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DEVELOPMENT AND TESTING OF A COMPUTER MODEL FOR PREDICTING THE AMOUNT AND TIMING OF NITROGEN RELEASE FROM SOIL

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DEVELOPMENT AND TESTING OF A COMPUTER MODEL FOR PREDICTING THE AMOUNT AND TIMING OF NITROGEN RELEASE FROM SOIL

by

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CONTENTS

Abstract

A computer model has been developed to establish the mineral nitrogen status of the soil throughout the year. The model runs on a weekly time-step using total weekly rainfall and evaoptranspiration, and mean weekly air temperature. It simulates the release of nitrogen by mineralization, its loss by denitrification and volatilization, and its subsequent removal from the soil system through crop uptake, immobilization and leaching. The model has been designed to specify how much fertilizer nitrogen should be applied to spring or winter cereals growing in a particular field in a particular year and requires only simple inputs. These include the soil type, previous cropping history and the expected yield from the field in question, given an average season and allowing for the likelihood of weed or disease problems. An account is kept of all the nitrogen flows within the model so it can be used, for example, to compare cumulative annual losses under different agronomic systems. Nitrogen may be 'labelled' within the model so that the fate of fertilizer N can also be traced.

The model was tested using data from experiments conducted at Rothamsted, Woburn and Saxmundham experimental farms in which a pulse of ^{15}N-labelled fertilizer was applied to winter wheat. The fate of this labelled N was followed for up to four years. Over this period, the agreement between modelled and measured values of labelled N remaining in the soil and recovered by successive crops was acceptable for all three sites, for N applications ranging from 48 to 192 kg N/ha. The model was also tested against data from experiments involving applications of FYM and ^{15}N-labelled fertilizer to spring barley. Again, model simulations of the fate of residual labelled N in soil agreed well with measurements. Experiments with ^{15}N-labelled fertilizer pose a particularly stringent test of such models, since the model has to mimic the behaviour of both labelled and unlabelled nitrogen.

Comparison of model simulations with measurements of residual labelled nitrogen in inorganic form have indicated that the processes causing loss of fertilizer N in the period immediately following application are complex and are probably highly sensitive

to temperature and moisture conditions in the soil. Although the model simulates loss of nitrate by denitrification in wet soil, it appears that other processes, such as the formation of nitrous oxide during nitrification, may cause significant losses of fertilizer in moist but aerobic soil conditions. Further experimental work is needed to clarify the interactions between the factors which govern the loss of fertilizer N.

OBJECTIVES

Our primary objective was to produce a model that can predict how much nitrogen will be released by the soil in a particular field (and when it will be released), from a knowledge of the soil, its agricultural history and the weather during the preceeding year.

During the course of the work, we extended our model so that it could be used to specify how much fertilizer N is required to attain a specified yield of spring or winter cereals on a particular field in a particular year.

INTRODUCTION

Advice to farmers on how much nitrogen fertilizer to use has long been based on the idea of the 'economic optimum' - the quantity of fertilizer that gives the maximum profit from the crop. However, in recent years it has become increasingly apparent that nitrate leaching increases sharply once the capacity of a crop to accumulate nitrogen is exceeded. This means that N fertilizer requirements need to be more finely tuned, avoiding both under-use of N, which is unprofitable, and over-use, which is environmentally unwelcome.

The quantity of N taken up by a cereal crop of a particular size is relatively well known. What is less well known is how much N the soil will supply to the crop during the growing season, and how efficiently the plant can use both soil and fertilizer N. Our long-term aim was to give cereal growers a soundly-based estimate of the amount of N required by a particular crop growing in a particular field, based on a computer model for the behaviour of N in the crop/soil system that can generate this information. We think this is a better approach than basing nitrogen recommendations on soil analysis, which is expensive and difficult to organise inside the short period in early spring when sampling must be done.

METHODS

The construction, tuning and testing of the model is fully described in the paper which is attached as an Appendix. The paper has been submitted for publication in the Journal of Agricultural Science, Cambridge. The methods use to construct and validate the model are summarized below.

The model parameters were set by tuning to data from an experiment in which ^{15}N-labelled fertilizer was applied to the Broadbalk Continuous Wheat Experiment at Rothamsted. Results from *one plot alone*, that receiving fertilizer at 192 kg N/ha, were used in the tuning exercise. The model was then tested against data not used in the tuning exercise including that from other Broadbalk plots receiving ^{15}N-labelled fertilizer, and from ^{15}-N experiments at Woburn on sandy loam soil and at Saxmundham on heavy clay.

The model was also tested against data from field experiments which formed part of a MAFF-funded project to investigate the leaching of nitrate from arable land (MacDonald et al., 1991). In this project, ^{15}N-labelled fertilizer was applied in 1987 and 1988 to a range of crops on four contrasting soil types at Rothamsted and Woburn. Details of the soils and experiments are summarized in Table 6. Total and inorganic labelled N remaining in the soil and crop recovery of labelled N were measured at harvest in the application year and in the first residual year. In addition, measurements of inorganic N were taken at intervals over the cropping season. Under winter wheat, recovery of labelled N in crop plus soil averaged 72% of that applied in 1987 and 80% in 1988. A separate set of data from labelled nitrogen experiments on the long-term trial at Hoosfield were used to extend the model to cover spring barley.

A menu-driven version of the model was developed so that it could be used for demonstration purposes.

The project results are described here in two parts. Part I covers the period from June

1987 to September 1991 during which time the construction and initial testing of the model was carried out. Part II describes an extension to June 1992 when some further testing and revision of the model was carried out.

RESULTS - PART I

The fitting of the model to field data from 15N experiments on winter wheat at Rothamsted, Woburn and Saxmundham experimental farms is fully dealt woith in the Appendix; here we are concerned with the application of the model thus fitted and tested to other experiments.

Simulation of soil mineral N

In the MAFF-funded project (see above), soil mineral nitrogen was monitored during the growth of a winter wheat crop and in the two succeeding (fallow) years.
Two sites were used: Claycroft (clay loam) at Rothamsted and Butt Close (sandy loam) at Woburn. In 1987, the first year of the trial, the crop at Claycroft received 224 kg N/ha and yielded 7 t/ha, with a total recovery of nitrogen of 204 kg N/ha. At Butt Close the crop received 173 kg N/ha but yielded only 1.8 t/ha, with a nitrogen recovery of 98 kg N/ha. Figs. 1 and 2 show a comparison of the model simulations with data from these two sites. The model over-estimates the amount of inorganic N remaining at harvest of winter wheat. Subsequently, model calculations of mineral N in the fallow period fit well with measurements, suggesting that simulation of the underlying mineralization/immobilization processes are acceptable. The model predicts that, on average, leaching would have increased from 35 kg N/ha under the wheat crops in the first winter to 93 kg N/ha in the third winter after the field had lain fallow for a year and a half.

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Using the model for spring cereals

Spring crops generally give lower yields than winter-sown ones, mainly because of their shorter growing period; their total offtake of nitrogen is also lower. The model has been modified so that the fertilizer requirements of spring cereals can also be predicted. In making these modifications we have concentrated on investigating the relationship between yield and N requirement (below and above ground), the course of N uptake and the turnover of organic matter under spring crops.

Relationship between N offtake and yield

Originally, data from several winter wheat trials were used to give a relationship between yield and total N recovery by the crop, namely :

$$U_T = 230(e^{0.075G}-1) \qquad \text{(Appendix, p.58)}$$

where :

U_T = above-ground crop N at harvest (kg N/ha)

G = grain yield of crop (t/ha)

This curve was also found to give a good fit to results on total N recovery and yield of spring barley from data sets 1 to 7 (Table 1). The curve (Fig. 3) was found to explain 78% of the variance in the data : changing the parameters of the equation did not significantly improve the fit. It was concluded that this relationship is satisfactory for spring as well as winter-sown crops.

Uptake of N by spring barley

Results from the experiment at Bush in 1988 (data set 7, Table 1) were used to find suitable parameters to describe the uptake of nitrogen by spring barley. In this experiment, the nitrogen content of the crop was measured on six occasions at approximately 3-week intervals from the end of May until harvest at the end of August.

We found that a generalized logistic curve of the form :

$$U = U_T/\{1+w(e^{(-f(d-dm))})\}^{1/w}$$

where :

U = N in crop (kg N ha^{-1})

U_T = N in above-ground crop at harvest (kg N ha^{-1})

w = power function

f = rate constant

d = cumulative day-degrees since sowing (day-°C)

dm = inflection point of curve (day-°C)

(analogous to that used to simulate uptake of nitrogen by winter crops, Appendix, p.58), could also be used for spring crops. Fig 4. shows such a curve fitted to the Bush data from the treatments in which 120 kg N/ha was applied in various splits, and from the 150 kg N ha^{-1} treatment. With parameters : $U_T = 130$, $w = 0.011$, f = 0.006, and dm = 470, 96% of the variance was explained.

Using the same parameters, this curve was also fitted to results from the 120 kg N/ha and 150 kg N/ha treatments at Lintlaw in 1987 and Middlestot in 1988 (data sets 5 & 6), and was found to explain 80% of the variance in the data.

Turnover of organic matter under spring barley

Spring barley has been grown every year on Hoosfield at Rothamsted since 1852. One set of plots receives only inorganic fertilizer, with nitrogen applied at various rates, whilst another set receives 35 t/ha of farmyard manure each year in addition to the inorganic N treatments (Table 1, data sets 1 to 4). In 1986, in Phase I of the experiment, labelled N was applied to microplots at the same rate as on the main plot, and the fate of this nitrogen in the soil and in succeeding crops was followed over two residual years. The experiment was repeated in 1987 using different microplots (Phase II).

When simulations from the model in its existing form were compared to the Hoosfield data, it was apparent that the relationship used to estimate the root nitrogen requirement of a winter cereal crop (Appendix, p.56) overestimated the amount recovered by a spring crop. In order to tune this part of the model for spring crops, the root N requirement was varied systematically until the best fit was obtained to measurements from Phase I of the experiments of labelled N in the soil and its recovery by successive crops. (The fitting procedure was as described in the Appendix, p.66). Fig. 5 shows the resulting relationship between the yield of a spring crop and the nitrogen requirement of its roots. With this modification, the model also gave a good fit to data from Phase II of the experiment. Figs 6 to 9 show the comparison between measured and modelled values for the decline of labelled N in the soil and the recovery of residual labelled N by successive crops in the two phases of the experiment and on plots receiving only inorganic N, as well as on plots receiving FYM in addition to the inorganic treatments.

Demonstration Version

A P.C. version of the model was demonstrated at the Cereals 91 event, as part of the AFRC/ADAS exhibit on 'Living with Nitrates'. This version is designed to present results from the model in a way which will be informative to farmers and non-specialists. An alternative format could be designed for use by agronomists and advisors.

The display runs through several stages. A series of menus (Table 2) prompts the user to enter information for a particular field on, for example, soil type, cropping history and yield expectation, the latter being used to calculate a target nitrogen requirement for the crop in question. Table 3 sets out the inputs for two contrasting sites - a loamy soil growing a second winter wheat in the Eastern region (Site A) and a site in the North-West growing spring barley on a sandy soil (Site B). Using this information, the model runs through from the previous anthesis up to the week when a prediction of fertilizer requirement is needed, say, in early March. For demonstration purposes, the model reads weekly rainfall, evapotranspiration and temperature from an internal file of meteorological data, so that the behaviour of nitrogen over a complete crop year can be considered; when in use as an advisory tool, current meteorological data will be input weekly.

The screen then displays graphs of simulations of soil mineral N, net mineralization, leaching and denitrification, and crop uptake of N over the months to March. Next, the model runs forward from March to the following harvest, using a set of 30-year mean meteorological data for the region specified (MAFF 1976), and predicts the likely contribution of soil N from mineralization, and the amount which may be lost by denitrification. The screen now displays a balance sheet which gives a prediction of fertilizer N required using the formula :

$$N_f = N_c - (N_{cs} + N_m + N_s) + (N_d + N_l)$$

where :

N_f = Fertilizer N required

N_c = Crop target N (including a portion which may be lost as NH_3 during senescence)

N_{cs} = N taken up by crop by spring

N_m = N mineralized between spring and anthesis

N_s = Available N in soil in spring

N_d = N lost by denitrification between spring and anthesis

N_l = N lost by leaching between spring and anthesis (usually negligible)

(all terms in kg N/ha)

In the examples shown here (Table 4), the model predicts a fertilizer requirement of 169 kg N/ha for the winter wheat at Site A and 103 kg N/ha for spring barley at Site B. The model can then be re-run with the predicted amount of N fertilizer being 'applied' at an appropriate time. When the run is complete, graphs are plotted showing the simulated amounts of total mineral N (i.e. soil-derived plus fertilizer-derived) and fertilizer N in the soil from January onwards, and similarly, the simulated crop uptake of total mineral N and fertilizer N.

Three further screens of results are displayed. Firstly, a comparison of simulations of crop uptake, mineralization and denitrification using mean and real meteorological data for the March-harvest period is shown. Secondly, there is a nitrogen balance for the year from previous harvest to current harvest (Tables 5a and 5b). In this example it is interesting to note that the sandy soil (Site B) contains less organic N and hence mineralizes less N than the loam. There is also more denitrification and leaching in the wetter climate of the North-West. Finally, a pie diagram (Fig. 10) shows the fate of the applied fertilizer N.

RESULTS - PART II

In this part of the project, we examined model simulations of labelled N remaining in the soil at all four sites in the MAFF experiment and in both application years (1987 and 1988). It was clear that the model consistently over-estimated the amount of labelled N remaining in the inorganic form at harvest of the winter wheat crop. This led us to re-evaluate the modelling of N loss processes, namely denitrification, leaching and volatilization. The sub-model for each process is described in detail in the Appendix; the main points are summarized below.

i) Denitrification

Denitrification occurs in each 5cm layer down to a depth of 50cm. The amount of N lost each week is dependent upon a denitrification coefficient, the moisture and nitrate content of the soil layer, and the O_2 demand in the layer during a particular week. (O_2 demand is taken to be equivalent to the amount of CO_2 produced by mineralization). The denitrification coefficient will increases with depth.

ii) Leaching

Bypass flow may occur when, shortly after application, fertilizer is exposed at the soil surface and is subject to heavy rainfall. In the model, fertilizer NO_3-N can be lost by bypass flow in the three weeks following application if rainfall exceeds a critical value, (set at 15mm), in any one week. A diminishing fraction of the fertilizer N is at risk during this period and a particular application of fertilizer is at risk to bypass flow only once.

iii) Volatilization

Fertilizer in the form of ammonium sulphate or urea is at risk to volatilization from the soil surface if applied in dry conditions. In the model, 15% of the fertilizer may be lost in this way. A small amount of NH_3-N may also be lost by volatilization from the crop canopy during senescence.

In addition to the above changes, the treatment of the return of crop residues to the soil and the crop nitrogen uptake function were simplified to good effect on the overall operation of the model.

Figures 11 to 18 show measurements and simulations of mineral N in soil at four experimental sites under winter wheat with applications of ^{15}N-labelled fertilizer in 1987 or 1988. Tables 7 & 8 show the measured and modelled fate of the labelled fertilizer at the harvest following the applications, and Table 9 shows the fate of labelled fertilizer at harvest in the first residual year after each application.
In this series of experiments, the amounts of labelled N recovered in the soil organic matter at harvest were generally higher than those observed in the experiments described by Powlson et al.(1986). This suggests that, at the higher rates of application used in 1987 and 1988, root growth and root uptake of both labelled and unlabelled N were promoted, even though crop yields were low in 1987. In the current version of the model, a maximum of 60 kg N/ha, (labelled plus unlabelled), can be taken up by the roots of a high-yielding crop, however, on the heavy clay at Broadmead, 68 kg/ha of labelled N alone was recovered in the soil from both the 1987 and 1988 applications. Clearly, we may need to re-evaluate the parameters for uptake of N by roots.
The model still tends to over-estimate the amount of labelled N remaining in the soil in inorganic form at harvest. The worst case of this was at Butt Close in 1987, however the crop was severely affected by take-all in that experiment, yielding only 1.8 tonne grain ha^{-1}. It is likely that model parameters such as those controlling the rate of uptake of N by the crop and the cycling of dead root material and other plant debris back to soil organic matter differ significantly in a disease-affected crop. This being said, the processes controlling loss of fertilizer N shortly after application are not adequately described in the model. Whilst we allow for conversion of NO_3^- to N_2O and N_2 during denitrification, it is possible that N_2O is also produced as a by-product of the conversion of $NH4^+$ to $NO3^-$ during nitrification (Klemendtsson et al., 1988). This loss process

may be important when the soil is moist but not wet enough to promote rapid denitrification.

