday^{-1} in the chalky soil and 3.4×10^{-4} nday^{-1} in the loamy soil. The much smaller value in the chalky soil is attributed to the protective effect of fine $CaCO_3$ on organic matter decomposition (Muller & Védy, 1978; Delphin, 1986). The model can be used in similar experiments (bare soils without crop residues) to characterize the specific mineralization rate which is thought to depend mainly on soil texture.

Another interesting feature of the model is to allow comparison between field and laboratory mineralization, using exactly the same temperature and moisture functions. Results obtained in Experiment 2 indicated that laboratory incubation data could be extrapolated to field conditions. The immobilization of N was found in both situations during the first 50 ndays and could be attributed to the decomposition of barley residues with a rather large C:N ratio. These results will have to be confirmed in other field experiments. Notice that they are highly dependent on the temperature function adopted, since the incubation was made at a higher temperature (28°C) than the reference temperature (15°C) which was itself more than the annual mean soil temperature (9.5°C). For example, using a coefficient $Q_{10} = 2.00$ (e.g. Stanford *et al.*, 1973) instead of our value $Q_{10} = 3.17$ would have overestimated the *in situ* mineralization by 80%.

The model has been applied with success to various agricultural conditions to calculate N mineralization from agro-industrial wastes (Justes *et al.*, 1998) and N leaching at the catchment scale (Mary *et al.*, 1997). It can also be used in a purely predictive mode when the rates of evaporation and the mineralization are known. So far it has been included in a management-oriented soil–plant simulation model called STICS (Brisson *et al.*, 1998) which aims to simulate water and nitrogen at the field and regional scale. In their review of models, Vachaud *et al.* (1993) and Addiscott (1995) indicated that this type of capacity model has modest requirements for input data, most of which can be obtained independently of the test data. They mention that capacity parameters are much less variable spatially than rate parameters which gives them an advantage for large areas and makes them potentially well adapted for management purposes.

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