

Modelling the fate of nitrogen in crop and soil in the years following application of ^{15}N -labelled fertilizer to winter wheat

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(Revised MS received 18 January 1993)

SUMMARY

A computer model is presented that describes the flow of nitrogen between crop and soil on the field scale. The model has a compartmental structure and runs on a weekly time-step. Nitrogen enters via atmospheric deposition and by application of fertilizer or organic manures, and is lost through denitrification, leaching, volatilization and removal in the crop at harvest. Organic nitrogen is contained within three of the model compartments – crop residues (including plant material dying off through the growing season), soil microbial biomass and humus. Inorganic nitrogen is held in two pools as NH_4^+ or NO_3^- . Nitrogen flows in and out of these inorganic pools as a result of mineralization, immobilization, nitrification, leaching, denitrification and plant uptake. The model requires a description of the soil and the meteorological records for the site – mean weekly air temperature, weekly rainfall and weekly evapotranspiration. The model is designed to be used in a ‘carry forward’ mode – one year’s run providing the input for the next, and so on. The model also allows the addition of ^{15}N as labelled fertilizer, and follows its progress through crop and soil. Data from a Rothamsted field experiment in which the fate of a single pulse of labelled N was followed over several years were used to set the model parameters. The model, thus tuned, was then tested against other data from this and two contrasting sites in south-east England. Over a period of 4 years, the root mean square (R.M.S.) difference between modelled and measured quantities of labelled N remaining in the soil of all three sites was *c.* 7.5 kg N/ha, on average. The root mean square error in the measurements was *c.* 2.5 kg/ha. Similarly, the R.M.S. difference between modelled and measured recovery of labelled N by the crop was 0.6, compared with 0.3 kg/ha in the measurements themselves.

INTRODUCTION

In this paper, the behaviour of ^{15}N -labelled fertilizer nitrogen applied in spring to winter wheat is modelled, both in the year of application and in succeeding (‘residual’) years. The model was tuned using the data from the preceding paper (Hart *et al.* 1993), which presents the results from field applications of ^{15}N -labelled fertilizer to winter wheat, grown continuously in three sites for a number of years. The labelled fertilizer was applied once only and the fate

of the labelled N remaining in the soil at harvest then followed for several years in the soil and in subsequent crops. Such data are particularly useful in developing and tuning models because the model has to mimic the behaviour of both labelled and unlabelled N, a much more stringent test than if unlabelled N alone was used.

In modelling the N cycle, the representation of processes and the choice of parameters and inputs will vary according to the intended use of the model. Some models aim to examine the overall effects of management practices on carbon and nitrogen flow through the whole soil/plant/animal system (Thornley & Verberne 1989), or on long-term changes in soil nitrogen dynamics (Wolf *et al.* 1989). Others provide a complete nitrogen balance for a particular system (Aslyng & Hansen 1985) or concentrate on mineral nitrogen (Verbruggen 1985; Addiscott &

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Whitmore 1987). Several authors have developed their models to provide fertilizer recommendations (Neeteson *et al.* 1987; Richter *et al.* 1988). A detailed examination of current models for the behaviour of N in the crop/soil system has recently been published: 14 different models were compared, all running on the same data set (Groot *et al.* 1991).

Our philosophy in constructing the model was to make sure it dealt with *all* the major processes affecting the behaviour of N in the cereal/soil system, even though each individual process is expressed in greatly simplified form. As far as possible, the model is modular in structure; if a particular module, for example that representing leaching, proves unsatisfactory at a later stage, it can be replaced by a more sophisticated module without rewriting the whole model. A central feature is that the model is designed to be used in a 'carry-forward' mode. It is constructed and tuned so that it does not, for example, allow soil organic N to build up to unrealistic levels, however long it is run. Needless to say, it has many ideas in common with other contemporary N models, particularly with SOILN (Bergstrom *et al.* 1991), ANIMO (Rijtema & Kroes 1991), DAISY (Hansen *et al.* 1991) and NCSOIL (Molina *et al.* 1983).

Some features of this paper may seem strange without reference to our long-term aim. The model described here is designed to be part of a system specifying how much fertilizer N is required to grow a particular crop in a particular field in a particular

year and when this N should be applied. This specification is to be made in early spring, from the farmer's estimated target grain yield. This is why, for example, N uptake is specifically related to grain yield (Eqn (11)), rather than to other plant or soil measurements.

STRUCTURE OF THE MODEL

Compartments

The model has 13 compartments in all, as shown in Fig. 1. Five of these are transformation compartments, into and out of which N flows: the nitrate-N compartment, the ammonium-N compartment, the plant-N compartment (which contains all the N taken up by the crop, including that in roots), the BIO compartment, which comprises the N in the soil microbial biomass and, lastly, the HUM compartment, which contains the N in the soil humus (Fig. 1). That part of the plant-N compartment returned to the soil is termed the RO compartment, which therefore includes N in dead roots, root exudates, plant debris shed during the growth of the crop, chaff and stubble. If straw is returned to the soil, the N it contains will also enter the RO compartment, although this possibility will not be considered further in this paper, as straw was removed in all the experiments described by Hart *et al.* (1993). There are three input compartments: chemically combined N from the atmosphere,

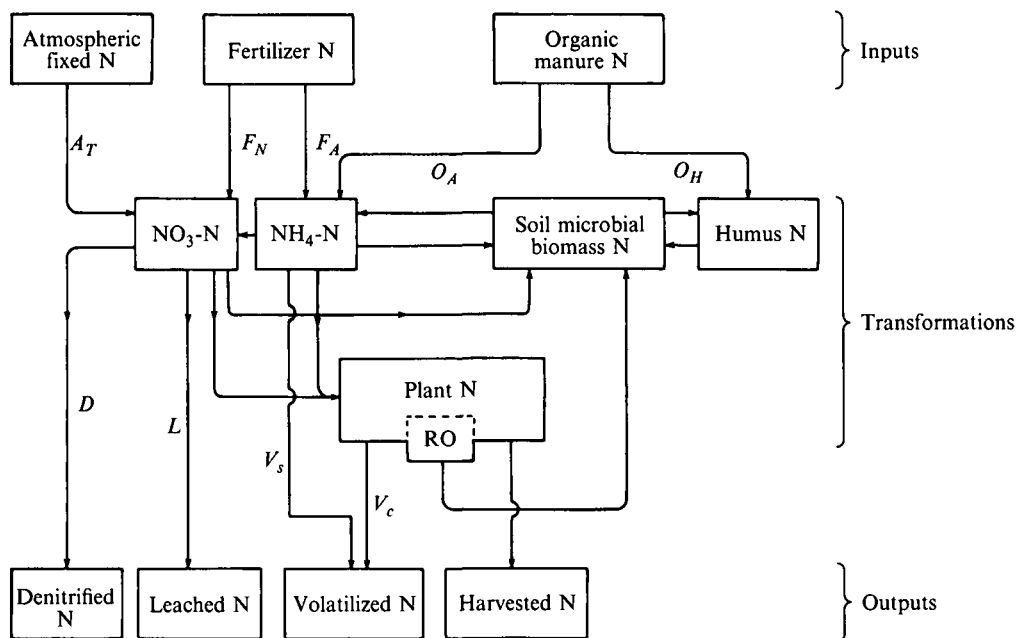


Fig. 1. Flow diagram for nitrogen in the model. RO is the portion of the plant N returned to the soil each year: it may or may not include straw N.

inorganic fertilizer N (which can enter as nitrate, or ammonium, or both), and N in organic manures, part (O_A) of which enters the ammonium compartment and part (O_H) the humus N compartment. Again, inputs of organic N will not be considered further in this paper, since organic manures were not used by Hart *et al.* (1993). There are four output compartments: denitrified N, leached N, volatilized N and harvested N, which contains the N in grain, plus that in the straw, if the straw is burnt or removed. The model runs in weekly steps: at the end of a week, the N content of each compartment is updated on the basis of the flows of N into and out of that compartment during the week.

Soil layers

The model divides the soil profile into four layers; 0–25, 25–50, 50–100 and 100–150 cm. Rooting below 150 cm is ignored. The top two layers are each subdivided into five slices, each 5 cm in thickness. Eighty percent of the soil organic matter (and of each year's input of fresh organic matter) is assumed to be evenly distributed in the 0–25 cm layer: the remaining 20% evenly throughout the 25–50 cm layer. Mineralizable organic matter, microbial biomass and root dry matter are all assumed to be negligible below 50 cm, although roots (if present) can take up water (and nitrate) to a depth of 150 cm.

Weather data

Weekly mean temperature, rainfall and evapotranspiration were taken from the records of the local weather stations at Rothamsted, Woburn and Saxmundham.