CONCLUSIONS

1) The model contains representations of all the major flows of nitrogen into and out of the soil/crop system, even though some of the processes are treated very simplistically. It requires only simple inputs and runs on a weekly time-step. It may be used in retrospect, (i.e. where weather data is known), or to predict the fertilizer requirement of a particular crop using long-term mean weather data.

2) The model is able to account for all the nitrogen flows in the soil/plant system week by week, so that (for example) cumulative annual losses can be assessed. In this way the model could be used to compare the 'nitrogen tightness' of different agronomic systems, winter cereals v. spring cereals, for example.

3) This model gives a good account of the fate of ^{15}N-labelled fertilizer applied to winter wheat or spring barley in a range of soil types. It has been more successful in simulating results from long-term field experiments in which the amount of fertilizer applied to each plot is kept constant, as in these experiments, there appears to be some relationship between crop yield and the amount of N in the roots. This relationship does not seem to hold particularly where the crop is affected by weed competition or by disease. Further work is needed on the amount of N held in roots and on the partitioning of nitrogen between crop and roots.

4) The model gives acceptable fits to measurements of soil mineral N from field experiments with successive winter wheat crops or with a winter wheat crop followed by a two-year bare fallow.

5) Comparisons with ^{15}N data have indicated that the processes causing gaseous loss of fertilizer N shortly after application are complex and are probably highly sensitive to moisture and temperature conditions in the soil. We now intend to investigate this point by laboratory and field experimentation.

6) As a result of this project, two MAFF Open Contracts have been gained by Rothamsted. In one of these, the model is being used to study nitrogen dynamics under different farming systems in Nitrate Sensitive Areas. As part of this project, an improved and extended menu-driven system has been devised for the P.C. version of the model (Smith 1992). In the other project, model recommendations of fertilizer requirement are being compared to those generated by the ADAS Fertiplan system. Both these projects will involve a detailed evaluation of the model in a wider range of crops and soils. Eventually, we would hope to recommend the model for general use by advisors.

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Table 1. Details of spring barley data sets

No.	Location	Year	Soil Type	Treatments
1	Hoosfield, Rothamsted	1986-1988	Silty clay loam	N0:0, N1:48, N2:96, N3:144 kg N/ha ^{15}N applied 1986
2	Hoosfield, Rothamsted	1986-1988	Silty clay loam	35 t/ha/annum FYM + N0,N1,N2,N3 treatments as above. ^{15}N applied 1986
3	Hoosfield, Rothamsted	1987-1989	Silty clay loam	As 1 above. ^{15}N applied 1987
4	Hoosfield, Rothamsted	1987-1989	Silty clay loam	As 2 above. ^{15}N applied 1987
5	Lintlaw, Berwickshire	1987	Loam	N0:0, N1:60, N2:90, N3:120, N4:150 kg N/ha 4 sub-treatments of N3 as 3 split applications at seedbed, brairding & tillering : 120-0-0, 60-60-0, 60-0-60, 0-120-0. ^{15}N applied in all treatments.
6	Middlestot, Berwickshire	1988	Sandy clay loam	Treatments as 5 above.
7	Bush, Midlothian	1988	Alluvial fan complex	Treatments as 5 above.

Data sets 1 to 4 : P. Poulton, IACR Rothamsted (pers. comm.).

Data sets 5 to 7 : (McTaggart & Smith 1992)

Table 2. Menu choices available for entering field information

Region	North East, North West, West, Midlands, East,South West, South East, South
Soil Type	Sand, Loam, Clay
Rooting Depth	50cm, 100cm, 150cm
Previous Crop	Winter Cereal, Spring Cereal, Oilseed Rape, Legume, Potatoes, Sugar Beet
Previous Yield	(enter in t/ha)
Previous Harvest	(enter date DD/MM)
Current Crop	Winter Wheat, Winter Barley, Spring Wheat, Spring Barley
Sowing Date	(enter date DD/MM)
Expected Yield	(enter in t/ha)
FYM applied	(enter in t/ha)
FYM application	(enter date DD/MM)

Table 3. Example of model demonstration for two sites

	Site A	Site B
	Early-sown winter cereal in Eastern region	Spring Barley in North-Western region
Region	East	North-West
Soil Type	Loam	Sand
Rooting Depth	150cm	150cm
Previous Crop	Winter cereal	Winter cereal
Previous Yield	8 t/ha	6 t/ha
Previous Harvest	05/08	25/08
Current Crop	Winter Wheat	Spring Barley
Sowing Date	10/09	10/03
Expected Yield	8 t/ha	4 t/ha
FYM applied	0 t/ha	0 t/ha
Date applied	00/00	00/00

Table 4. Comparison of N fertilizer prediction for two sites

	Site A	Site B
TARGET		
Expected Yield of crop *	8	4
Crop N target (N_c)	263	131
N recovered by crop (Sowing-Spring) (N_{cs})	70	9
Crop N required (Spring-Harvest) (N_c - N_{cs})	193	122
INPUTS		
Available Soil Mineral N in Spring (N_s)	0	0
Predicted Mineralization (Spring-Anthesis) (N_m)	17	12
Atmospheric input (Spring-Anthesis) (N_a)	10	10
Total inputs ($N_s + N_m + N_a$)	27	22
LOSSES		
Predicted Denitrification (Spring-Anthesis) (N_d)	3	3
Predicted Leaching (Spring-Anthesis) (N_l)	0	0
Total Losses ($N_d + N_l$)	3	0
BALANCE		
Total Mineral N available from soil ($N_s + N_m + N_a$) - ($N_d + N_l$)	24	19
Fertilizer N required (N_f)	169	103

* in t/ha; remaining values in kg N/ha

Table 5a. Annual Nitrogen Balance (Harvest to Harvest) for Site A

Initial soil N			Final soil N		
	Total	Fertilizer		Total	Fertilizer
Organic N	4039	0	Organic N	4038	30
Mineral N	63	0	Mineral N	50	2
Total N in Soil	4102	0	Total N in soil	4088	32
Inputs			Losses		
Fertilizer N	169	169	Denitrification	20	2
Stubble N	25	0	Senescence	28	18
Atmospheric N	46	0	Crop offtake	189	117
			Leaching	17	0
Total inputs of N	240	169	Total Losses	254	137
Initial N + inputs of N	4342	169	Final soil N + losses of N	4342	169
N mineralized*	76	1			

Table 5b. Annual Nitrogen Balance (Harvest to Harvest) for Site B

Initial soil N			Final Soil N		
	Total	Fertilizer		Total	Fertilizer
Organic N	2388	0	Organic N	2400	29
Mineral N	33	0	Mineral N	47	3
Total N in Soil	2421	0	Total N in soil	2447	32
Inputs			Losses		
Fertilizer N	103	103	Denitrification	31	3
Stubble N	27	0	Senescence	12	8
Atmospheric N	46	0	Crop offtake	80	60
			Leaching	27	0
Total inputs of N	176	103	Total Losses	150	71
Initial N + inputs of N	2597	103	Final soil N + losses of N	2597	103
N mineralized*	57	4			

* Mineralization is a transfer process so does not appear separately in the sum of inputs.

Table 6 Details of sites & ^{15}N applications to wheat in MAFF project 'Nitrate Leaching from Arable Land'

Site	Soil type	1987 Application Year		1988 Application Year	
		^{15}N Applied kg/ha	Yield* t/ha	^{15}N Applied kg/ha	Yield* t/ha
Rothamsted					
Claycroft	Clay loam	224	7.0	215	6.3
Webbs	Chalky loam	223	4.5	218	7.1
Woburn					
Butt Close	Sandy loam	173	1.8	176	6.2
Broadmead	Heavy clay	222	4.2	227	5.7

* Yield at 85% dry matter

Table 7. Harvest 1987 : fate of ^{15}N-labelled fertilizer applied to winter wheat in spring 1987

		Crop N					Soil ^{15}N at harv				Inorg N harv	
	kg ^{15}N/ ha	Total		^{15}N		Depth	Total		Inorg			
		Obs[1]	Sim[2]	Obs	Sim		Obs	Sim	Obs	Sim	Obs	Sim
Claycroft	224	204	204	124	132	0-23	40	25	3.4	1.2	34	26
						23-50	3	10	0.9	3.9	9	11
						50-70	1	<0.1	0.6	<0.1	3	20
						70-100	2		0.7		4	
						Total	46	35	5.6	5.1	50	57
Webbs	223	174	174	112	115	0-23	39	29	3.0	5.6	31	36
						23-50	10	11	0.7	5.0	19	13
						50-70	10	<0.1	0.6	<0.1	8	20
						70-100	3		0.5		9	
						Total	62	40	4.8	10.6	67	69
Butt Close	173	98	96	67	60	0-23	43	19	3.3	1.8	18	15
						23-50	2	36	3.3	31.1	17	45
						50-70	2	7	3.0	6.6	13	17
						70-100	1		2.8		11	
						Total	48	62	12.4	39.5	59	77
Broadmead	222	184	184	82	115	0-23	64	23	6.0	1.1	55	30
						23-50	1	18	0.3	11.2	18	23
						50-70	1	3	0.2	2.8	7	31
						70-100	2		0.5		7	
						Total	68	54	7.0	15.1	87	84

[1] Observed
[2] Simulated

Table 8. Harvest 1988 : fate of ^{15}N-labelled fertilizer applied to winter wheat in spring 1988

		Crop N					Soil ^{15}N at harv				Inorg N harv	
	kg ^{15}N/ ha	Total		^{15}N		Depth	Total		Inorg			
		Obs[1]	Sim[1]	Obs	Sim		Obs	Sim	Obs	Sim	Obs	Sim
Claycroft	215	198	197	123	140	0-23	36	32	2.8	5.3	32	42
						23-50	1	16	0.6	9.6	16	22
						50-70	0	0	0.2	0.0	6	20
						70-100	0		0.1		7	
						Total	37	48	3.7	14.9	61	84
Webbs	218	206	206	134	146	0-23	39	34	2.8	7.3	27	37
						23-50	1	18	0.5	10.6	15	26
						50-70	0	0	0.1	0	3	20
						70-100	0		0.1		2	
						Total	40	52	3.5	17.9	47	83
Butt Close	176	155	150	111	106	0-23	36	33	2.5	7.5	18	32
						23-50	0	13	0.6	6.7	11	13
						50-70	0	0.3	0.2	0.3	5	11
						70-100	0		0.1		6	
						Total	36	46.3	3.4	14.5	40	56
Broadmead	227	201	201	130	140	0-23	65	36	6.6	9.3	63	46
						23-50	3	16	0.2	8.8	27	23
						50-70	0	0	0.1	0	7	30
						70-100	0		0.1		4	
						Total	68	52	7.0	18.1	101	109

[1] Observed
[2] Simulated

Table 9. Fate of ^{15}N-labelled fertilizer at harvest in first residual year from applications to winter wheat in 1987 and 1988.

1st residual year		Series I 1988				Series II 1989			
	Residual crop	^{15}N in soil		^{15}N in crop		^{15}N in soil		^{15}N in crop	
		Obs[1]	Sim[1]	Obs	Sim	Obs	Sim	Obs	Sim
Claycroft	Wheat	37	35	3	2.5	34	39	4	5.1
Webbs	Wheat	48	35	3	2.6	31	30	2	4.2
Butt Close	Wheat	57	25	4	2.5	17	37	3	2.7
Broadmead	Wheat	57	35	2	2.5	42	40	1	2.2

[1] Observed

[2] Simulated

Fig. 1 Measured and modelled values of soil mineral N (0–100cm)
Claycroft 1986–89

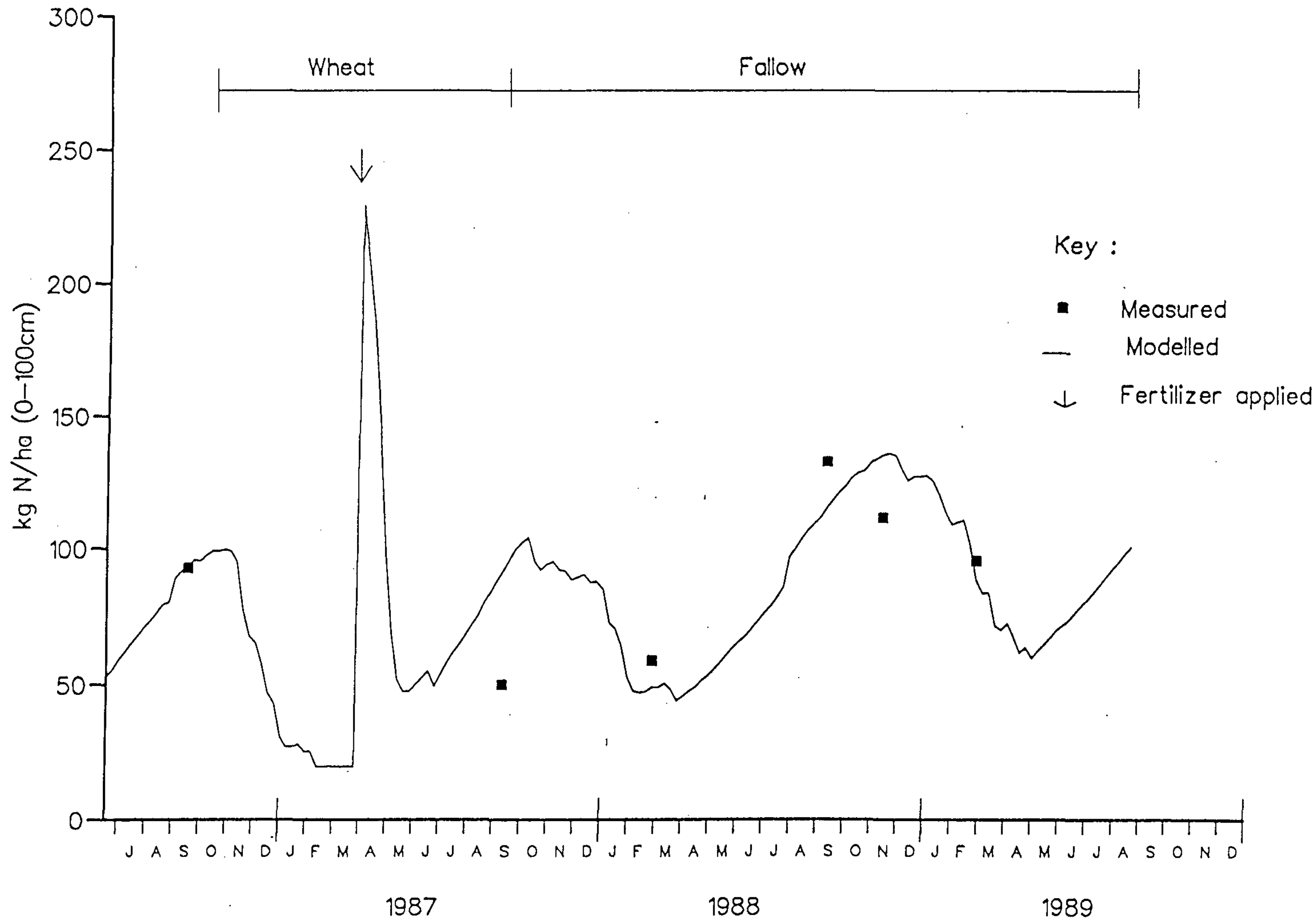


Fig. 2 Measured and modelled values of soil mineral N (0–100cm)
Butt Close 1986–89