Movement of water through the soil

The available water holding capacities (AWHC) of the three soils are given in Table 1. Only 50% of the AWHC in the 50–100 cm layer and 25% of the AWHC in the 100–150 cm layer is deemed to be used by the winter wheat (Weir 1988). Water enters the soil from the top. With the exception noted below, leaching occurs as a 'piston flow' process, water successively filling each layer down the profile, before draining to the layer below. Soil water is subject to evapotranspiration after any filling by rainfall or drainage has occurred. Evapotranspiration (taken as the meteorological data for evaporation over grass in that particular week) takes place successively from layers down the profile as the upper layers are emptied. If the soil is bare, only the top 5 cm slice loses water: once this slice is emptied of water, no further loss occurs (i.e. there is no upward movement of water from below). An alternative to 'piston flow' (bypass flow, see Addiscott & Whitmore 1991) is

Table 1. *Water relationships for the Rothamsted, Woburn and Saxmundham soils*

Soil layer (cm)	Available Water Holding Capacity* (mm)		
	Rothamsted	Woburn	Saxmundham
0–25	45 (20)†	30 (20)	45 (20)
25–50	45 (20)	30 (20)	45 (20)
50–100	60	30	60
100–150	60	30	60

* AWHC (ψ_f) is taken to be the water held between Field Capacity and -15 bar. The data are rounded values based on work by Salter & Williams (1969), Hodge (1972), Hall *et al.* (1977) and French & Legg (1979).

† Values in parentheses are for water held between Field Capacity and -1 bar (ψ_r).

allowed if the rainfall in a particular week exceeds a specified threshold value (R_{CRT}). The rules governing N loss by bypass flow are specified in the section on leaching of nitrate.

The part of the model concerned with soil moisture starts in the first week of January of the crop year prior to that for which the simulations are being made, at which time the soil moisture deficit (SMD) is assumed to be zero. Each week thereafter the water balance is updated by adding the rainfall and subtracting evapotranspiration for that week.

INPUTS OF NITROGEN IN THE MODEL

Crops receive chemically combined N from seed, rain, dry deposition, symbiotic and non-symbiotic fixation. The total of these inputs (A_T , kg N/ha/week), is set at 0.8 kg N/ha/week, a value derived from work on N inputs to the Broadbalk Continuous Wheat Experiment (Powlson *et al.* 1986). For simplicity, it is assumed to be distributed evenly throughout the year and to be exclusively in the nitrate form, although the model can handle other inputs. Fertilizer can be added in any week and can be nitrate (F_N , kg N/ha) or ammonium (F_A , kg N/ha) or both, in any proportion.

NITROGEN TRANSFORMATIONS IN THE MODEL

Priorities for N transformation

For the model to work, certain priorities must be specified. These are, for ammonium:

immobilization > nitrification > plant uptake

For nitrate the priorities are:

immobilization > denitrification > plant uptake > leaching

Ammonium is immobilized in preference to nitrate and nitrification must perforce occur before denitrification. Crops are assumed to take up nitrate and ammonium impartially. Field measurements show that soil profiles are rarely completely depleted of mineral N, so a minimum N content is set, below which mineral N is unavailable to any process. This minimum level (N_{RESA} for ammonium N and N_{RESN} for nitrate N), depends on soil type.

Nitrification

Ammonium N enters the soil in two ways: from mineralization of soil organic N (M kg N/ha/week in a specified soil layer) and from ammoniacal fertilizers (F_A kg N/ha). It is then nitrified by a first-order process (disregarding the nitrite intermediate), according to the equation:

$$P = N_A(1 - e^{-smq}) \quad (1)$$

where P is the quantity of nitrate formed in one week, in kg $\text{NO}_3\text{-N/ha}$; m is the temperature rate modifier (see Eqn (3) below); s is the soil moisture rate modifier (see Eqn (4) below); q is a rate constant (set provisionally at 0.6/week, by fitting Eqn (1) to Addiscott's (1983) data); and N_A is the quantity of ammonium present in the soil layer (in kg $\text{NH}_4\text{-N/ha}$) at the beginning of the week. This treatment assumes that the soil always contains sufficient nitrifiers for nitrification to proceed according to Eqn (1); this may not be true in the period immediately after addition of

large quantities of fertilizer N, when nitrification may well be of zero order.

Decomposition of organic matter

The model first simulates the decomposition of organic carbon as it moves through the various compartments and then calculates the nitrogen content of these compartments from the appropriate C:N ratios. Although this procedure has the disadvantage that C inputs from roots (and the distribution of these inputs throughout the year) are not well known, it has the great advantage that it allows substrate-driven processes such as denitrification and immobilization to be modelled in a very direct way.

A three-compartment model, based on that described for N by Jenkinson & Parry (1989) is used to simulate decomposition of organic C in soil (Fig. 2). The carbon in the RO compartment, which includes stubble, chaff and straw (if straw is not removed or burnt) decomposes to give microbial biomass (in compartment BIO), humus (in compartment HUM) and CO_2 by a first-order process with rate constant r /week. The material in the BIO compartment decomposes in turn, to give further BIO, HUM and CO_2 , by a first-order process with rate constant b /week. Humus in the HUM compartment decomposes likewise, with rate constant h /week, to give BIO, more HUM and CO_2 . Carbon undergoing decomposition in all three of these compartments is converted to BIO in fraction α , to HUM in fraction β and to CO_2 in fraction $(1 - \alpha - \beta)$.

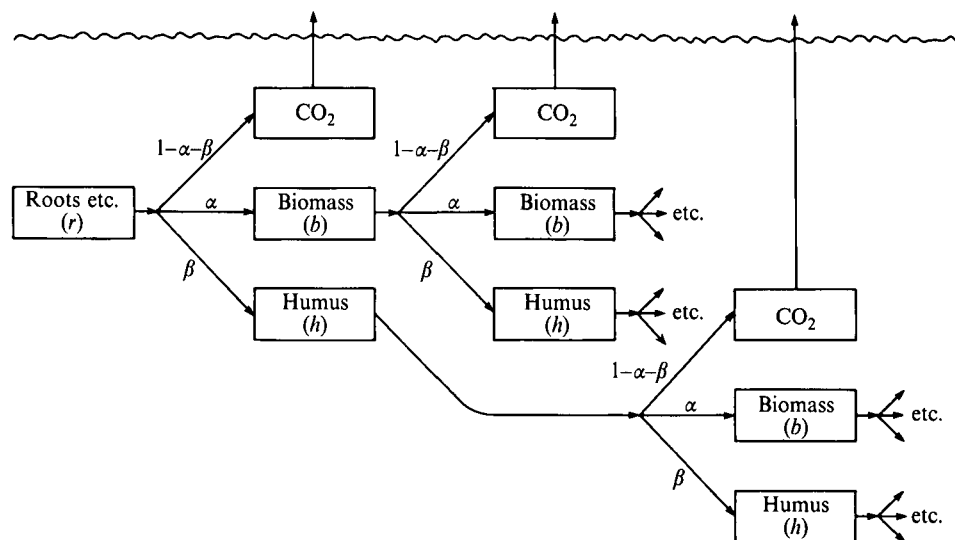


Fig. 2. Scheme for the decomposition of organic carbon in soil. Rate constants for the different compartments are given in parentheses: α is the fraction of incoming substrate converted to soil microbial biomass carbon (BIO) and β the fraction to humus carbon (HUM).

All three rate constants are modified to allow for the actual temperature and soil water content of the soil during the particular week in question, using the relationship:

$$\text{Decomposition in unit time (1 week)} = C_o(1 - e^{-smr}) \quad (2)$$

where C_o is the amount of material present in compartment RO at the beginning of the week, m is the temperature rate modifying factor and s the moisture rate modifying factor. Similar relationships are used for BIO and HUM.

The relationship used to establish m is:

$$m = 47.9 / (1 + e^{106/(T+18.3)}) \quad (3)$$

where T is the mean air temperature for the relevant week in °C (Jenkinson *et al.* 1987).

The rate constant modifier (s) for soil moisture content is obtained from the relationship

$$s = 1 - (1 - s_o)(\psi_c - \psi_i) / (\psi_f - \psi_i) \quad (4)$$

where s_o is the rate modifier at -15 bar, ψ_c is the calculated deficit in a particular soil layer, ψ_i is the deficit in that layer at -1 bar (as given in Table 1) and ψ_f is the available water holding capacity of the layer (again as given in Table 1). If $\psi_c < \psi_i$, then $s = 1$. In this treatment, we assume that decomposition proceeds at its maximum rate as the soil dries from Field Capacity to -1 bar, but then slows until the soil is at -15 bar (AWHC being defined as the water held between Field Capacity and -15 bar), at which stage it is running at 60% of the maximum rate (i.e. $s_o = 0.6$). Soils are not allowed to dry to more than -15 bar. This value for s_o is set from measurements of the effects of moisture on N mineralization made by Stanford & Epstein (1974). Taking a mean of all their nine soils, the ratio for (mineral N accumulated at -15 bar)/(mineral N accumulated at -0.3 bar) was 0.59.

Soil texture also influences the turnover of organic C and N in soil. The effects of texture are handled in a special way in the model: the fraction of the incoming substrate converted to CO_2 decreases as clay content increases. The ratio ($\text{CO}_2 - \text{C}$ formed per unit substrate decomposed)/(BIO-C + HUM-C formed per unit substrate decomposed) is $(1 - \alpha - \beta) / (\alpha + \beta)$, with α and β defined as above. Then:

$$(1 - \alpha - \beta) / (\alpha + \beta) = 0.714(1.85 + 1.60 e^{-0.0786K}) \quad (5)$$

where K is the % clay ($< 2 \mu\text{m}$) in the 0–50 cm layers. For soils, such as that at Rothamsted, in which there is a sharp change in texture just below the plough layer, the clay content of the plough layer is used instead. The part of this relationship inside the bracket on the right-hand side of the equation is based (see Jenkinson *et al.* 1987) on Sorensen's (1975) experiments on the decomposition of ^{14}C -labelled

cellulose in soils of different texture. A value of 0.4 was selected by iteration for $(\alpha + \beta)$ in Rothamsted soil during the fitting of the model parameters (see below), giving a ratio of 1.5 for $(1 - \alpha - \beta) / (\alpha + \beta)$. A scaling factor of 0.714 was then necessary to balance Eqn (5) for Rothamsted soil (23.5% clay). Using the same scaling factor (0.714) and taking the clay content of the 0–50 cm layer at Woburn to be 10%, gives a value of 0.35 for $(\alpha + \beta)$: the corresponding value for Saxmundham (40% clay) is 0.42.

Annual return of organic C and N to the soil from the crop

Material enters RO in two ways: from stubble and chaff at harvest (and straw, if it is incorporated), and from dead roots, root exudates and other plant debris returned to the soil during the growing season. The overall return of C (in dead roots, root exudates, stubble and chaff) to the soil is calculated as:

$$C_{Ao} = 1.25 [1 + 1.12 (1 - e^{-0.22G})] \quad (6)$$

where C_{Ao} is annual return of C to the soil (in t/ha) and G is grain yield (in t/ha) at 85% dry matter. This relationship is based on estimates of the annual return of organic C to the top 25 cm of soil by wheat at Rothamsted (Jenkinson *et al.* 1987). The scaling factor 1.25 allows for carbon returned to the 25–50 cm layer. Equation (6) will slightly overestimate the return of C in Hart *et al.*'s (1993) work, where chaff was removed from the central (harvested) areas of the ^{15}N microplots. All three sites used by Hart *et al.* (1993) have long been arable and it is unlikely that large changes in soil organic matter content were occurring in any of them during the period the ^{15}N experiments were under way. The relationship between the yield of the crop and the amount of C in stubble and chaff is taken to be:

$$C_{sc} = 1.4 (1 - 0.96 e^{-0.165G}) \quad (7)$$

where C_{sc} is stubble + chaff carbon (in t/ha) and G is grain yield (in t/ha) as above. Equation (7) is based on data on grain yields and on the amounts of C in stubble and chaff, as given by Powlson *et al.* (1986).

The overall return of N (in dead roots, root exudates, dead tillers, stubble and chaff) is given by

$$N_{Ao} = \text{N returned in roots, root exudates and dead tillers} + \text{N returned in chaff and stubble} \\ = 60 (1 - e^{-0.5G}) + 0.12 (U_G + U_S) \quad (8)$$

where N_{Ao} is the annual return of N to the soil (in kg/ha), G the grain yield (in t/ha), U_G is N in grain at harvest and U_S is N in straw, chaff and stubble. The term $60 (1 - e^{-0.5G})$ was obtained by fitting grain yields to estimates of N returned to the soil in roots, root exudates and dead tillers from five field experiments done at Rothamsted in which ^{15}N labelled nitrate was

applied to winter wheat (Powlson *et al.* 1986, 1992). In these experiments, root N, root exudate N and N in dead tillers was taken as (labelled organic N in soil at harvest) \times (total N in stubble)/(labelled N in stubble). The term $0.12(U_G + U_S)$ is the N returned in chaff and stubble; likewise set from field experiments with labelled fertilizer (Powlson *et al.* 1986).

Stubble and chaff C (and N) are added to the RO pool at harvest. To estimate the amounts of C in plant roots and debris, the calculated amounts of C in stubble and chaff are subtracted from the total C (as given by Eqn (6)) returned during the year.

The return of roots and plant debris to RO during the growing season is distributed as follows:

$$C_c = (C_{AO} - C_{sc})e^{-c(w-g)} \quad \text{for carbon} \quad (9)$$

$$\text{and } N_c = (N_{AO} - N_{sc})e^{-n(w-g)} \quad \text{for nitrogen} \quad (10)$$

where C_c and N_c are the cumulative C and N inputs up to the current (gth) week; C_{sc} and N_{sc} are stubble + chaff C and N; c and n are rate constants; and w is the number of weeks between sowing and harvest.

By altering the relative rates of return of C and N, some manipulation of the C:N ratio of plant material entering RO is possible. Following validation of the model (see below), c and n were set to 0.15 and 0.10 respectively. Thus shortly after sowing, the C:N ratio is very narrow (perhaps 5:1 for roots that die early in the development of the crop), and it widens gradually up to harvest, when it might be over 70:1.

Plant uptake of N

The quantity of N required to grow the crop includes that in the grain (U_G) and in the straw, stubble and chaff at harvest (U_S), plus the N present in roots at harvest, plus any N returned to the soil during growth, in dead tillers, dead roots, root exudates, etc. Where U_G and U_S are known (as in Hart *et al.*'s 1993 experiments), U_m , the target crop requirement, in kg N/ha, is given by

$$U_m = (1 + \phi_c)(U_G + U_S) + 60(1 - e^{-0.5G}) \quad (11)$$

where G is the grain yield (in t/ha) as before and ϕ_c is the N lost by volatilization during crop senescence, expressed as a fraction of the above-ground crop N at harvest (see Eqn (18)). The term $60(1 - e^{-0.5G})$ gives the N in roots at harvest, plus N previously returned to the soil in dead tillers etc: as has already been defined (Eqn (8)).

If the above-ground uptake of N in Eqn (11) is not known, another version of this equation is used:

$$U_m = (1 + \phi_c)230(e^{0.075G} - 1) + 60(1 - e^{-0.5G}) \quad (12)$$

In Eqn (12), both above-ground and below-ground uptakes of N are related to grain yield. The term $230(e^{0.075G} - 1)$ was derived empirically by fitting

measured uptake of N in grain and straw to grain yield from seven field experiments on winter wheat at Rothamsted (Powlson *et al.* 1986, 1992). Each experiment tested a range of N applications: all were protected against weeds, foliar disease and insect pests.

The time course of nitrogen uptake

This is calculated by the equation proposed by Whitmore & Addiscott (1987). The N taken up by a particular time is given by:

$$U = (U_m^{-1/p} + e^{-fd})^{-p} \quad (13)$$

where U is cumulative crop uptake of N (in kg/ha); U_m is final N target of crop (in kg/ha); p is a shape factor, which relates the rate of uptake to the point of inflection of the uptake curve; d is cumulative week-degrees since sowing; and f is a rate constant.

Note that f is set during the iterative parameter fitting process (see below), not as calculated by Whitmore & Addiscott (1987). The value assigned to f governs the 'take off' of N uptake in spring; a value greater than that set for the Rothamsted ^{15}N experiments (0.004) should be used for a 'forward' crop, a value less than this for a 'backward' crop.

The rules for uptake of N by plants are:

- (1) There is no uptake before sowing, or when the mean weekly air temperature is $< 0^\circ\text{C}$.
- (2) Crops can only deplete each 50 cm soil layer to the specified minimum of $\text{NH}_4\text{-N}$ (N_{RESA}) and of $\text{NO}_3\text{-N}$ (N_{RESS}) for each soil type.
- (3) Crops deplete each layer of $\text{NO}_3\text{-N}$ and $\text{NH}_4\text{-N}$ before abstracting N from the layer below.
- (4) Root growth occurs at a rate of 5 cm/week, starting from the date of sowing.
- (5) To allow time for roots to explore the lower two layers, they must reach a depth of 75 cm before starting to deplete the 50–100 cm layer, and to 125 cm for the 100–150 cm layer. They terminate at 150 cm in the three soils used by Hart *et al.* (1993).
- (6) Uptake stops 5 weeks before harvest.