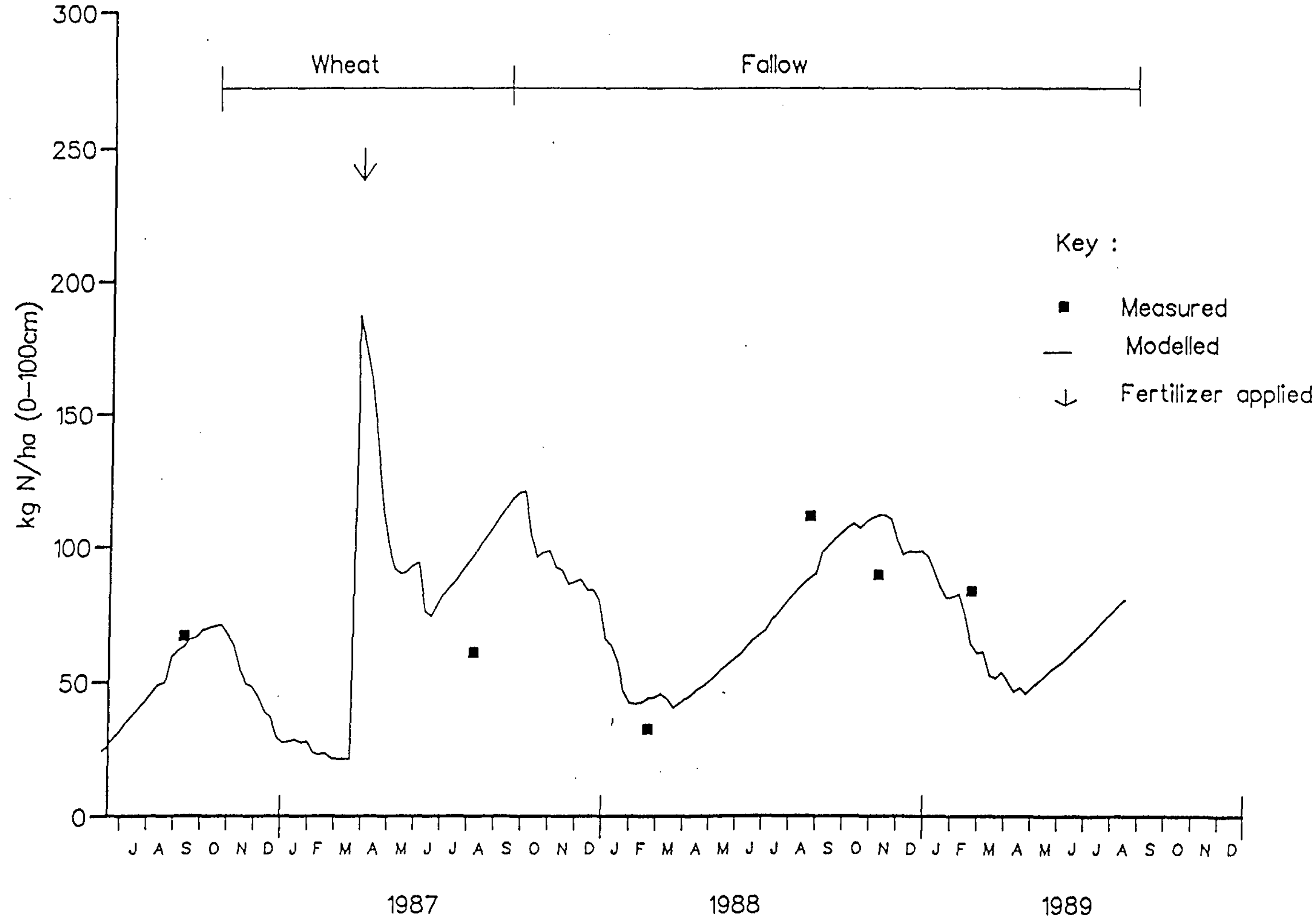


Fig. 3 Relationship between grain yield of Spring Barley and total N in crop at harvest

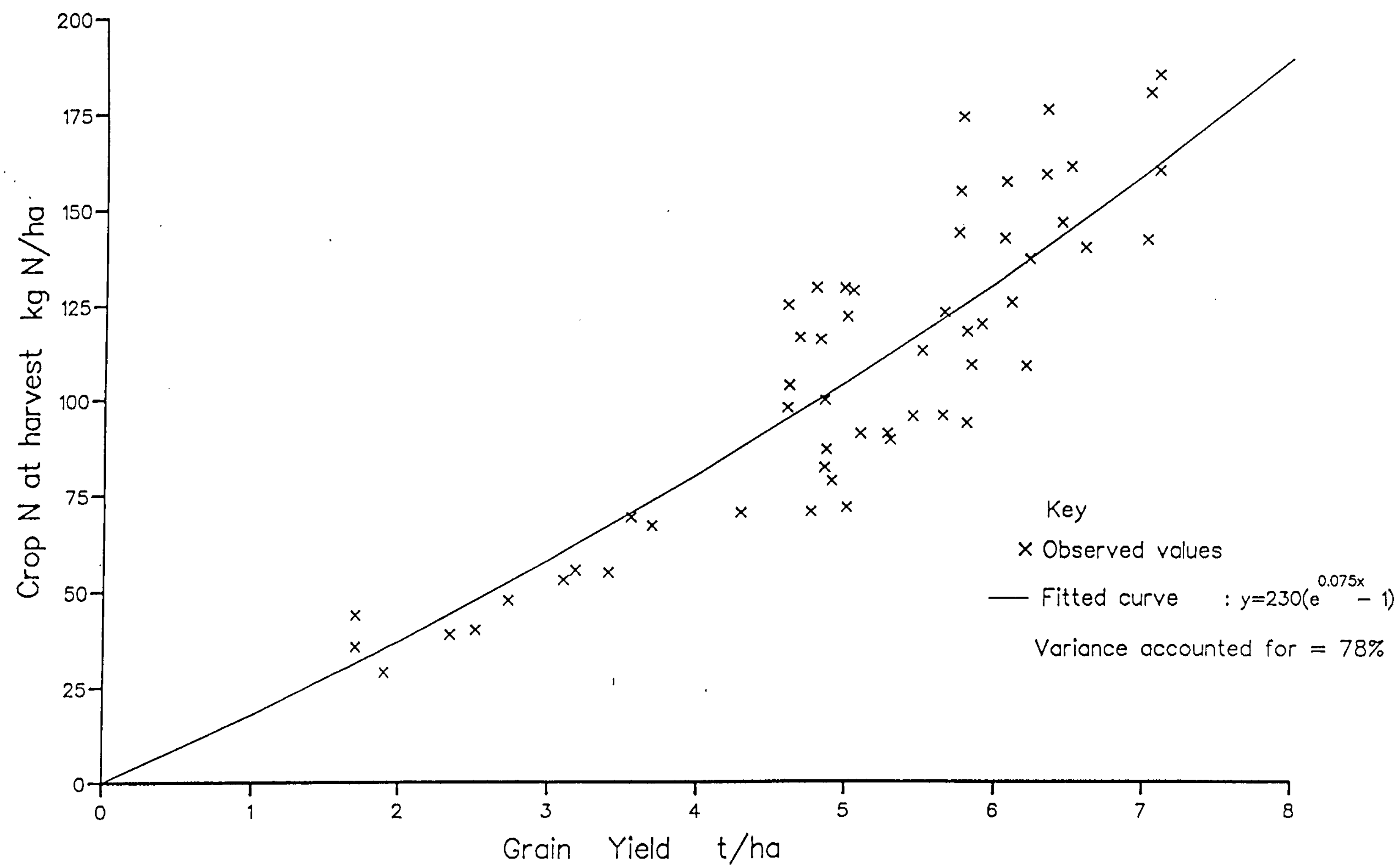


Fig. 4 Relationship between nitrogen uptake by spring barley and day–degrees : Bush 1988

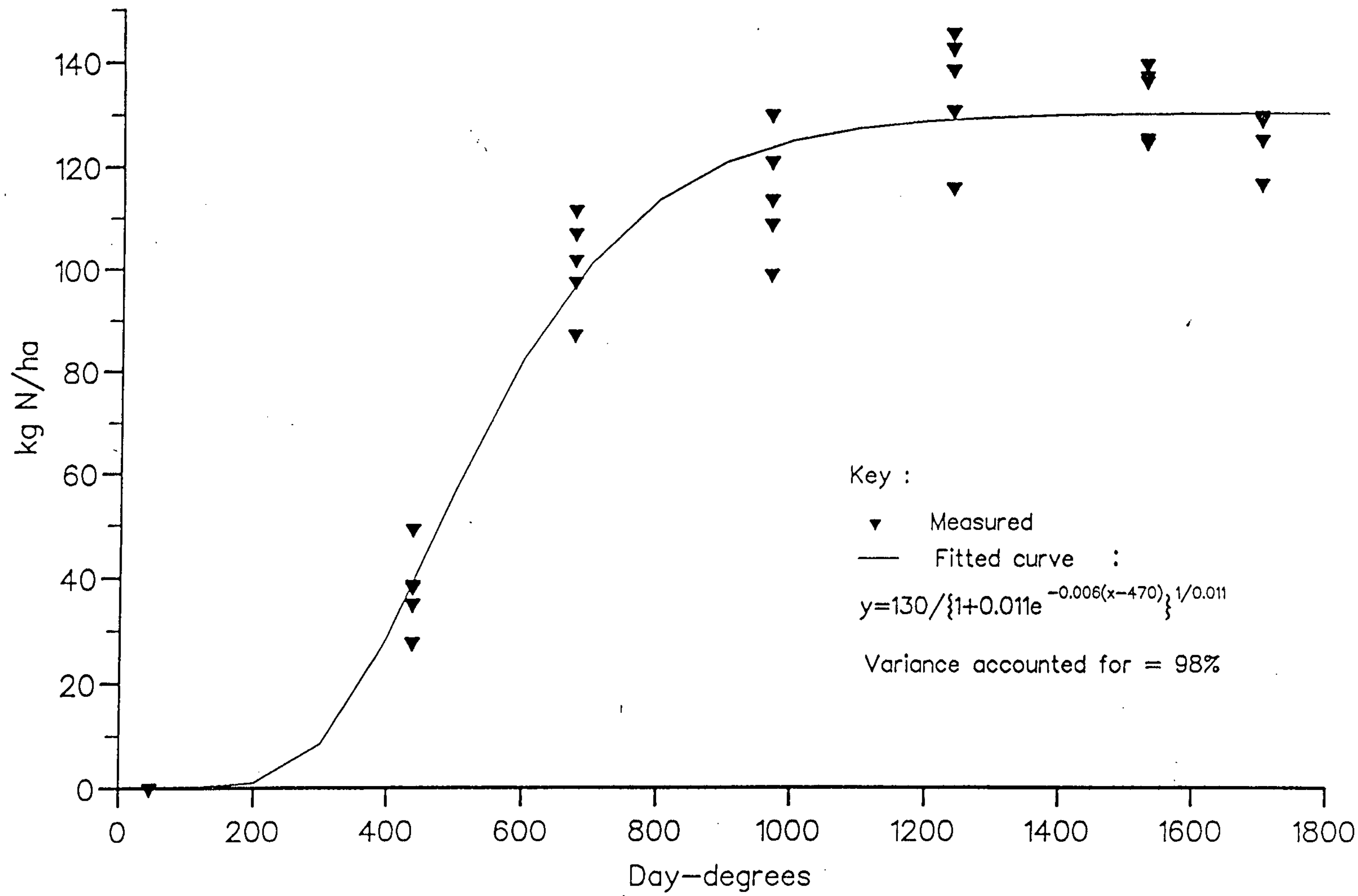


Fig. 5 Root nitrogen requirement vs. yield of spring barley

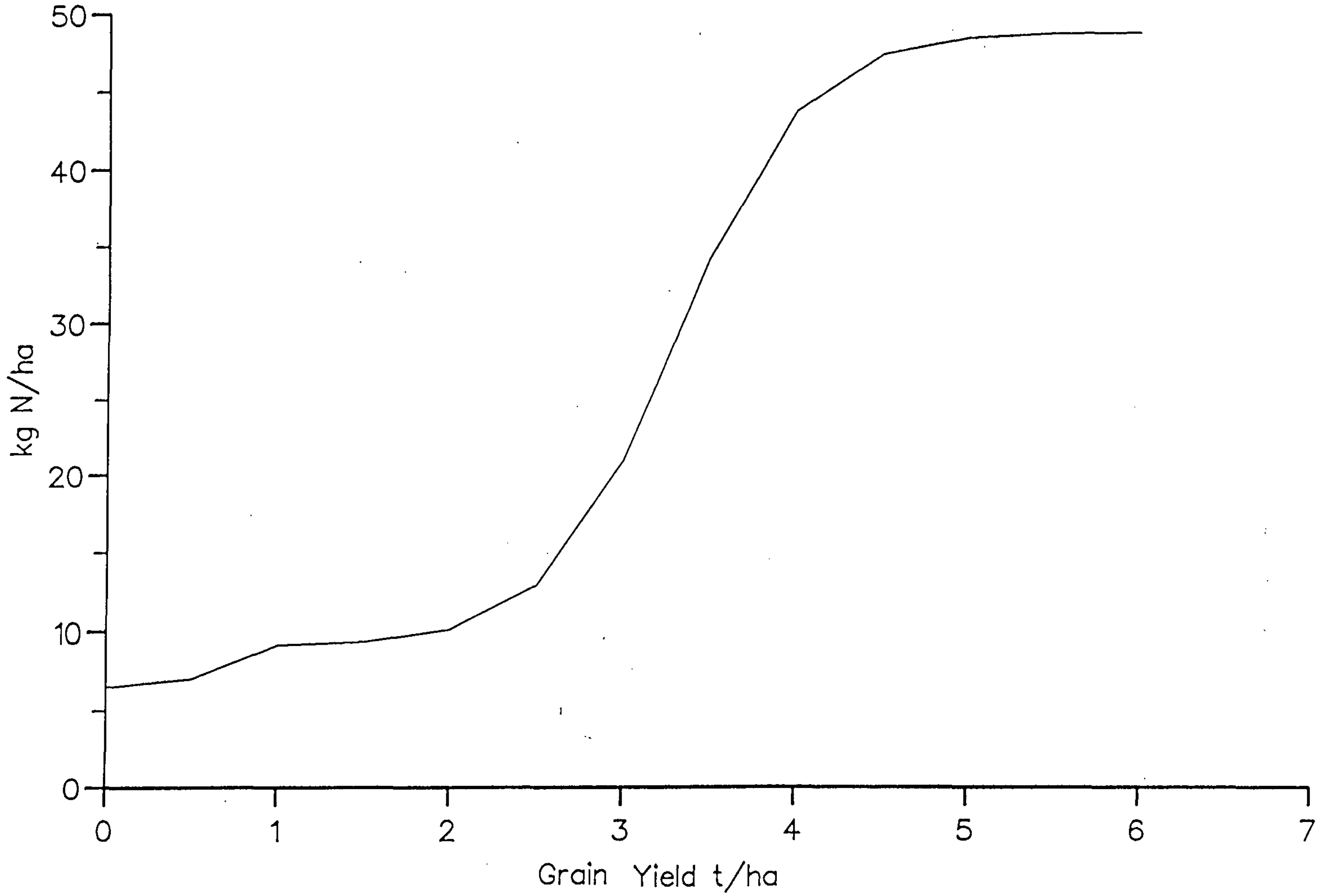


Fig. 6 Measured and modelled values for the decline of labelled N in soil and uptake of residual labelled N by successive crops : Hoosfield 1986–88

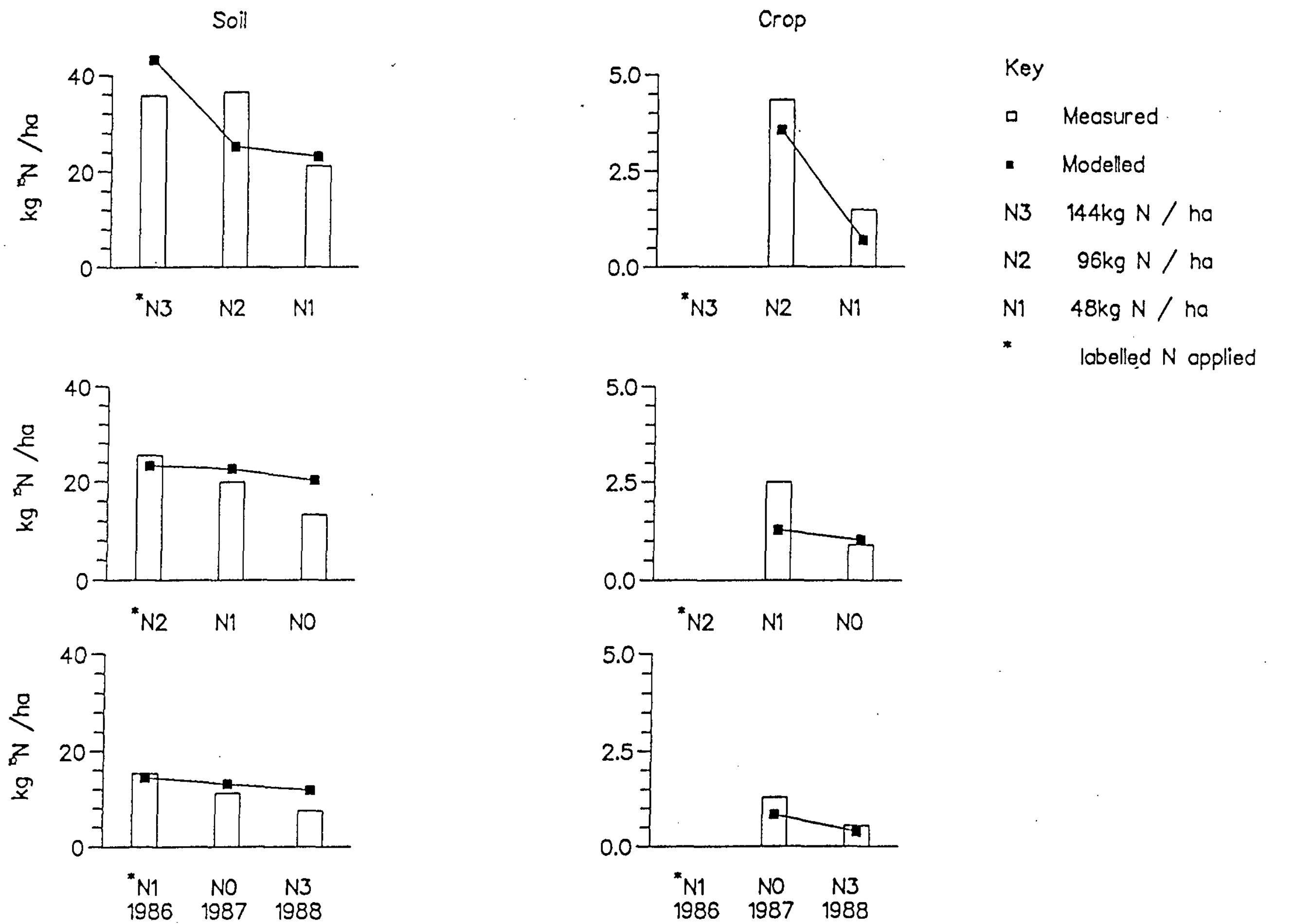


Fig. 7 Measured and modelled values of the decline of labelled N in soil and uptake of residual labelled N by successive crops : Hoosfield 1987–89

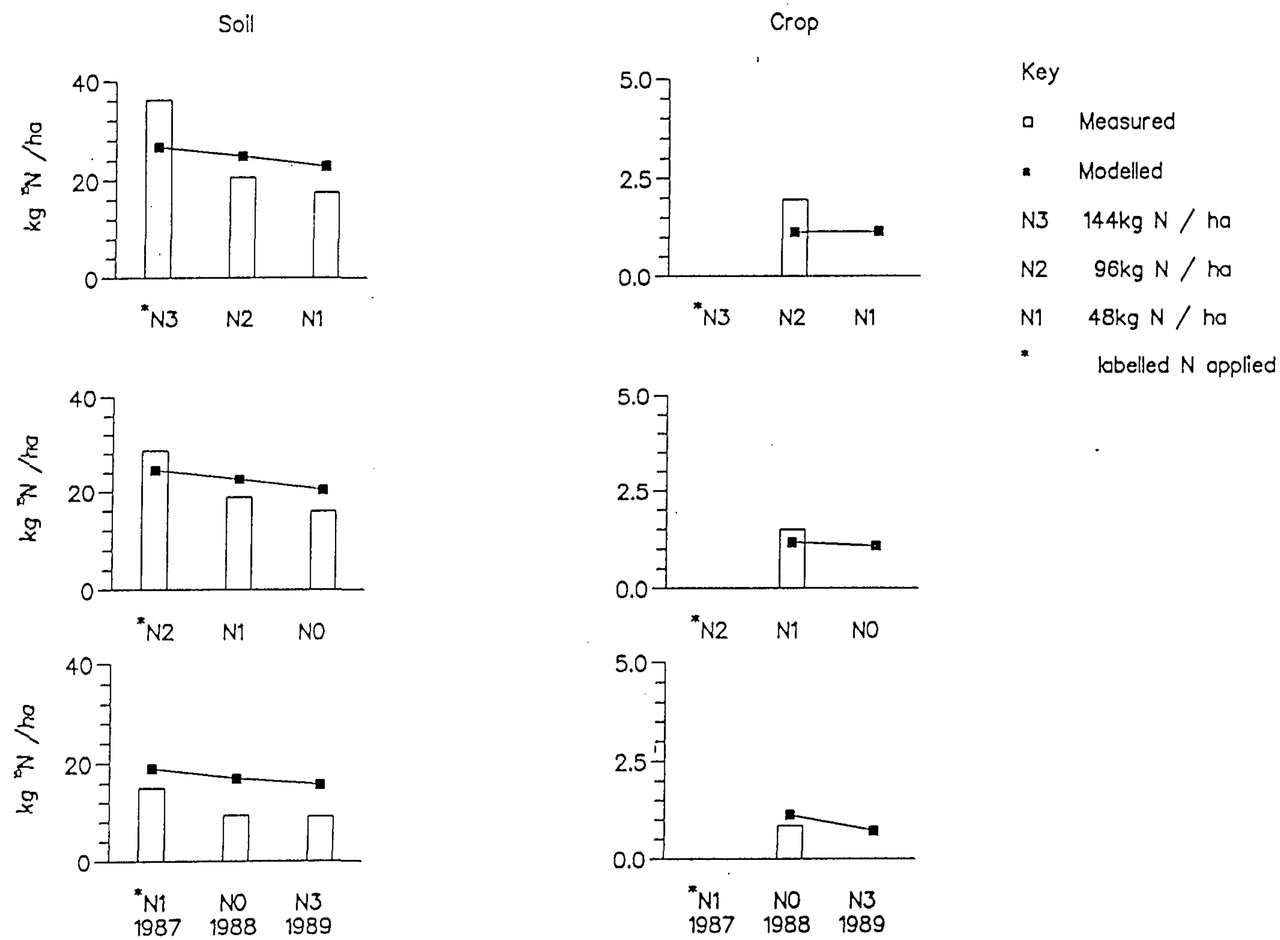


Fig. 8 Measured and modelled values for the decline of labelled N in soil and uptake of residual labelled N by successive crops : Hoosfield 1986–88 (Plots receiving 35 t/ha FYM annually)

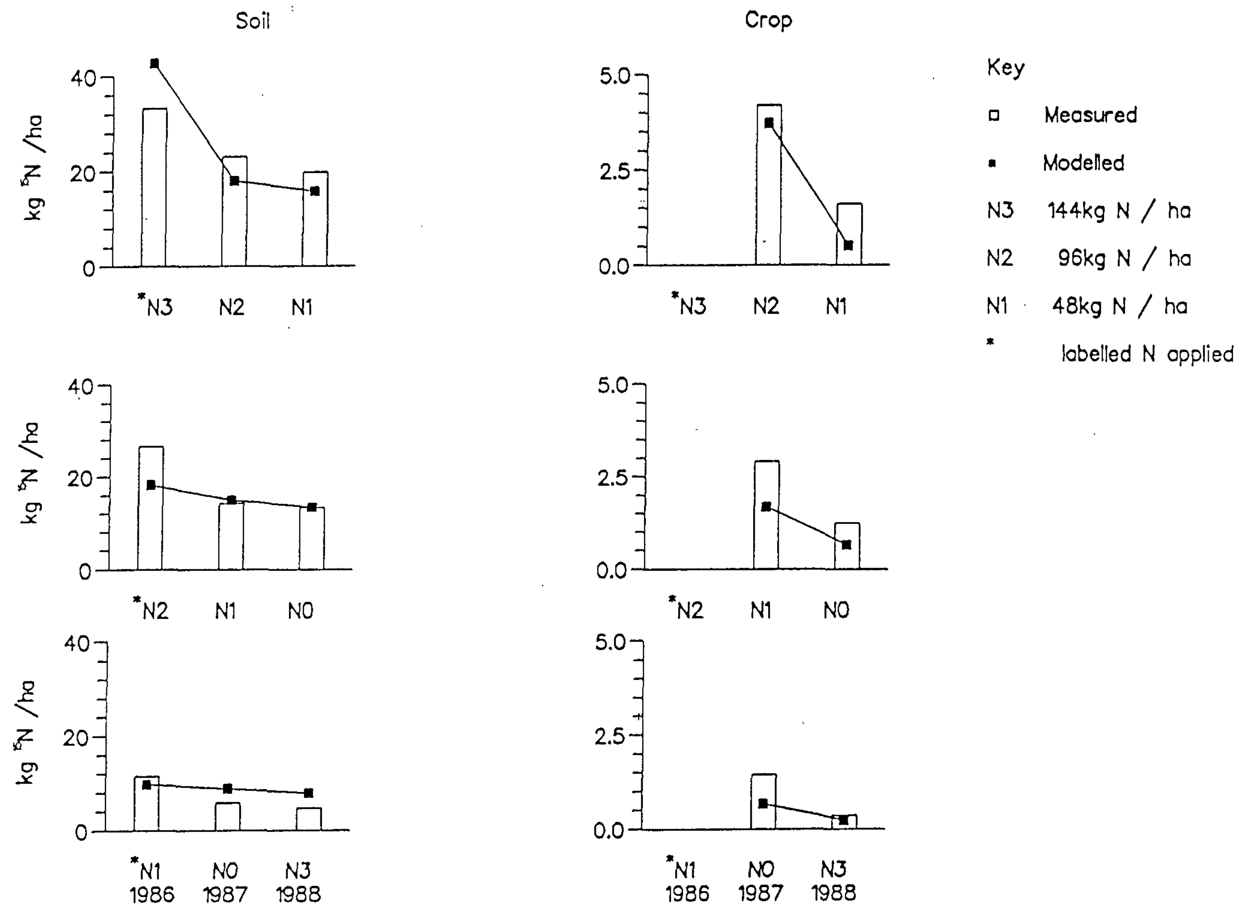


Fig. 9 Measured and modelled values for the decline of labelled N in soil and uptake of residual labelled N by successive crops : Hoosfield 1987–89 (Plots receiving 35 t/ha FYM annually)

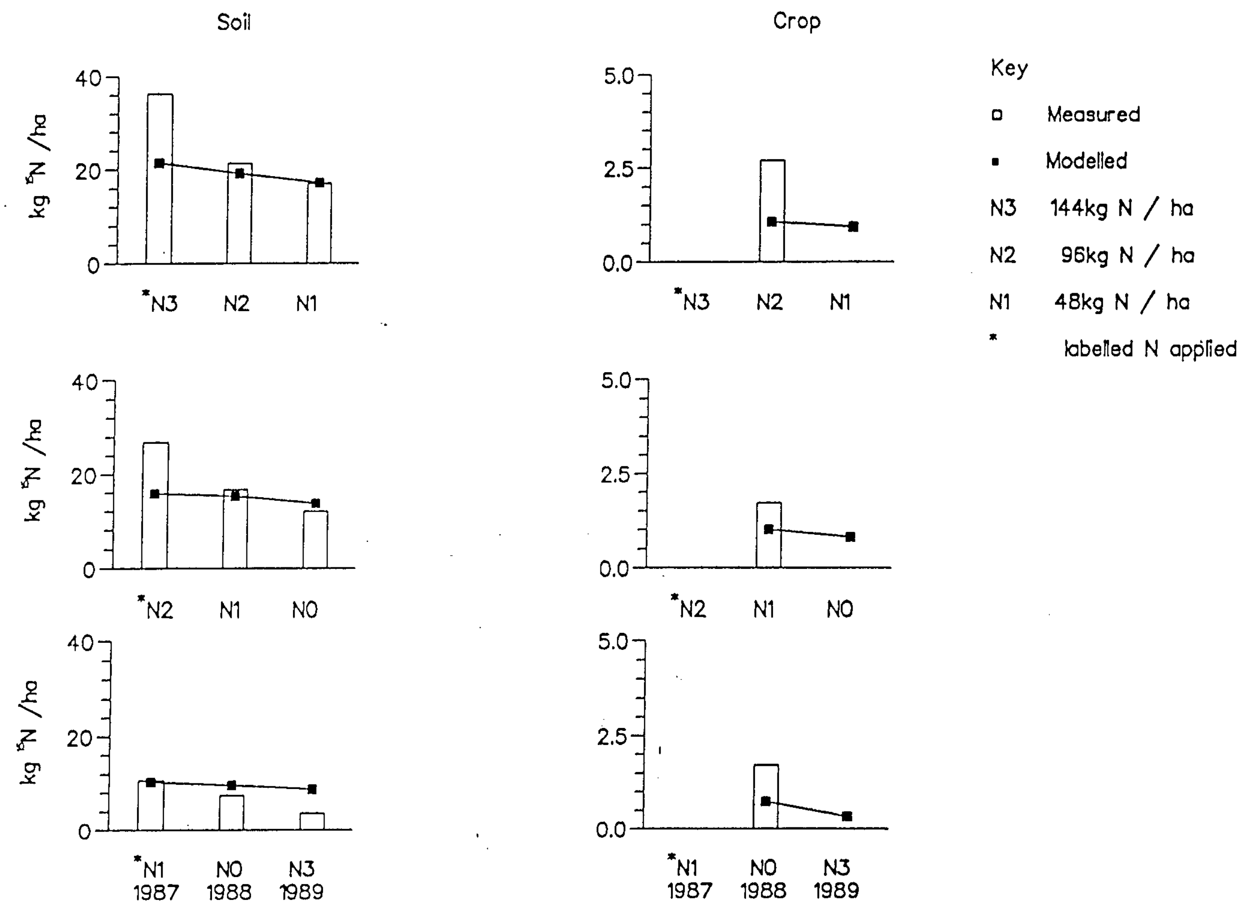


Fig. 10 Fate of fertilizer N
over the application-harvest period

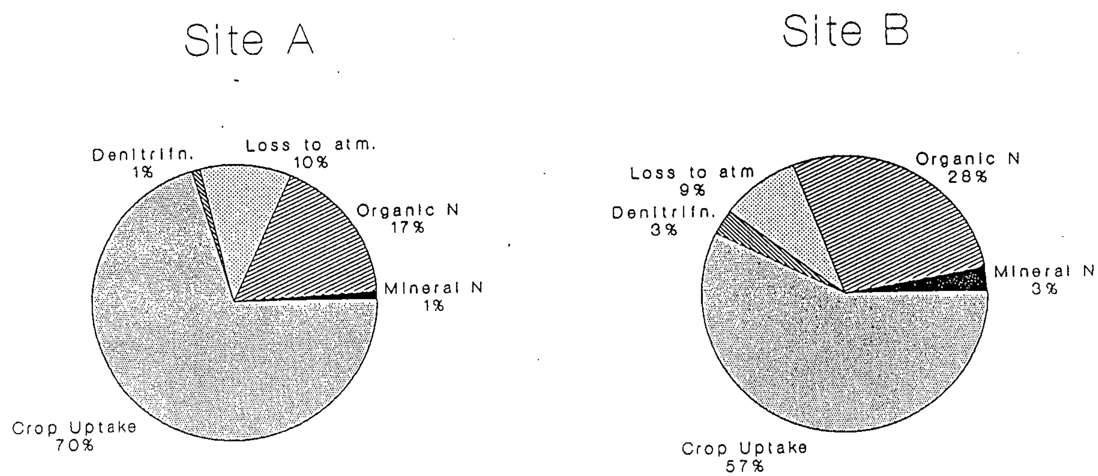


Fig. 11 Comparison of Simulated and Observed Soil Mineral N
Claycroft: 1986-89: Winter Wheat