Mineralization of organic N and immobilization of inorganic N

The rules for the behaviour of organic N are obtained directly from those for organic C (see section above; Decomposition of Organic Matter), by setting C:N ratios for the various compartments. For simplicity, the BIO and HUM compartments are both assumed to have the same C:N ratio (set at 8.5) and both C and organic N are mineralized from these compartments in this ratio. This value is a mean of the C:N ratio proposed by Jenkinson (1988) for microbial biomass in arable soils (6.7) and that of soil organic matter in the 0–23 cm layer of the Broadbalk plots receiving N (10.2). The BIO and HUM compartments,

both relatively rich in N, each decompose at their characteristic (but different) rates, whether or not the inorganic-N compartments are empty.

The rules for mineralization of N from the RO compartment are more complex, because its C:N ratio depends on that of the input and the compartment may be deficient in N. Let the reciprocal of the C:N ratio of the BIO and HUM compartments be x ($= 1/8.5$) and that of the RO compartment during the current week be z . During unit time (1 week), the gross release of N from this compartment will be $zC_o(1 - e^{-smr})$. However, part of this gross release will have been built into new BIO ($= x\alpha C_o(1 - e^{-smr})$) and part into new HUM ($= x\beta C_o(1 - e^{-smr})$). If $z > x(\alpha + \beta)$, then there is a net release of N during the decomposition of RO; if $z = x(\alpha + \beta)$ there is no flow out of or into the decomposing RO compartment and if $z < x(\alpha + \beta)$, N is immobilized, first from the ammonium-N compartment and then from the nitrate-N compartment. If both soil mineral N compartments become empty during any week, the model retraces its steps and makes $r = 0$ for that week, stopping decomposition of the RO compartment alone, until mineral N reappears.

OUTPUTS OF NITROGEN FROM THE CROP/SOIL SYSTEM

Leaching of nitrate

Nitrate is assumed to be infinitely soluble in water and to move downwards at the same rate as the water in which it is dissolved. Ammonium N is not leached, nor is any form of organic N. Nitrate is not allowed to move by diffusion to zones of lower nitrate concentration. If the soil is not at field capacity, incoming rainfall (R_w) fills each soil layer from the top down until it is. When nitrate is leached from a layer, the amount of nitrate N moving into the layer immediately below is given by an expression for simple 'piston flow':

$$L = N_N R / R_{FC} \quad (14)$$

where L is the amount of $\text{NO}_3\text{-N}$ moving into the layer below, N_N is the amount of $\text{NO}_3\text{-N}$ in the layer, R is excess water entering the layer (in mm), over and above that needed to saturate it, and R_{FC} the amount of water held in the soil layer at field capacity (also in mm). A small quantity (N_{RESN}) of $\text{NO}_3\text{-N}$ in each of the 0–50, 50–100 and 100–150 cm layers is never leached; N_{RESN} depends on soil type.

Fertilizer $\text{NO}_3\text{-N}$ can be lost by bypass flow (or by surface runoff: both processes are modelled in the same way) in the 3 weeks after fertilizer addition. Lawes *et al.* (1882) showed that fertilizer N moves rapidly to the Broadbalk drains if fertilizer application is followed by heavy rain. Losses by bypass flow diminish as fertilizer N moves away from the surface

and into the soil fabric. The quantity thus lost is calculated from the relationship

$$L_B = \sigma \epsilon F_N (R - R_{CRIT}) \quad (15)$$

where L_B is the amount of fertilizer $\text{NO}_3\text{-N}$ leached by bypass flow, σ is the bypass flow factor per mm excess rain, F_N is the quantity of fertilizer $\text{NO}_3\text{-N}$ originally added, R is weekly rainfall, R_{CRIT} the level of rainfall above which bypass flow takes place and ϵ is the fraction of F_N at risk during a particular week. The value of ϵ is set at 1 for the week during which the fertilizer is applied, at 0.67 during the following week, 0.33 for the next week and zero thereafter. A particular application of fertilizer N is at risk to bypass flow only once. The bypass factor σ will depend on both the bulk properties of the soil, for example the proportion of large cracks, and its surface properties, which will determine the likelihood of surface runoff. Any $\text{NO}_3\text{-N}$ lost by bypass flow immediately joins the $\text{NO}_3\text{-N}$ leached from the bottom of the soil profile.

Denitrification

The quantity of N denitrified by a particular layer in a particular week is assumed to be proportional to the quantity of CO_2 produced by that layer during that week and also to its $\text{NO}_3\text{-N}$ content. CO_2 evolution is used rather than O_2 consumption because the model generates CO_2 evolution: see Hansen *et al.* (1991) for a similar approach. If, as is usually the case, the Respiratory Quotient of soil is *c.* 1, CO_2 evolution will give a good measure of O_2 consumption, which is the real driving force for denitrification. Since CO_2 evolution, as modelled, depends on temperature, it is not necessary to adjust denitrification rates for temperature.

The rules for denitrification are:

- (1) Denitrification only occurs in the 0–25 cm layer, where 80% of the organic matter entering the soil each year is decomposed.
- (2) The maximum rate of denitrification occurs when a particular layer (5 cm in thickness) is at its maximum water holding capacity. If the layer is not fully filled, the rate of denitrification decreases, in proportion $(\psi_f - \psi_c) / \psi_f$.
- (3) Denitrification cannot reduce the $\text{NO}_3\text{-N}$ content of a particular layer below its N_{RESN} value.
- (4) Loss of N by denitrification during one week in a particular 5 cm layer (D kg N/ha) is given by

$$D = \theta (W/5) N_N [(\psi_f - \psi_c) / \psi_f] \quad (16)$$

where θ is the denitrification factor and W is the combined evolution of $\text{CO}_2\text{-C}$ during that week by the RO, BIO and HUM compartments in the 0–25 cm layer, in kg/ha.

Volatilization of NH_3

Ammonia can be lost from the soil after the

application of fertilizer or organic manure, and also from the senescing plant (Sharpe *et al.* 1988). Ammonium fertilizers are particularly subject to ammonia loss if (a) they remain on the surface of a damp (but drying) calcareous soil, and (b) the fertilizer anion forms an insoluble calcium salt, for example CaSO_4 (Fenn & Hossner 1985). In the experiments described by Hart *et al.* (1993), two of the soils were calcareous. Furthermore, the labelled nitrogen was applied as a mixture of $(^{15}\text{NH}_4)_2\text{SO}_4$ and K^{15}NO_3 , so that sulphate was always present. Powlson *et al.* (1986) examined the fate of labelled N applied either as $^{15}\text{NH}_4$ or $^{15}\text{NO}_3$. In 1980, 100% of the nitrate-derived N was accounted for in the crop plus soil at harvest, whilst only 76% of the ammonium-derived N was recovered. In 1981, however, c. 80% of the labelled N was accounted for, whether applied as ammonium, nitrate or as a mixture. This suggests that ammonia volatilization was significant in the dry conditions of 1980 but was not repeated in the much wetter spring of 1981 (Powlson *et al.* 1986).

Fertilizer $\text{NH}_4\text{-N}$ (F_A) can be lost by volatilization, according to the equation

$$V_s = \phi_s F_A \quad (17)$$

where V_s is N loss by volatilization (in kg N/ha) and ϕ_s is the fraction of the fertilizer N volatilized. It only occurs in the week of fertilizer application if the rainfall is < 5 mm in that week and if the fertilizer is applied as ammonium sulphate or urea.

After anthesis, the total N content of the crop may decline (Schjørring *et al.* 1989). In the model, losses during senescence can only occur during the last 5 weeks before harvest and are modelled by assuming that once crop N reaches its target value (U_m), a fraction of the N present in the tops can be released as NH_3 in the period up to harvest, so that

$$V_c = \phi_c (U_G + U_S)/5 \quad (18)$$

where V_c is N loss in one week by volatilization, in kg N/ha, ($U_G + U_S$) is the N content of the above-ground part of the crop at harvest and ϕ_c is the fraction of the above-ground crop N lost by volatilization. Volatilization only occurs if the above-ground part of the crop contains more N than ($U_G + U_S$).

If by 5 weeks before harvest the crop has not recovered its target N but uptake has exceeded ($U_G + U_S$), then

$$V_c = [U_T - (U_G + U_S)]/5 \quad (19)$$

where U_T is the N content of the above-ground part of the crop at that time.

Rules for the behaviour of ^{15}N labelled fertilizer in the model

In fitting the model to the results in the preceding paper (Hart *et al.* 1993), half the ^{15}N -labelled fertilizer enters the $\text{NH}_4\text{-N}$ compartment (minus any volatil-

ization losses) and half enters the $\text{NO}_3\text{-N}$ compartment. Thereafter ^{15}N -labelled N is nitrified, leached, immobilized, denitrified, taken up by plants or volatilized, exactly as for unlabelled N. If, for example, a particular soil layer is denitrifying D kg N/ha/week and a fraction, μ_N , of the nitrate compartment N is labelled at the beginning of the week, then the labelled N denitrified during the week is taken as $\mu_N D$ kg N/ha/week and the unlabelled as $(1 - \mu_N)D$. At the end of the week the nitrate compartment is updated on the basis of all the flows of labelled and unlabelled N into and out of it and a new value (μ'_N) struck for the fraction of labelled fertilizer N in that compartment for use in the following week. All other compartments (except RO) are treated similarly.