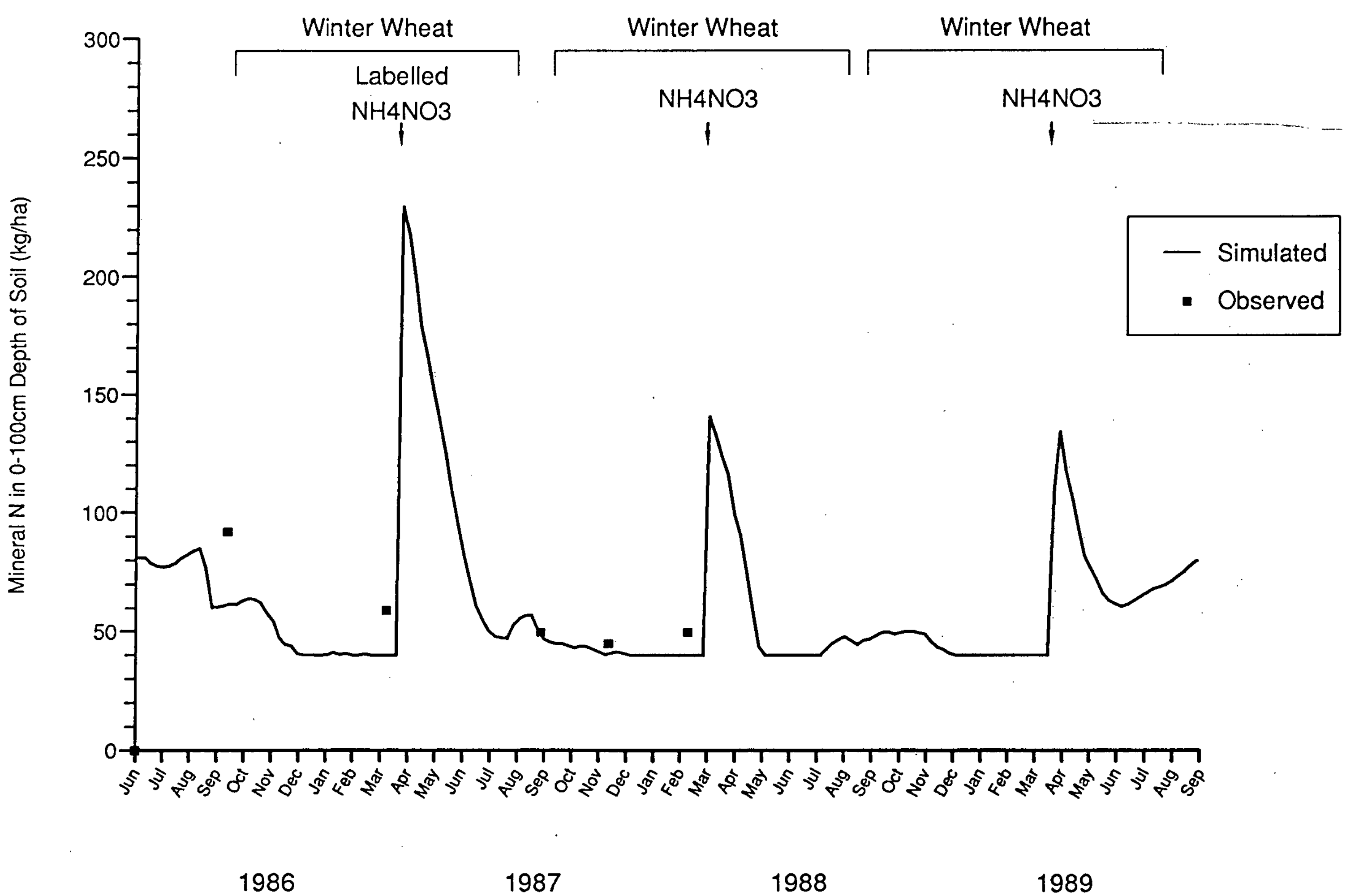


Fig. 12 Comparison of Simulated and Observed Soil Mineral N

Butt Close: 1986-89: Winter Wheat

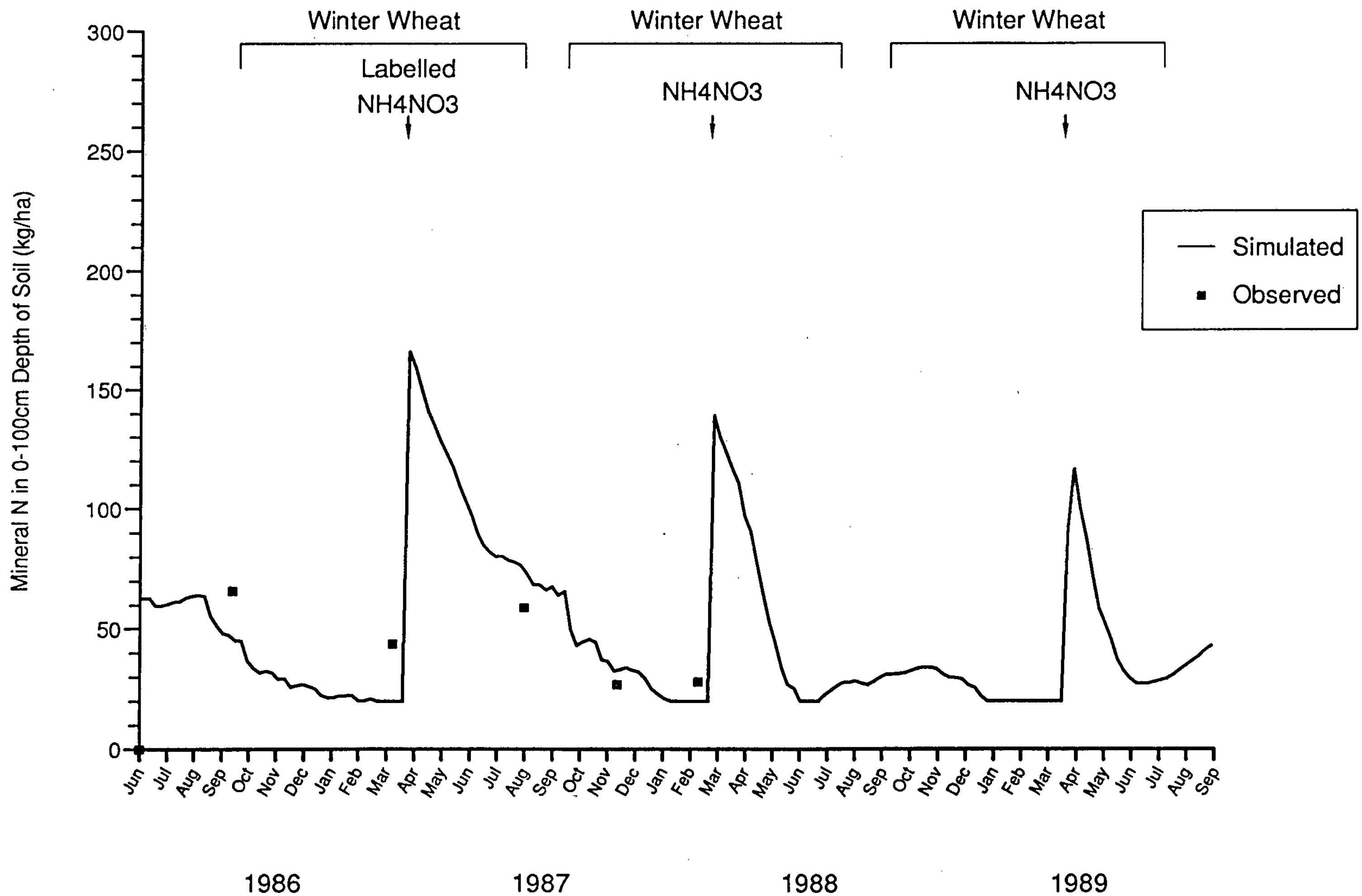


Fig. 13 Comparison of Simulated and Observed Soil Mineral N

Webbs: 1986-89: Winter Wheat

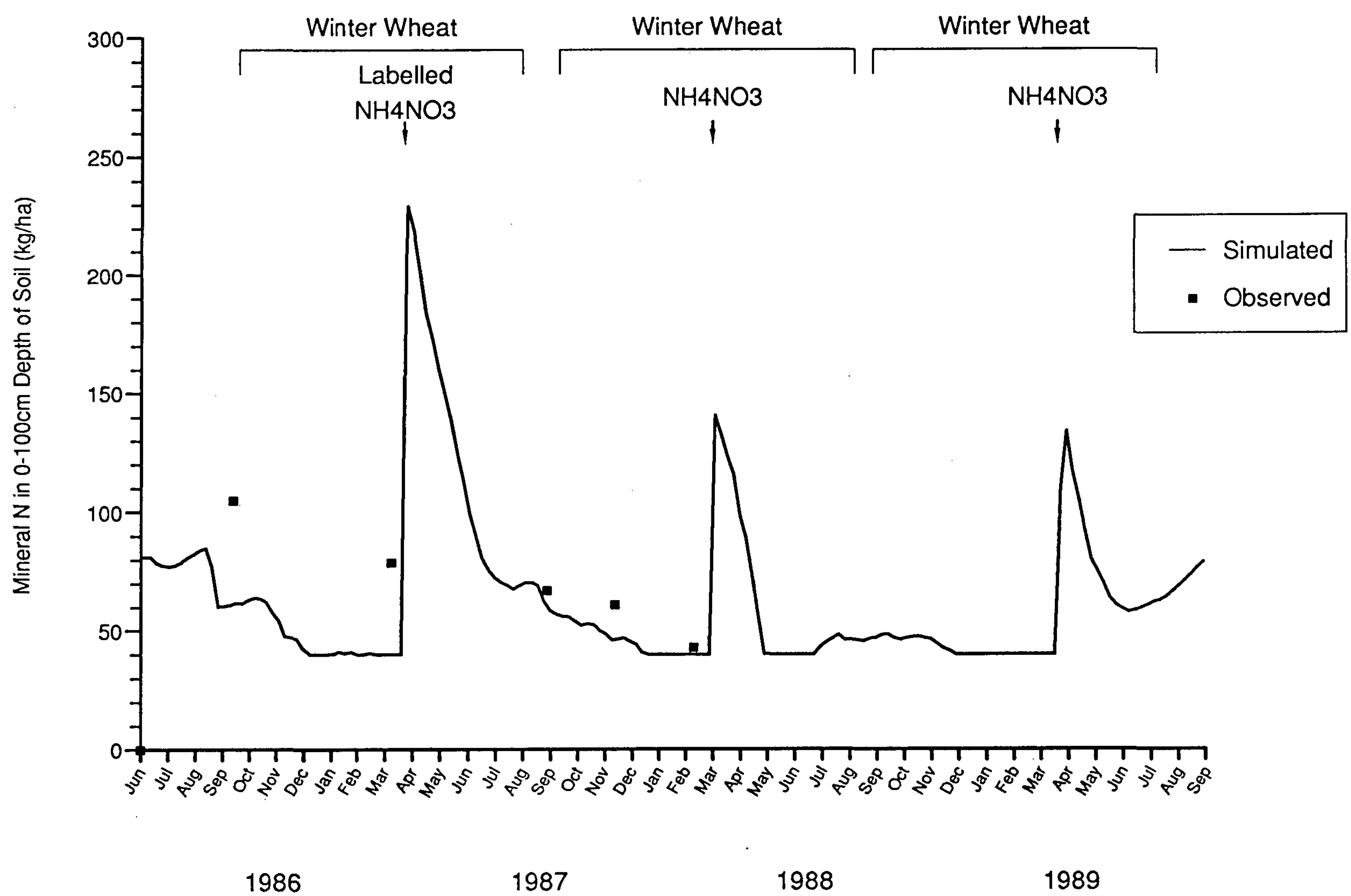


Fig. 14 Comparison of Simulated and Observed Soil Mineral N
Broadmead: 1986-89: Winter Wheat

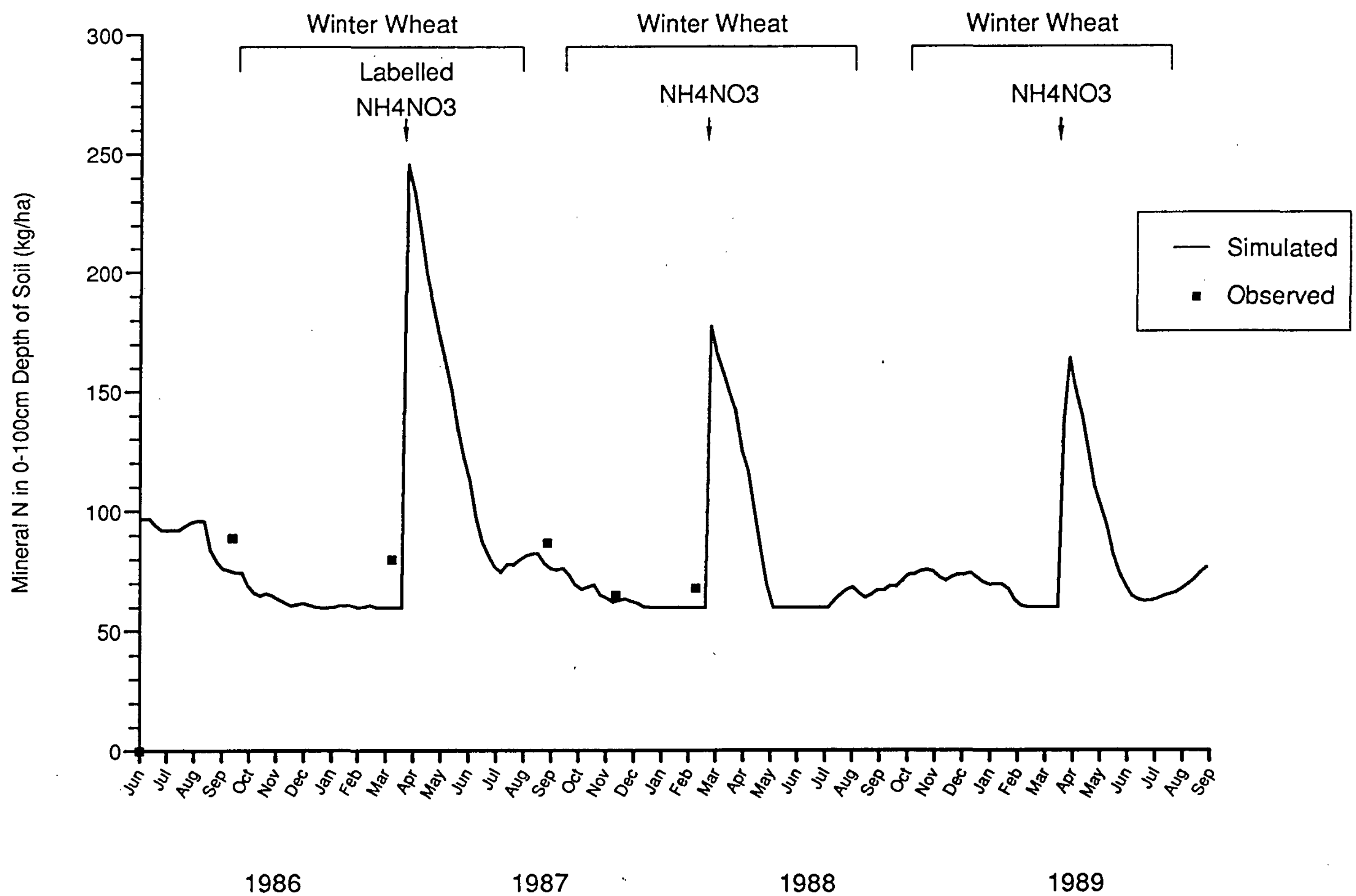


Fig. 15 Comparison of Simulated and Observed Soil Mineral N
Claycroft: 1987-90: Winter Wheat