The net quantity of labelled N released from the RO compartment in one week is

$$\mu_{RO} C_o (z - x (\alpha + \beta))(1 - e^{-smr})$$

the corresponding net quantity of unlabelled N is

$$(1 - \mu_{RO}) C_o (z - x (\alpha + \beta))(1 - e^{-smr})$$

where μ_{RO} is the fraction of the N in RO that is labelled at the beginning of the week, C_o is the quantity of organic C present at the beginning of the week, with z the reciprocal of its C:N ratio at the beginning of that week, x the (unchanging) reciprocal of the C:N ratio of both the BIO and HUM compartments, α and β the proportions of C going to biomass and humus respectively (see Fig. 2) and r the rate constant for decomposition of the RO compartment. The BIO compartment releases

$$\mu_{BIO} B_o (x - x (\alpha + \beta))(1 - e^{-smb})$$

and the HUM compartment

$$\mu_{HUM} H_o (x - x (\alpha + \beta))(1 - e^{-smh})$$

μ_{BIO} being the fraction of BIO N that is labelled at the beginning of the week and μ_{HUM} that of HUM N. If $z < x (\alpha + \beta)$, net immobilization occurs, and both labelled and unlabelled N is taken up from the inorganic N compartments. Labelled (and unlabelled) inorganic N then enters the BIO and HUM compartments in proportions $\alpha/(\alpha + \beta)$ and $\beta/(\alpha + \beta)$, respectively, first from the ammonium compartment and then from the nitrate compartment. However, during net immobilization, the proportion of labelled N in the inorganic-N compartments is calculated in a special way. For example, if the ammonium pool is undergoing depletion, the fraction of labelled N in the ammonium pool is taken not as μ_A , the fraction at the beginning of the week, but as $(\mu_A + \mu'_A)/2$ where μ'_A is the calculated fraction at the end of the week.

Computing

The model is programmed in FORTRAN77 and can be

run on a mainframe computer or on an IBM-compatible PC. Special rules are used to initiate the model. Calculations of soil moisture start during the first week of January of the previous season. Five and a half months later, in mid-June, but still several months before the first crop to be modelled is sown, the main N model starts. Mid-June is chosen because mineral N levels under cereals are then at or near their annual minimum.

Fitting and testing the model

Whitmore (1991) partitioned the residual sum of squares between model and measurement into two components and calculated the mean squares from these sums of squares. The first is shown in Eqn (20) and arises from the experimental error in the measurements:

$$\sum_{j=1}^N \sum_{i=1}^{n_j} (y_{ij} - \bar{y}_j)^2 / \sum_{j=1}^N (n_j - 1) \quad (20)$$

where y_{ij} is the i th replicate in the j th experiment, \bar{y}_j the mean of the n_j replicate measurements and N the total number of experiments. The other mean square summarizes the systematic difference between model and measurement; in other words the lack of fit between model and data. With the notation above and where x_j is the simulation of the j th experiment this may be written:

$$\sum_{j=1}^N n_j (\bar{y}_j - x_j)^2 / N \quad (21)$$

The square roots of the lack of fit and error (root mean squares (R.M.S.): see, for example, Loague *et al.* 1988) express the deviation in the measurements (or between model and measurements) in the same units as the measurements themselves, in this work kg/ha. Mean squares may be compared using the variance ratio test (F -test) to see if one is significantly larger than the other. In this way we compared values of the lack of fit mean square (Eqn (20)) to see if changes made while building the model led to a significant improvement.

The model was tuned (i.e. values selected for the various constants within the model so as to minimize the lack of fit), using data from the experiment in which labelled fertilizer was applied to the Broadbalk Continuous Wheat Experiment at Rothamsted (Powlson *et al.* 1986; Hart *et al.* 1993). Only data from plot 09 (receiving 192 kg N/ha/year) of this experiment were used during the tuning process: data from the other plots, which received less N, were reserved for testing. There were some instances in which increasing the value of a constant or parameter reduced the lack of fit of the model to the measured labelled N content of the soil, but increased the lack of fit to the measured uptake of labelled N by the crop. Where

this was so, the ratio of lack of fit to error of labelled crop N and labelled soil N simulations was minimized simultaneously: that is to say Eqn (21) divided by Eqn (20). In other cases the effect of changing one constant or parameter was closely linked with the change in a related one: for example the retention of C or N in BIO depends on the relative sizes of α and β ; however the total amount of material retained in both BIO and HUM together is determined by the size of $(\alpha + \beta)$. Here we chose the combination of values of (α/β) and $(\alpha + \beta)$ that gave the least lack of fit.

An overriding consideration in setting certain key parameters is the need to maintain the organic N content of the soil at levels that are realistic for old arable land. Thus if h , the rate constant for the HUM compartment, is set too large for a given input of organic matter, the model will slowly but steadily run down soil organic N. The annual input of organic matter to the RO compartment and the rate constants h and b were matched so that the model neither depleted nor increased soil organic C and N in the three soils. All three have been arable for many years and their organic C and N contents can reasonably be assumed to be near equilibrium.

Another, and related, restriction was that the inputs of N must balance the outputs over a run of years. This considerably narrows the range over which certain parameters can vary: thus if the denitrification coefficient θ is increased, less N is available for removal in crop, by leaching and by volatilization as NH_3 .

The parameters finally set in matching the model to data from plot 09 of the Broadbalk Continuous Wheat Experiment were: r , 0.16/week; b , 0.0127/week; h , 0.0004/week; θ , 0.005/kg $\text{CO}_2\text{-C/ha}$; ϕ_c , 0.05; ϕ_s , 0.15; the ratio α/β was 1.1. For Rothamsted soil ($\alpha + \beta$) was 0.40, for Woburn 0.35 and for Saxmundham 0.42. The rate constant for release of dead plant C to soil (c) was 0.15/week: for dead plant N to soil (n) it was 0.10/week. The rate constant for uptake of N by plants (f) was 0.004: the shape factor (p), 1.5. The level above which rainfall contributes to bypass flow (R_{CRIT}) was 15 mm and the factor for loss of solute by bypass flow (σ) was 0.015/mm rain. N_{RESA} and N_{RESN} (the minimum permitted contents of ammonium N and nitrate N, respectively) were both set at 5 kg N/ha for each 50 cm layer of the Woburn soil. The corresponding figures for the Rothamsted soil are 10 and 10; for Saxmundham, 15 and 15.

Correspondence between measured and modelled data

Only when we had fixed the model structure and established the best values for its constants and parameters did we evaluate the model on ^{15}N data from other plots on Broadbalk (Fig. 3) and from the ^{15}N experiments at Woburn in Bedfordshire and

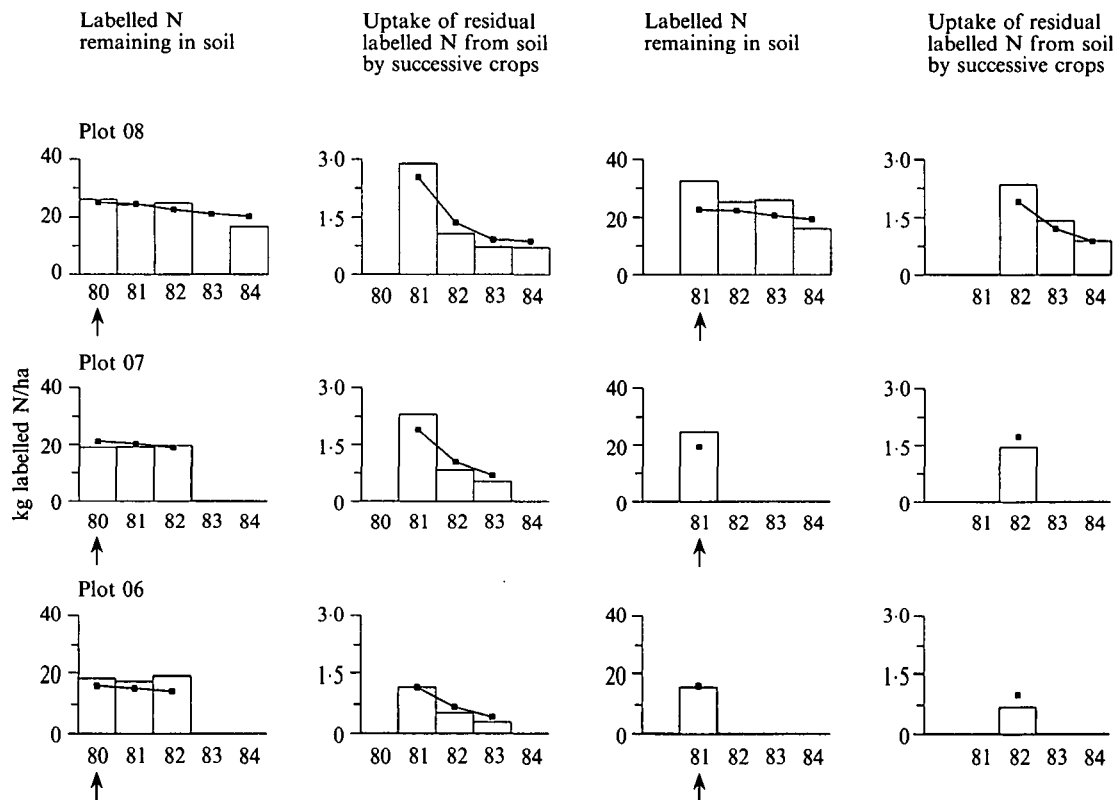


Fig. 3. Comparison of measured (histogram) and modelled (■) values for residual labelled N in the soil and for uptake of this residual labelled N by successive crops on Broadbalk. The results are for a single application of labelled fertilizer in either 1980 or 1981 to plot 06 (receiving an annual fertilizer application of 48 kg N/ha/year), plot 07 (96 kg/ha/year) and plot 08 (144 kg N/ha/year); for details of the experiments see Hart *et al.* (1993). The year of application of labelled fertilizer is shown by ↑; uptake of N by crop in the application year is calculated by Eqn (11).

Saxmundham in Suffolk (Fig. 4). Table 2 shows the mean squares, partitioned as above, between those due to error in the experimental data and those due to lack of fit between model and measurement. So that the model could be tested using data on the fate of labelled N in the crop/soil system, it was first set up using the *measured* above-ground crop total N (i.e. labelled plus unlabelled N) at harvest as an input. In a separate exercise, the model was also set up to *estimate* the total uptake of N from grain yield by Eqn (12): the latter results are given at the bottom of the Table.

Consider first the errors in measurement of residual labelled N in soil and in the model fit to these measurements, using measured above-ground crop N as input. The experimental error in the measurements of labelled soil N was almost the same at all sites in the year of application of labelled N and in each residual year. In all cases, the error mean square is *c.* 7, equivalent to a root mean square in the measurements of *c.* 2.5 kg labelled N/ha. The lack of fit of the simulated measurements was rather more

variable and at times significantly larger. The model is better at Rothamsted and Saxmundham than at Woburn and there are no statistically significant differences between its performance at Rothamsted and Saxmundham. Overall (with the exclusion of the Woburn 1981 result, for reasons explained below), the root mean square of the difference between the modelled and the measured values of labelled N in soil is *c.* 7.5 kg labelled N/ha.

It is clear that some results from Woburn present particular problems for the model. Grain yields at Woburn were severely depressed by take-all (*Gaeumannomyces graminis*), although straw yields and offtake of nitrogen were not as badly affected. In the 1981 application year, the model underestimates the quantity of labelled N remaining in the soil at harvest: the simulated retention for Woburn is 18.8 kg labelled N/ha, compared to a measured 34.4 kg. It seems likely that, due to disease, a larger amount of crop litter was returned to the soil during the growing season than would be normally estimated by the model, thereby increasing the labelled N remaining at

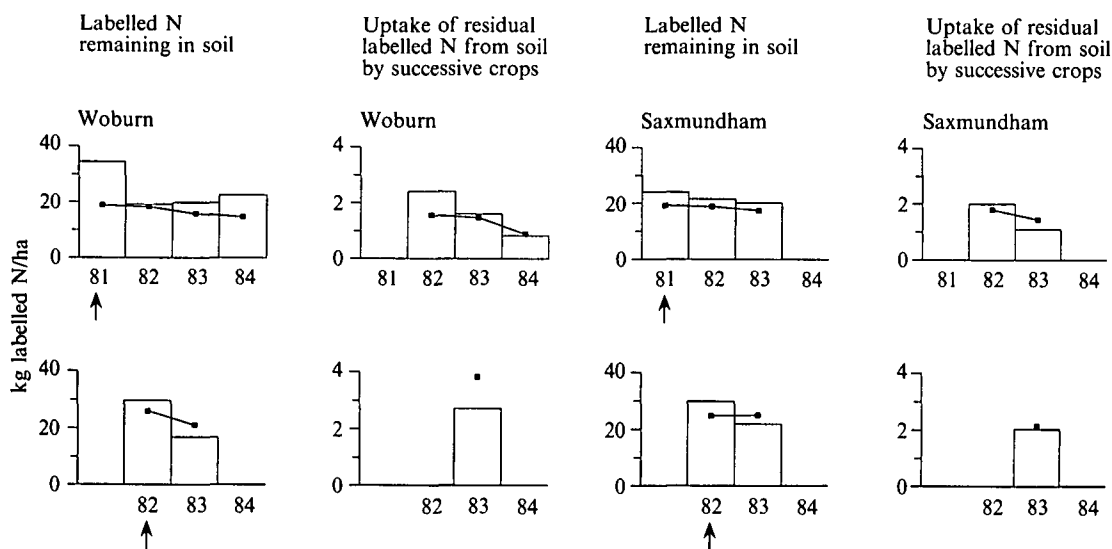


Fig. 4. Comparison of measured (histogram) and modelled (■) values for residual labelled N in the soil and for uptake of this residual labelled N by successive crops at Woburn and Saxmundham. The results are for a single application of labelled fertilizer in either 1981 or 1982; for details see Hart *et al.* (1993). Total fertilizer applications throughout the period were 150 kg N/ha/year at Woburn and 144 kg/ha/year at Saxmundham. The year of application of labelled fertilizer is shown by ↑; uptake of N by the crop in the application year is calculated using Eqn (11).

Table 2. Mean squares due to error in the experimental data and to lack of fit between model and measurement

Comparison		Mean squares			
		Residual labelled N in soil at harvest		Labelled N recovered by crop	
		Lack of fit (D.F.)	Experimental error	Lack of fit (D.F.)	Experimental error
Residual	Year 0	164.9 (10)	6.9 (24)	—	—
	Year 1	23.6 (8)	6.4 (20)	0.995 (10)	0.185 (24)
	Year 2	44.4 (6)	8.5 (14)	0.187 (6)	0.025 (14)
Site	Rothamsted	43.5 (16)	8.7 (32)	0.189 (15)	0.118 (28)
	Saxmundham	62.1 (5)	6.1 (15)	0.232 (3)	0.095 (9)
	Woburn	236.3 (6)	4.8 (18)	1.967 (4)	0.022 (12)
Measured uptake ^a	All data	89.8 (27)	7.0 (65)	0.518 (22)	0.086 (51)
	Excluding one result	55.8 (26)	7.2 ^b (62)	0.402 (21)	0.091 ^b (48)
Estimated uptake ^c	All data	232.1 (27)	7.0 (65)	5.133 (22)	0.086 (51)
	Excluding one result	69.1 (26)	6.9 ^d (62)	0.711 (21)	0.090 ^d (48)

^a Measured total uptake of N by above-ground part of crop (i.e. $U_G + U_S$) used to initiate model.

^b Excluding Woburn results from 1981 application year (soil) or first residual year (crop).

^c Estimated (using Eqn (12)) total uptake of N by above-ground part of crop used to initiate model.

^d Excluding Woburn results from 1982 application year (soil) or first residual year (crop).

harvest. It is also possible that the crop uptake parameters of a diseased crop are very different from those of a healthy crop.

Consider next the errors in measuring the uptake of residual labelled N by the crop and in the fit of the

model to these measurements, again using measured above-ground crop N as input to the model. The experimental error in the measurements of labelled N in crop was more variable than in soil; biggest at Rothamsted and least at Woburn. The model,

Table 3. Modelled losses of N for the three sites

	Rothamsted ^a					Woburn ^b				Saxmundham ^c		
	1980 ^d	1981	1982	1983	1984	1981 ^d	1982	1983	1984	1981 ^d	1982	1983
	kg total N/ha											
Volatilized ^e	10.6	0.0	0.0	0.0	0.0	4.2	2.8	3.5	5.5	12.7	2.4	0.0
Leached ^f	6.0	30.2	29.0	61.5	5.5	49.2	73.7	62.4	56.6	49.8	42.1	37.6
Denitrified	15.5	22.5	19.3	20.4	17.1	18.9	24.2	31.1	22.0	25.3	22.1	25.8
Total	32.1	52.7	48.3	81.9	22.6	72.3	100.7	97.0	84.1	87.8	66.6	63.4
	kg labelled N/ha											
Volatilized ^e	10.6	0.0	0.0	0.0	0.0	2.4	<0.1	<0.1	<0.1	12.7	<0.1	0.0
Leached ^f	0.0	0.2	0.6	1.0	0.2	18.9	26.2	2.3	0.6	23.7	2.6	0.5
Denitrified	1.1	0.7	0.4	0.3	0.1	8.0	0.7	0.6	0.3	5.7	0.5	0.3
Total	11.7	0.9	1.0	1.3	0.3	29.3	26.9	2.9	0.9	42.1	3.1	0.8

^a Receiving 141 kg labelled N/ha in spring 1980, 144 kg unlabelled N/ha each year thereafter.