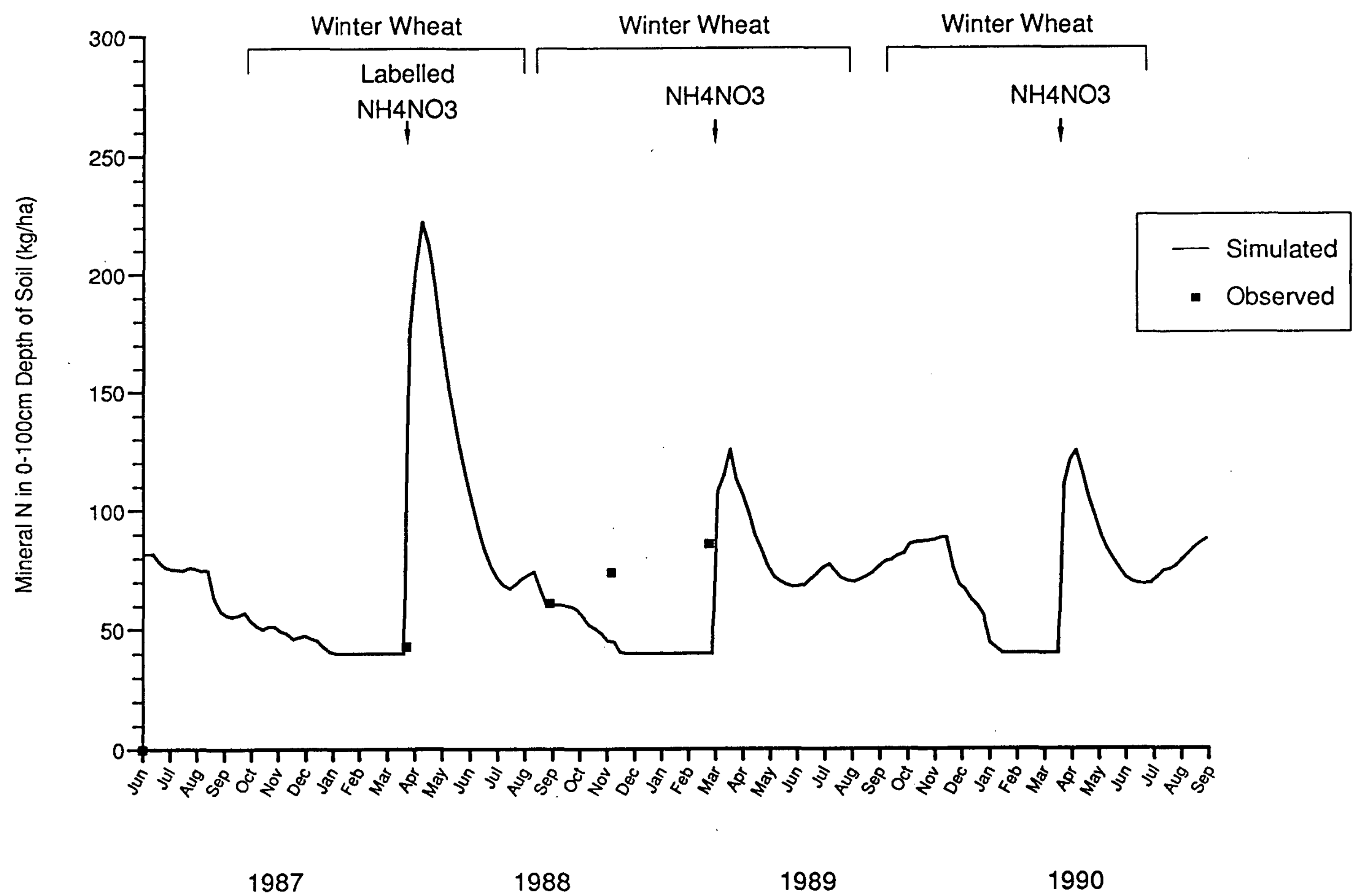


Fig. 16 Comparison of Simulated and Observed Soil Mineral N

Butt Close: 1987-90: Winter Wheat

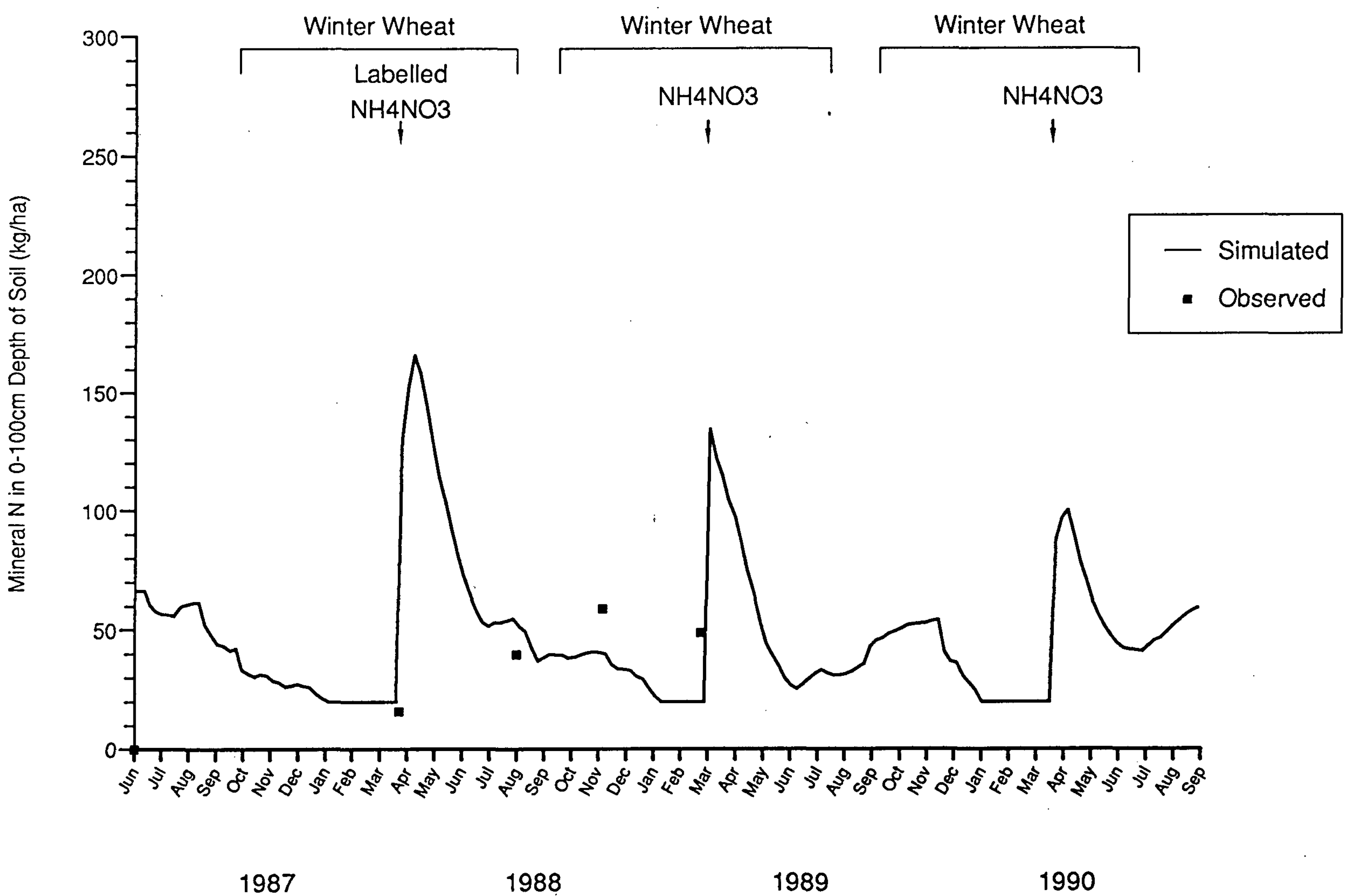


Fig. 17 Comparison of Simulated and Observed Soil Mineral N

Webbs: 1987-90: Winter Wheat

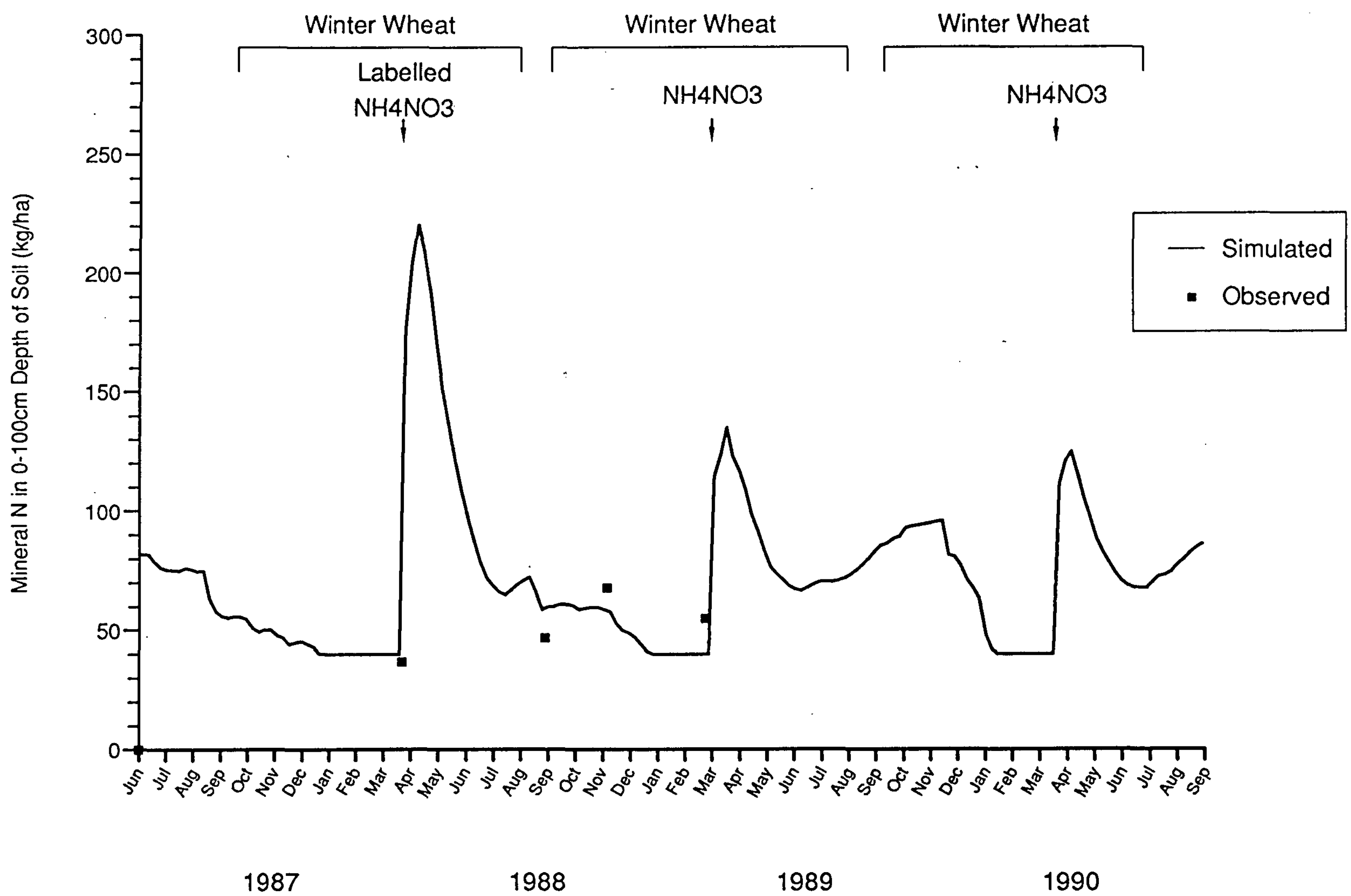
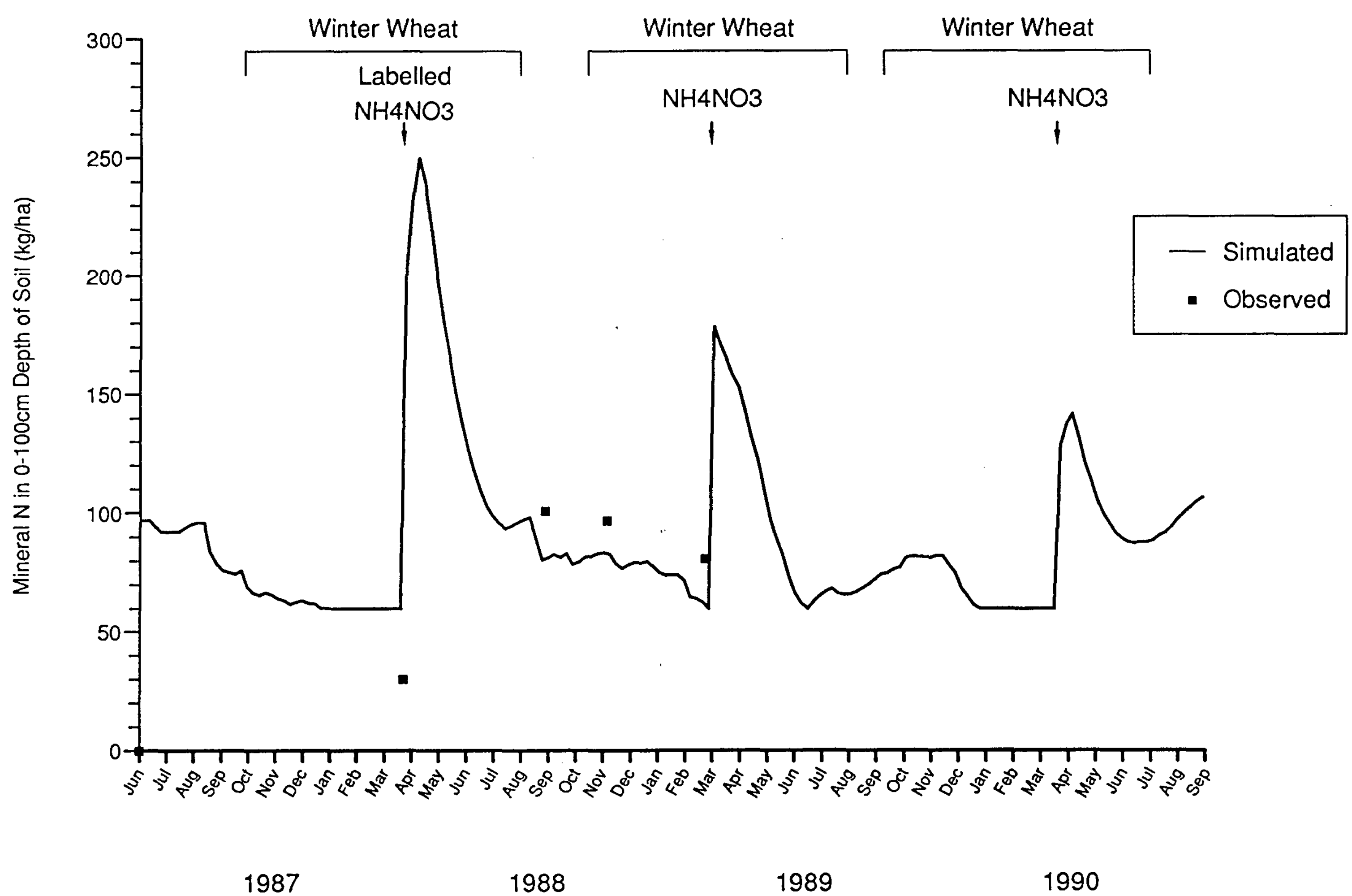


Fig. 18 Comparison of Simulated and Observed Soil Mineral N

Broadmead: 1987-90: Winter Wheat



APPENDIX

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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With: 39 Pages
3 Tables
6 Figures
\+ List of symbols

Short title: Modelling nitrogen in crop and soil

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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 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 root mean square difference between modelled and measured recovery of labelled N by the crop was 0.6 kg/ha and 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 is 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 on 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 & 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: fourteen 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 process 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, straw being removed in all the experiments described by Hart *et al.* (1993). There are three input compartments: chemically combined N from the atmosphere, 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 through 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 are 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 allowed if the rainfall in a particular week exceeds a specified threshold value (R_{CRIT}). 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:

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

where *P* is the quantity of nitrate formed in one week, in kg NO_3-N/ha, *m* is the temperature rate modifier (see equation 3 below), *s* the soil moisture rate modifier (see equation 4 below), *q* is a rate constant (set provisionally at 0.6/week, by fitting equation (1) to Addiscott's (1983) data) and N_A is the quantity of ammonium present in the soil layer (in kg NH_4-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 $(1-\alpha-\beta)$.

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:

Decomposition in unit time (1 week) $= C_o\,(1-e^{-smr})$ (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 (CO_2 - 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 ($< 2\ \mu m$) 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 equation (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:

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

where C_{AO} is annual return of C to the soil, in t/ha

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 25cm 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:

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

where C_{sc} is stubble + chaff carbon, in t/ha

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

$$N_{AO} = \text{N returned in roots, root exudates and dead tillers + N returned in chaff and stubble}$$

$$= 60\ (1 - e^{-0.5G}) + 0.12\ (U_G + U_S) \qquad (8)$$

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) x (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 is subtracted from the total C (as given by equation 6) returned during the year.

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

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

and

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

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, n are rate constants

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

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

where G is the grain yield, in t/ha, as before

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 16)

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: it 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:

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

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.

<u>The time course of nitrogen uptake</u>. This is calculated by the equation proposed by Whitmore & Addiscott (1987). The N taken up by a particular time is given by:

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

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

f is a rate constant

Note that f is set during the iterative parameter fitting process (see below), not calculated as 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°C.

(2) Crops can only deplete each 50 cm soil layer to the specified minimum of NH_4-N (N_{RESA}) and of NO_3-N (N_{RESN}) for each soil type.

(3) Crops deplete each layer of NO_3-N and NH_4-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 75cm before starting to deplete the 50-100 cm layer, and to 125 cm for the 100-150 cm layer. They terminate at 150cm in the three soils used by Hart *et al.* (1993).

(6) Uptake stops 5 weeks before harvest.

<u>Mineralization of organic N and immobilization of inorganic N.</u> The rules for the behaviour of organic N are obtained directly from those for organic C (see section above, headed 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 (1987) 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 $z\ C_o\ (1 - e^{-smr})$. 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':

$$L = N_N R/R_{FC} \tag{14}$$

where L is the amount of NO_3-N moving into the layer below, N_N is the amount of NO_3-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 NO_3-N in each of the 0-50, 50-100 and 100-150 cm layers is never leached: N_{RESN} depends on soil type.

Fertilizer NO_3-N can be lost by bypass flow (or by surface runoff: both processes are modelled in the same way) in the three weeks after fertilizer addition. Lawes, Gilbert and Warington (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

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

where L_B is the amount of fertilizer NO_3-N leached by bypass flow, σ is the bypass flow factor per mm excess rain, F_N is the quantity of fertilizer NO_3-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 NO_3-N lost by bypass flow immediately joins the NO_3-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 NO_3-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 approximately one, 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 percent 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 NO_3-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

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

where θ is the denitrification factor and W is the combined evolution of CO_2-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 $(^{15}NH_4)_2SO_4$ and $K^{15}NO_3$, so that sulphate was always present. Powlson *et al.* (1986) examined the fate of labelled N applied either as $^{15}NH_4$ or $^{15}NO_3$. 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, about 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 NH_4-N (F_A) can be lost by volatilization, according to the equation

$$V_S = \phi_S\ F_A \qquad (17)$$

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 less than 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

$$V_C = \phi_C(U_G + U_S)/5 \tag{18}$$

where V_C is N loss in one week by volatilization, in kg N/ha, $(U_G + U_S)$ 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 five weeks before harvest the crop has not recovered its target N but uptake has exceeded $(U_G + U_S)$, then

$$V_C = [U_T - (U_G+U_S)]/5 \tag{19}$$

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

<u>Rules for the behaviour of ^{15}N labelled fertilizer in the model</u>. In fitting the model to the results in the preceding paper (Hart *et al.* 1993), half the ^{15}N-labelled fertilizer enters the NH_4-N compartment (minus any volatilization losses), half the NO_3-N compartment. Thereafter ^{15}N-labelled N is nitrified, leached, immobilized, denitrified, taken up by plants, or volatilized, exactly as 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 enter 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:

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

where y_{ij} is the ith replicate in the jth experiment, 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 jth experiment this may be written:

The square roots of the lack of fit and error (Root Mean Squares: see, for example,

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

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 minimise 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/yr) of this experiment were used during the tuning process: data from the other plots, which receive 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 smallest 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 CO_2-C/ha; ϕ_C, 0.05; $\phi_S = 0.15$; 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) 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) are 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 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 about 7, equivalent to a root mean square in the measurements of about 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 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, 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. Figs 6*a* - 6*d* are 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 NH_3-N (ϕ_C); the proportion of NH_4-N fertilizer lost by volatilization (ϕ_S); the denitrification coefficient θ; the bypass flow factor (σ). Figs 6*e* and 6*f* show the effects of varying the critical level 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 increase in mineralisation will increase uptake of labelled N by the crop. This is demonstrated most noticeably in Figs 5*c* and 5*d*, where the relationships between C_{AO}, α and β are altered. Figs 5*c* and 5*d* show 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 successfully applied 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 (Figs 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 6*c*: 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 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.

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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 parenthesis are for water held between Field Capacity and -1 bar (ψ_i).

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	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[c] (62)	0.402 (21)	0.091[c] (48)
Estimated uptake[b]	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]*Estimated* (using equation 12) total uptake of N by above-ground part of crop used to initiate model.
[c]Excluding Woburn results from 1981 application year (soil) or first residual year (crop)
[d]Excluding Woburn results from 1982 application year (soil) or first residual year (crop)

Table 3. Modelled losses of N for the three sites.

	Rothamsted[d]					Woburn[e]				Saxmundham[f]		
	1980[a]	1981	1982	1983	1984	1981[a]	1982	1983	1984	1981[a]	1982	1983
	kg total N/ha											
Volatilized[b]	10.6	0.0	0.0	0.0	0.0	4.2	2.8	3.5	5.5	12.7	2.43	0.0
Leached[c]	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[b]	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[c]	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] Labelled fertilizer N applied
[b] From both soil and plant
[c] Including bypass flow
[d] Receiving 141 kg labelled N/ha in spring 1980, 144 kg unlabelled N/ha each year thereafter
[e] 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
[f] 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

Legends to Figures

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.

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).

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) or 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 equation 11.

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.

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) ○, ● the rate constant (r) for the input compartment (RO)

□, ■ the rate constant (b) for the biomass compartment (BIO)

△, ▲ the rate constant (h) for the humus compartment (HUM)

c and d) ○, ● 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 (C_{AO})

e and f) ○, ● the rate constant (c) for return of organic C to the RO compartment

□, ■ the rate constant (n) for return of organic N to the RO compartment

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) ○, ● the above-ground N in the crop at harvest ($U_G + U_S$)

□, ■ the rate constant (f) for crop N uptake

△, ▲ the fraction (ϕ_C) of the above ground-N released by the senescing crop as NH_3-N

c and d) ○, ● the denitrification factor (θ)

□, ■ the proportion of NH_4-N fertilizer lost by volatilization (ϕ_S)

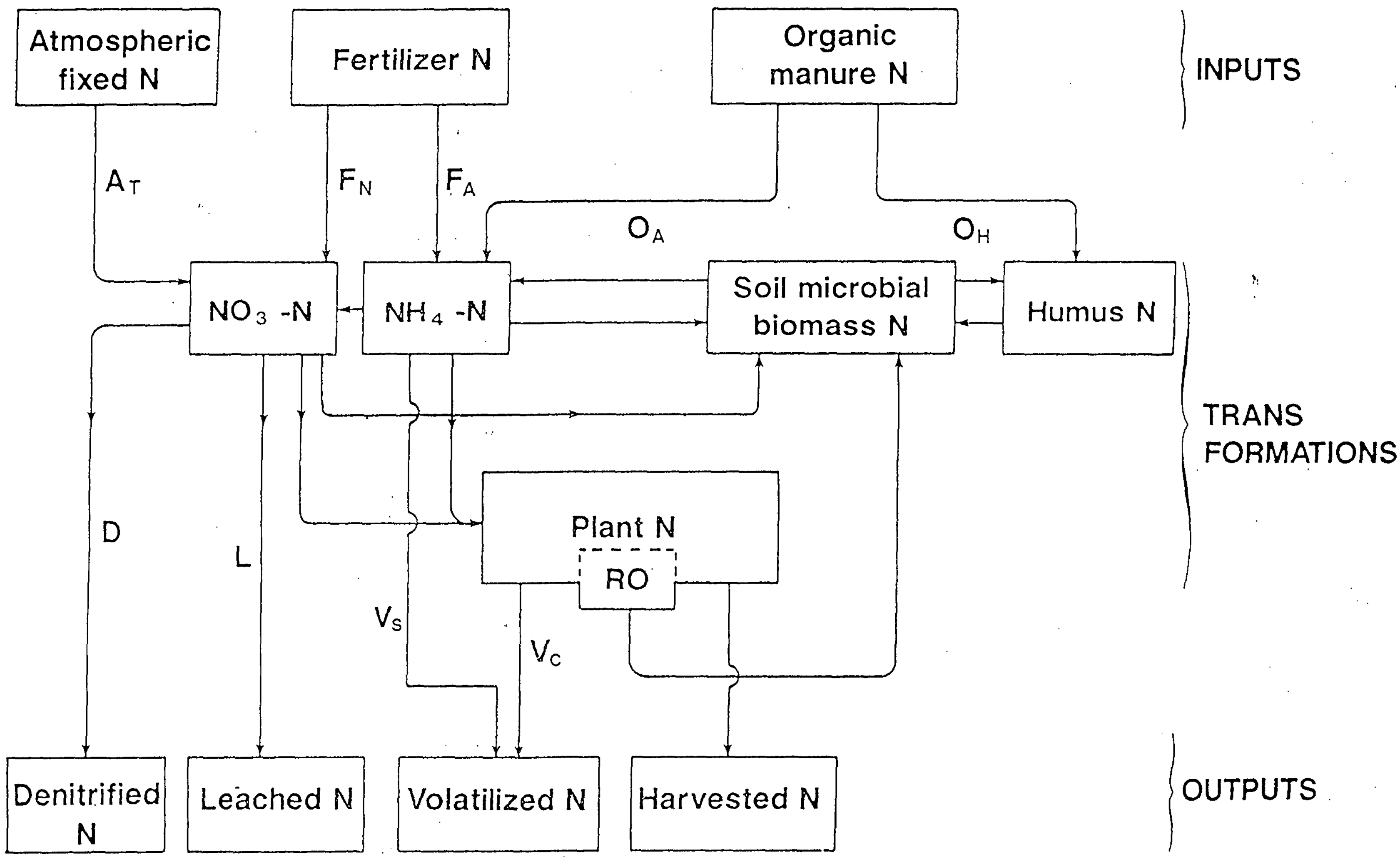
△, ▲ the bypass flow factor (σ)

e and f) ○, ● the level above which rainfall contributes to bypass flow (R_{CRIT})

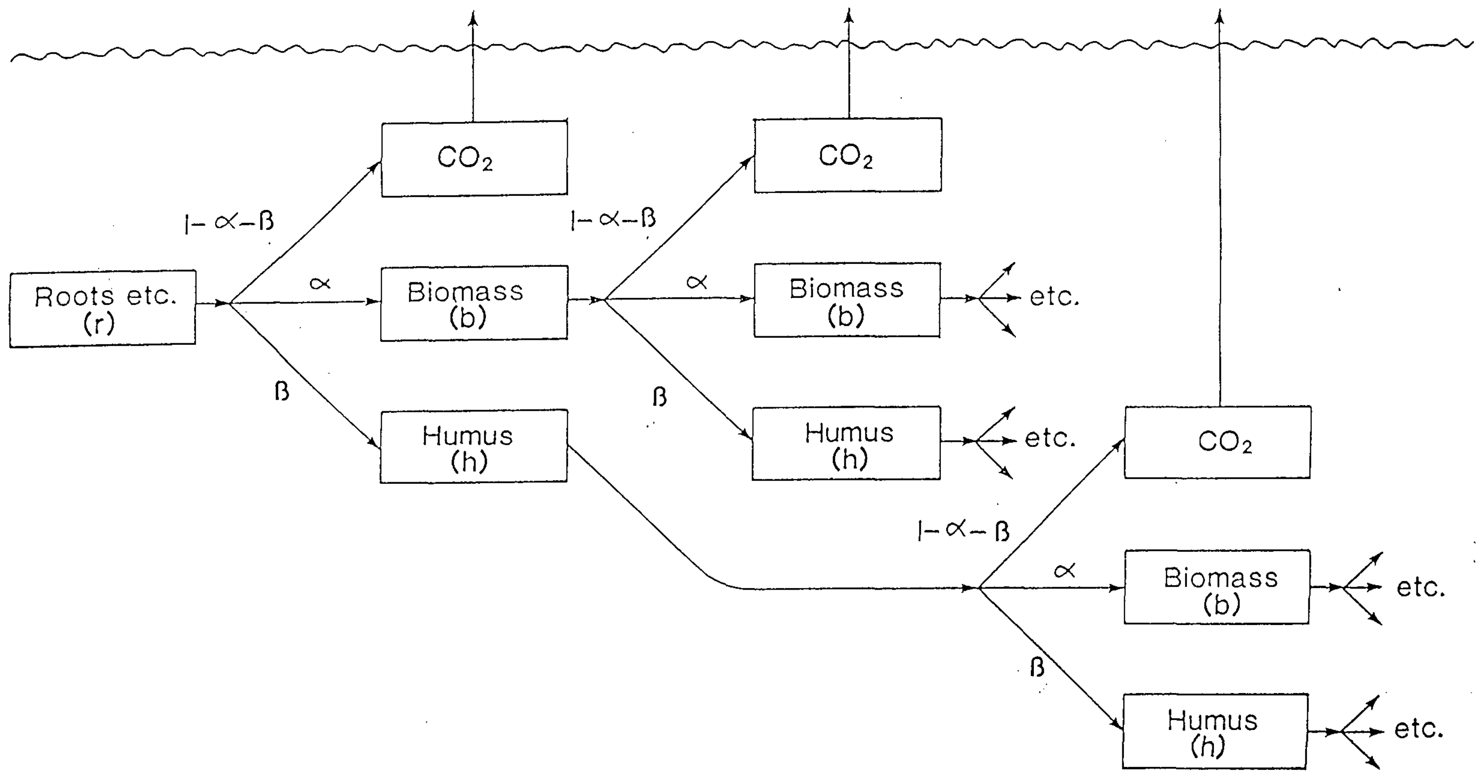
□, ■ weekly rainfall (R_W)