^b Receiving 28 kg unlabelled N/ha in autumn 1980, followed by 150 kg labelled N/ha in spring 1981, 150 kg unlabelled N/ha each year thereafter.

^c Receiving 40 kg unlabelled N/ha in autumn 1980, followed by 142 kg labelled N/ha in spring 1981, 144 kg unlabelled N/ha each year thereafter.

^d Labelled fertilizer N applied.

^e From both soil and plant.

^f Including bypass flow.

however, is best at Rothamsted and least good at Woburn.

Now consider the situation if the input to the model (above-ground crop N at harvest) is calculated from grain yield, rather than set from the actual measurements. Table 2 shows that this causes the residual mean squares due to lack of fit to increase greatly. However Table 2 also shows that this increase is mostly caused by the Woburn results, particularly those from labelled fertilizer applied in 1982. The grain yield was only 2.7 t/ha at Woburn in 1982, so that Eqn (12) predicted an above-ground uptake of 51 kg N/ha, much less than the measured recovery of 130 kg. This caused the model to overestimate the quantity of unused fertilizer remaining in the soil at harvest, in turn making the modelled recovery of labelled N by the subsequent crop much larger than measured. If these Woburn results are excluded, estimating above-ground crop N from grain yields is only a little worse than using the actual measurements: the root mean square difference between modelled and measured values of labelled N remaining in the soil increases from 7.5 to 8 kg N/ha.

Table 3 shows the modelled losses of N for the three sites, and how they are partitioned between volatilization, leaching and denitrification. In general, losses are greatest at Woburn and least at Rothamsted, with Saxmundham occupying an intermediate position. Again the model predicts very large losses of labelled N by leaching during the first residual year at Woburn, for reasons discussed above.

Sensitivity of the model output to changes in the model parameters

Two outputs were used to test the sensitivity of the model to changes in constants or parameters: the quantity of labelled N remaining in the soil after 4 years and the cumulative recovery of residual labelled N by the crop in succeeding years. Attention was mainly directed at parameters set during the fitting exercise: parameters set externally, for example q , the rate constant for nitrification, were not examined.

Fig. 5 shows the effects of varying the parameters that govern the transformations of organic matter in soil: the rate constants (r , b and h) for the input (RO), biomass (BIO) and humus (HUM) compartments, the fraction ($\alpha + \beta$) of the incoming substrate converted to biomass plus humus, the ratio (α/β) of biomass formed to humus formed, the annual C input of plant material and the rates at which organic C and N are returned to the soil. Fig. 6(a-d) is concerned with parameters that govern the transport of inorganic N out of the soil and out of the plant/soil system: the above-ground N in the crop at harvest ($U_G + U_S$); the rate constant f for N uptake by the crop; the fraction of N lost from the senescing crop as $\text{NH}_3\text{-N}$ (ϕ_C); the proportion of $\text{NH}_4\text{-N}$ fertilizer lost by volatilization (ϕ_S); the denitrification coefficient θ ; the bypass flow factor (σ). Fig. 6(e and f) shows the effects of varying the critical levels above which rainfall contributes to bypass flow (R_{CRIT}), the weekly rainfall (R_w) and T , the mean weekly air temperature.

In general, a change in a parameter which causes an

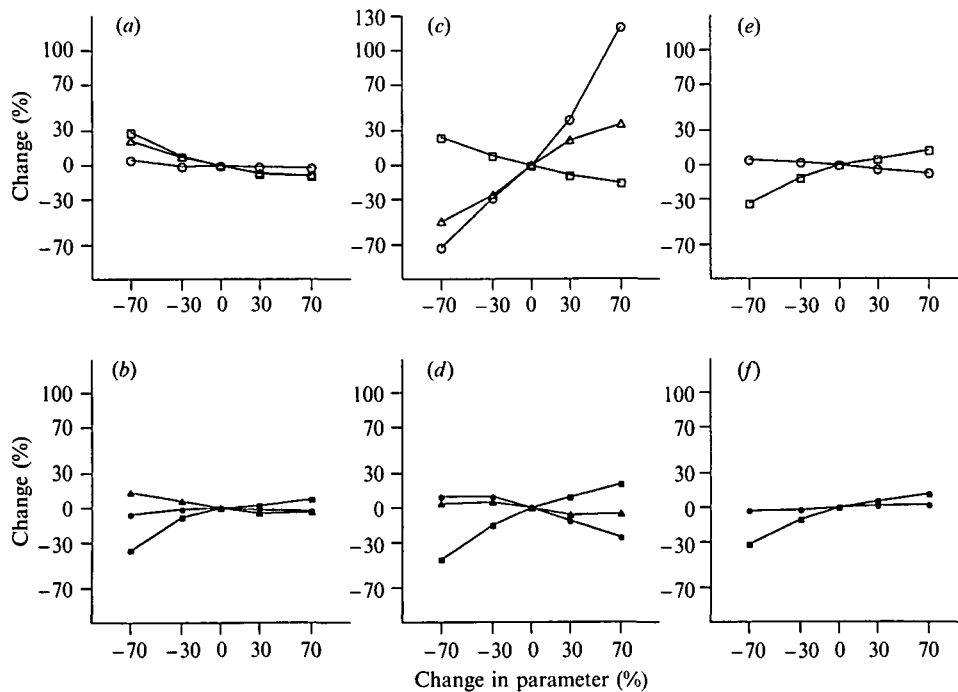


Fig. 5. Sensitivity of labelled N remaining in soil after 4 years (open symbols) and cumulative crop uptake in four years of residual labelled N (closed symbols), to changes in various parameters: (a and b) \circ , \bullet the rate constant (r) for the input compartment (RO); \square , \blacksquare the rate constant (r) for the biomass compartment (BIO); \triangle , \blacktriangle the rate constant (h) for the humus compartment (HUM). (c and d) \circ , \bullet the fraction ($\alpha + \beta$) of the incoming substrate converted to biomass plus humus; \square , \blacksquare the ratio (α/β) of biomass formed to humus formed; \triangle , \blacktriangle the annual C input (C_{AO}). (e and f) \circ , \bullet the rate constant (e) for return of organic C to the RO compartment; \square , \blacksquare the rate constant (n) for return of organic N to the RO compartment.

increase in mineralization will increase uptake of labelled N by the crop. This is demonstrated most noticeably in Fig. 5(c and d), where the relationships between C_{AO} , α and β are altered. Fig. 5(c and d) shows that the annual input of organic matter and the proportions of this input going to CO_2 , microbial biomass and humus, are particularly critical: good data will clearly be needed to establish these parameters if the model is to be applied successfully to other crops and soils.

Labelled N remaining in soil and recovery of residual labelled N by successive crops are quite sensitive to changes in mean weekly temperature (Fig. 6(e and f)). When temperature is reduced, crop uptake (driven by cumulative week-degrees) is also reduced, leaving unused fertilizer in the soil at risk to leaching and other loss processes. However, when temperature is increased, the rate of N uptake (f) also increases, allowing the crop to recover residual labelled N before it is lost by other means.

It should be stressed that all these sensitivity tests were run with real weather data for a specified run of years. For the tests illustrated in Figs 5 and 6, the start

year was 1980, a year in which there was little rain in the weeks following application of labelled fertilizer. This is why (for example) varying the denitrification factor θ had so little effect in Fig 6c: there was virtually no denitrification of labelled fertilizer N in 1980, so it did not matter whether θ was large or small. A very different result would have been obtained had 1981 been the start year.

CONCLUSIONS

The model described here provides a useful representation of the behaviour of a pulse of labelled N as it moves through the crop/soil system. Its principal strength is the ability to carry N forward from year to year: an erroneous prediction too small to be noticed over a single year can lead to a long-term prediction that is unacceptable.