△, ▲ mean weekly temperature, (T), varied by $\pm$ 5°C

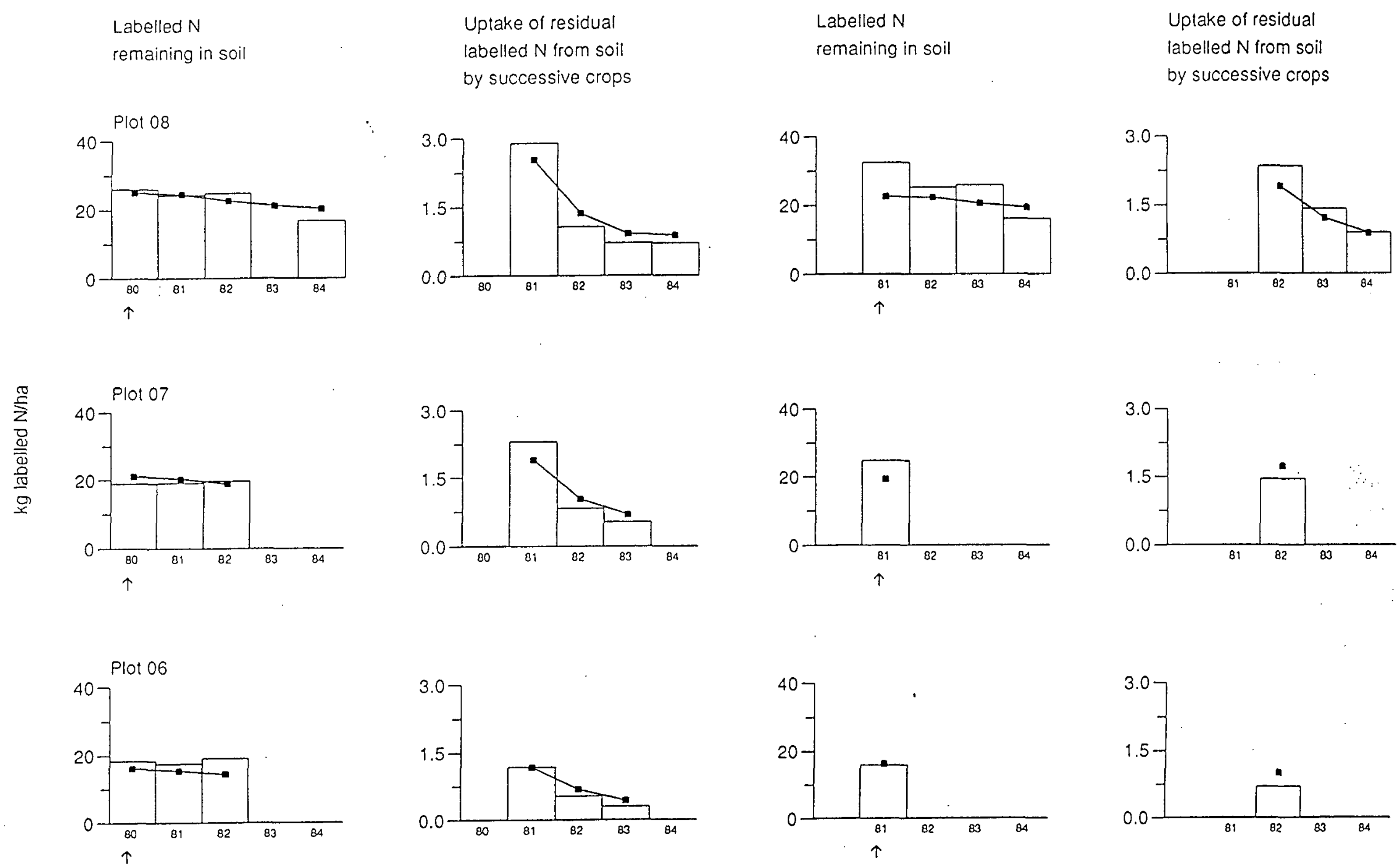
Appendix. Figure 1



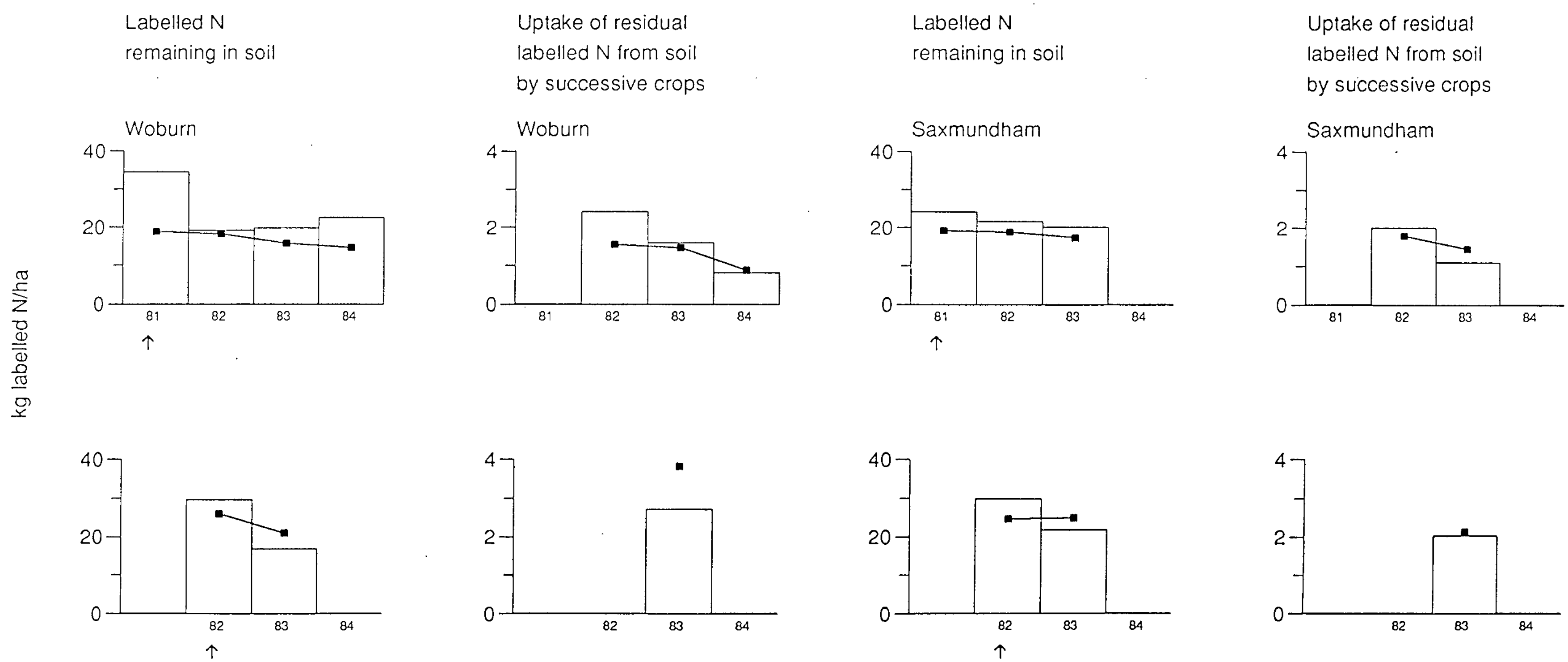
Appendix. Figure 2



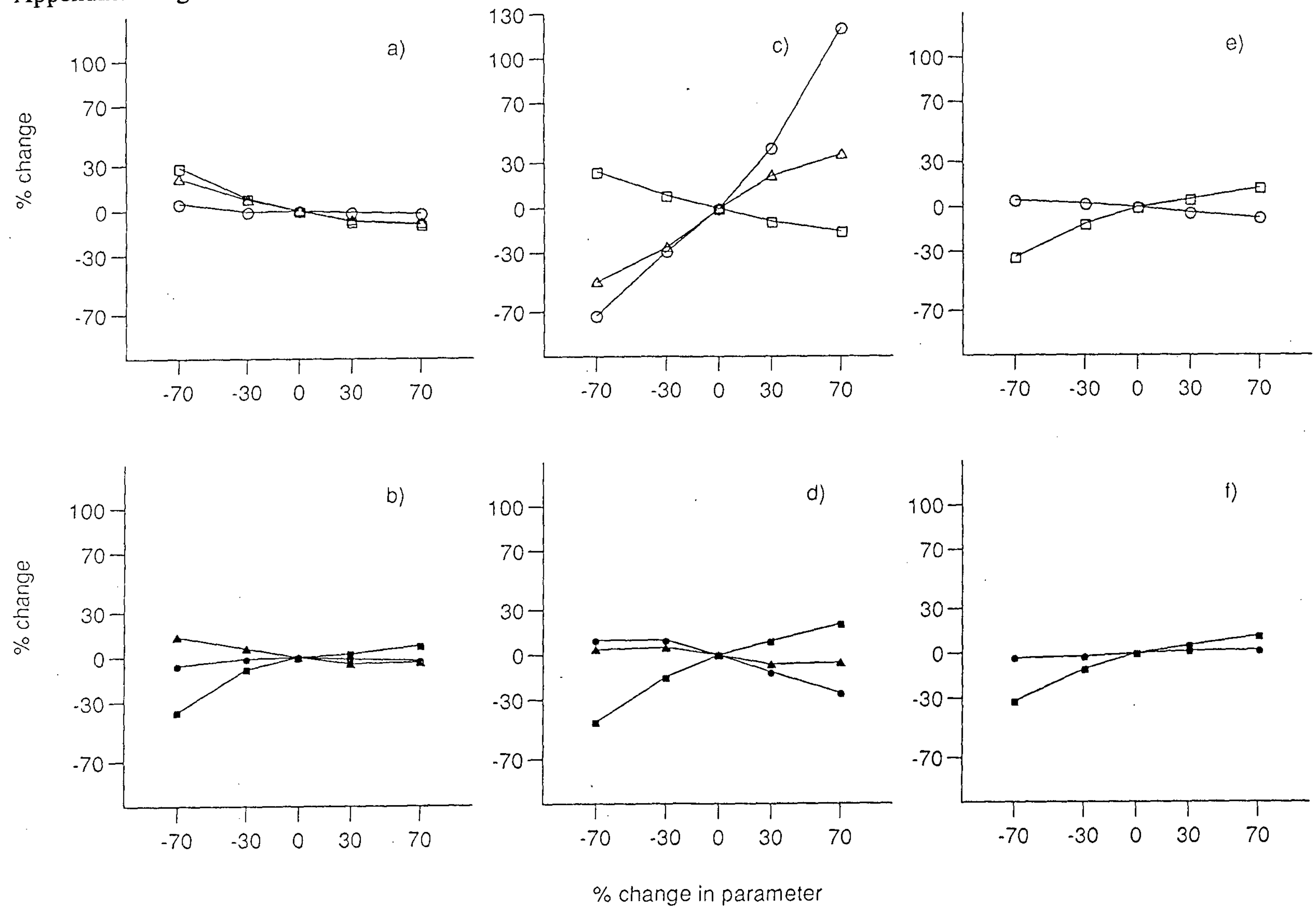
Appendix. Figure 3



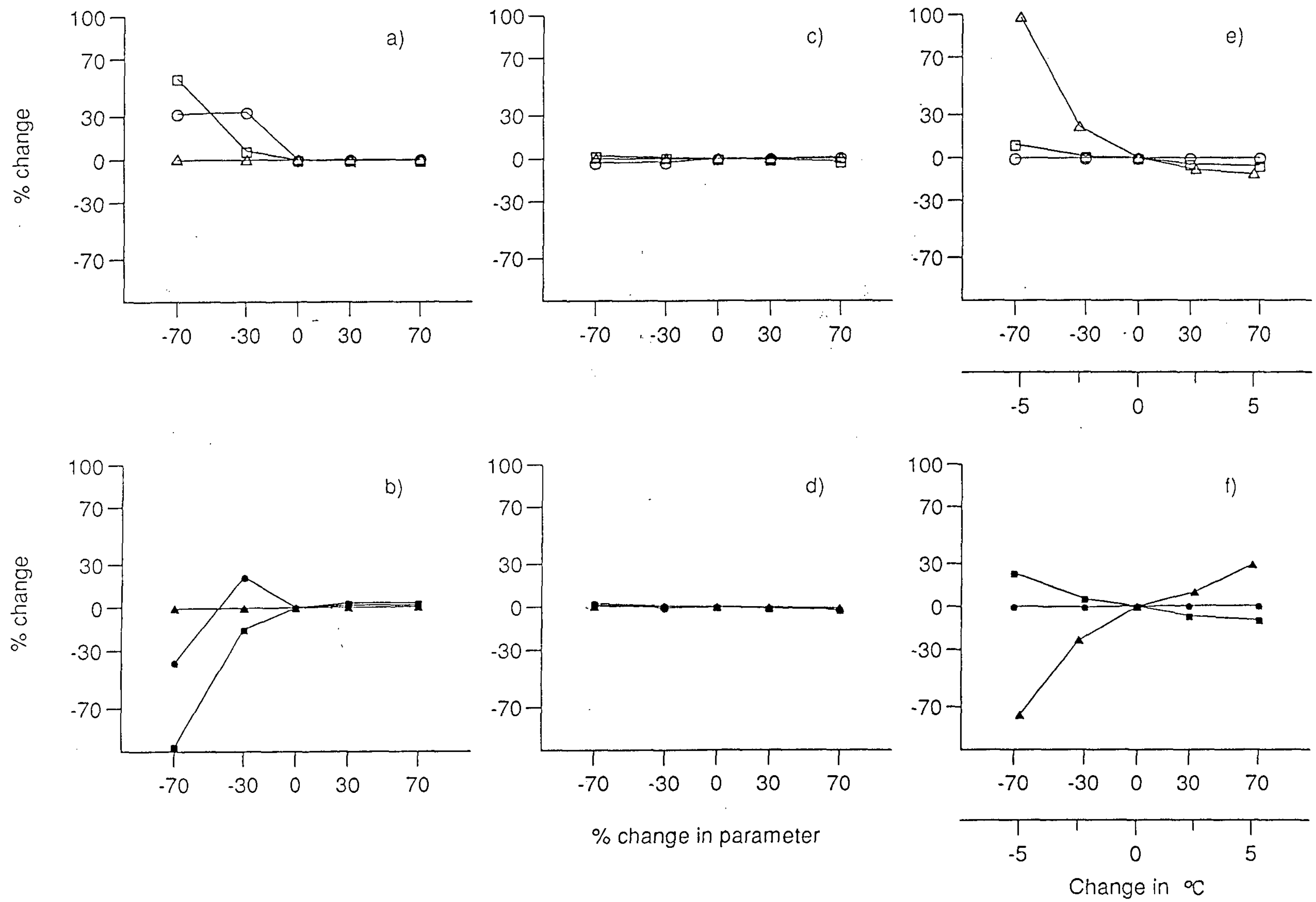
Appendix. Figure 4



Appendix. Figure 5



Appendix. Figure 6



Appendix 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 curent (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 fertiliser 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	Percent clay (<2μm) 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 C 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)	
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 RO 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	-
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 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	-