Our long-term aim is to use the model described and calibrated in this paper to predict how much N a soil could supply to a particular crop over its growing season, from a knowledge of the soil, its cropping history and the preceding weather. This information

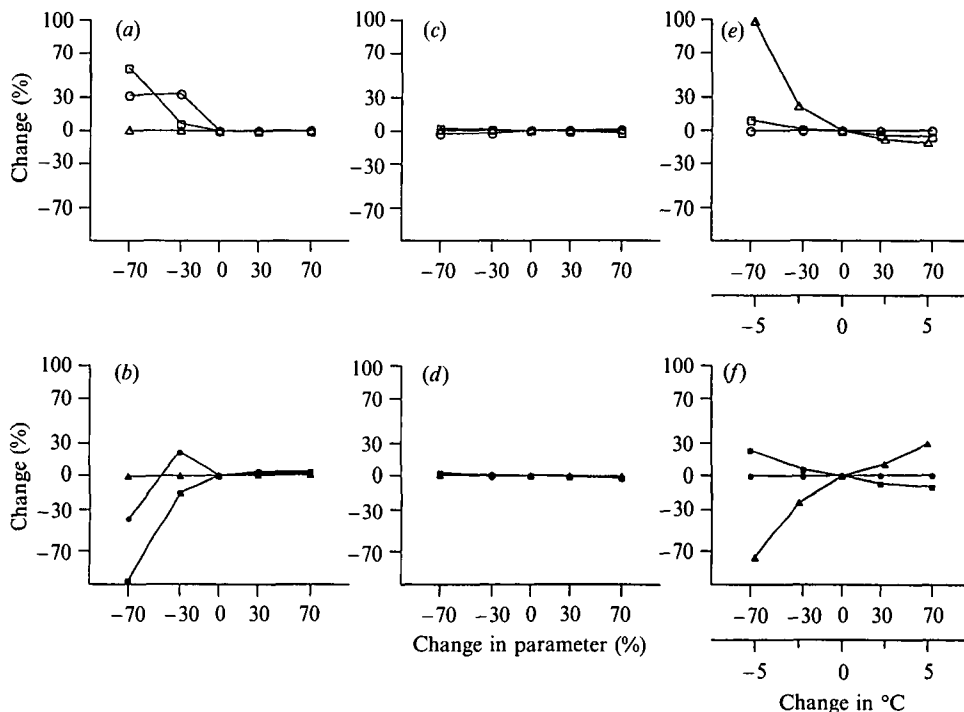


Fig. 6. Sensitivity of labelled N remaining in soil after 4 years (open symbols) and cumulative crop uptake in four years of residual labelled N (closed symbols), to changes in certain parameters and inputs: (a and b) \circ , \bullet the above-ground N in the crop at harvest ($U_G + U_S$); \square , \blacksquare the rate constant (f) for crop N uptake; Δ , \blacktriangle the fraction (ϕ_C) of the above-ground N released by the senescing crop as $\text{NH}_3\text{-N}$. (c and d) \circ , \bullet the denitrification factor (θ); \square , \blacksquare the proportion of $\text{NH}_3\text{-N}$ fertilizer lost by volatilization (ϕ_S); Δ , \blacktriangle the bypass flow factor (σ). (e and f) \circ , \bullet the level above which rainfall contributes to bypass flow (R_{CRIT}); \square , \blacksquare weekly rainfall (R_w); Δ , \blacktriangle mean weekly temperature, (T), varied by $\pm 5^\circ\text{C}$.

could, in turn, be used to give cereal growers a soundly-based estimate of how much nitrogen to apply to a particular crop growing in a particular field and when it should be applied, without the need for measurements of soil mineral N.

N. J. Bradbury and D. S. Jenkinson thank the Home-Grown Cereals Authority, which supported this work. N. J. Bradbury also thanks the Fertiliser Manufacturers' Association for a special grant. P. B. S. Hart thanks NRAC, New Zealand, for a study award.

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Appendix 1. Definition of symbols, units, etc. used in the model

Symbol	Definition	Dimension
A_T	Input of combined N from atmosphere	kg/ha/week
b	Rate constant for decomposition of microbial biomass compartment (BIO)	/week
B_o	C in biomass compartment (BIO) at beginning of week	kg C/ha
c	Rate constant for release of dead plant C to soil	/week
C_{AO}	Overall annual return of organic C to the soil from plant remains	t C/ha
C_c	Cumulative return of organic C to the soil up to the current (gth) week	t C/ha
C_o	C in input compartment (RO) at beginning of week	kg C/ha
C_{sc}	Annual return of stubble and chaff C to the soil	t C/ha
d	Cumulative degree-weeks above 0 °C since sowing	°C week
D	Denitrification in specified soil layer	kg N/ha/week
f	Rate constant for plant N uptake	/week
F_A	Input of fertilizer as ammonium	kg NH ₄ -N/ha
F_N	Input of fertilizer as nitrate	kg NO ₃ -N/ha
g	Weeks elapsed since sowing	—
G	Measured grain yield	t/ha at 85% DM
h	Rate constant for decomposition of humus compartment (HUM)	/week
H_o	C in humus compartment (HUM) at beginning of week	kg C/ha
K	Percentage clay (< 2 µm) in 0–50 cm layer	—
L	NO ₃ -N moving to layer below by piston flow	kg NO ₃ -N/ha/week
L_B	NO ₃ -N moving to bottom of profile by bypass flow	kg NO ₃ -N/ha/week
m	Temperature rate modifier	—
M	Mineralization of N in specified soil layer	kg N/ha/week
n	Rate constant for release of dead plant N to soil	/week
N_A	NH ₄ -N in specified soil layer at beginning of week	kg NH ₄ -N/ha
N_{AO}	Overall annual return of organic N to the soil from plant remains	kg N/ha
N_c	Cumulative return of organic N to the soil up to the current (gth) week	kg N/ha
N_N	NO ₃ -N in specified soil layer at beginning of week	kg NO ₃ -N/ha
N_{sc}	Annual return of stubble and chaff N to the soil	kg N/ha
N_{RESA}	Residual quantity of NH ₄ -N that cannot be removed from a soil layer	kg NH ₄ -N/ha
N_{RESN}	Residual quantity of NO ₃ -N that cannot be removed from a soil layer	kg NO ₃ -N/ha
O_A	NH ₄ -N added in organic manure	kg N/ha
O_H	Organic N added in organic manure	kg N/ha
p	Shape factor	—
P	Nitrification in specified soil layer	kg NO ₃ -N/ha/week
q	Rate constant for nitrification	/week
r	Rate constant for decomposition of input compartment (RO)	/week
R	Excess water entering specified soil layer in week	mm/week
R_{FC}	Water held in soil at Field Capacity	mm
R_w	Rainfall	mm/week
R_{CRIT}	Threshold rainfall above which N is lost by bypass flow	mm/week
s	Soil moisture rate modifier	—
s_o	Soil moisture rate modifier at –15 bar	—
T	Mean air temperature for a particular week	°C
U	N in crop, of which U_T is above ground and U_R below ground. At harvest U_T is divided between N in grain (U_G) and N in straw, chaff and stubble (U_S)	kg N/ha
U_m	Target N uptake of crop, including N in roots, N to be lost as NH ₃ during senescence and N lost from the growing plant through death of roots, tillers, etc.	kg N/ha
V_S	N lost by volatilization of F_A from soil	kg N/ha
V_C	N lost by volatilization from above-ground part of crop	kg N/ha/week
w	Weeks between sowing and harvest	week
W	CO ₂ -C released from soil in specified soil layer	kg CO ₂ -C/ha/week
x	Reciprocal of the C/N ratio of humus (HUM) and biomass (BIO) compartments	—
z	Reciprocal of the C/N ratio of the input compartment (RO)	—
α	Fraction of decomposing organic C going to microbial biomass compartment (BIO)	—
β	Fraction of decomposing organic C going to humus compartment (HUM)	—
θ	Denitrification factor	/kg CO ₂ -C/ha
μ_A	Fraction of the ammonium compartment labelled at the beginning of the week	—
μ_{BIO}	Fraction of the N in biomass compartment (BIO) labelled at beginning of the week	—
μ_{HUM}	Fraction of the N in humus compartment (HUM) labelled at beginning of the week	—

Symbol	Definition	Dimension
μ_N	Fraction of the nitrate compartment labelled at the beginning of the week	—
μ_{RO}	Fraction of the N in input compartment (RO) labelled at the beginning of the week	—
ϕ_S	Fraction of ammonium fertilizer N volatilized from soil as NH_3	—
ϕ_C	Fraction of N in above-ground part of the crop released as NH_3 during senescence	—
ψ_c	Calculated water deficit in specified soil layer	mm
ψ_f	Water held in specified soil layer between Field Capacity and -15 bar	mm
ψ_i	Water held in specified soil layer between Field Capacity and -1 bar	mm
σ	Bypass flow factor	/mm excess rain
ϵ	Fraction of F_N at risk to bypass flow during a particular week	—