114

Simulation of nitrogen behaviour of soil-plant systems

Papers of a workshop
Models for the behaviour
of nitrogen in soil
and uptake by plant.
Comparison between
different approaches
Wageningen, the Netherlands
January 28-February 1, 1980

Editors: M.J. Frissel and J.A. van Veen

pudoc

1981

Centre for Agricultural Publishing and Documentation
Wageningen

ISBN 90-220-0735-9

4.7 Use of tracers and computer simulation techniques to assess mineralization and immobilization of soil nitrogen

N.G. Juma and E.A. Paul

1. NAME OF MODEL

TRAMIN - Use of tracer and computer simulation techniques to assess mineralization and immobilization of soil nitrogen.

2. SYSTEM MODELED

The model describes the mineralization and immobilization of soil nitrogen during microbial growth and decay under laboratory conditions.

3. OBJECTIVES

The objectives of this investigation were to develop and test concepts of microbial growth and decay in soil and to study the mineralization and immobilization of soil N using tracer and computer simulation techniques.

4. TIME SCALE

The programme was designed to simulate the duration of the laboratory experiments which lasted from 42 to 84 days. The time resolution was fixed at 0.01 day.

5. DIAGRAM

The flow chart for transfer of C and N involved in the mineralization and immobilization processes is presented in Fig. 1. Four versions of the model are available depending on whether tracer ^{15}N and/or ^{14}C were used. In the basic version, C and N behavior in the mineralization-immobilization processes were simulated. In the other versions, the number of N and/or C integrals were doubled when ^{15}N and/or ^{14}C tracers were used.

6. LEVELS

See 7.

7. GOVERNING EQUATIONS

In models that describe soil organic matter turnover, the microbial biomass transforms C substrates in soil (Paul and Van Veen, 1978) and is directly involved in the N mineralization-immobilization processes. Microbial growth is primarily limited by substrate and nutrient availability and by the physical conditions prevailing in soil. Soil microorganisms grow on a variety of C substrates. For simulation purposes, the exogenous sub-

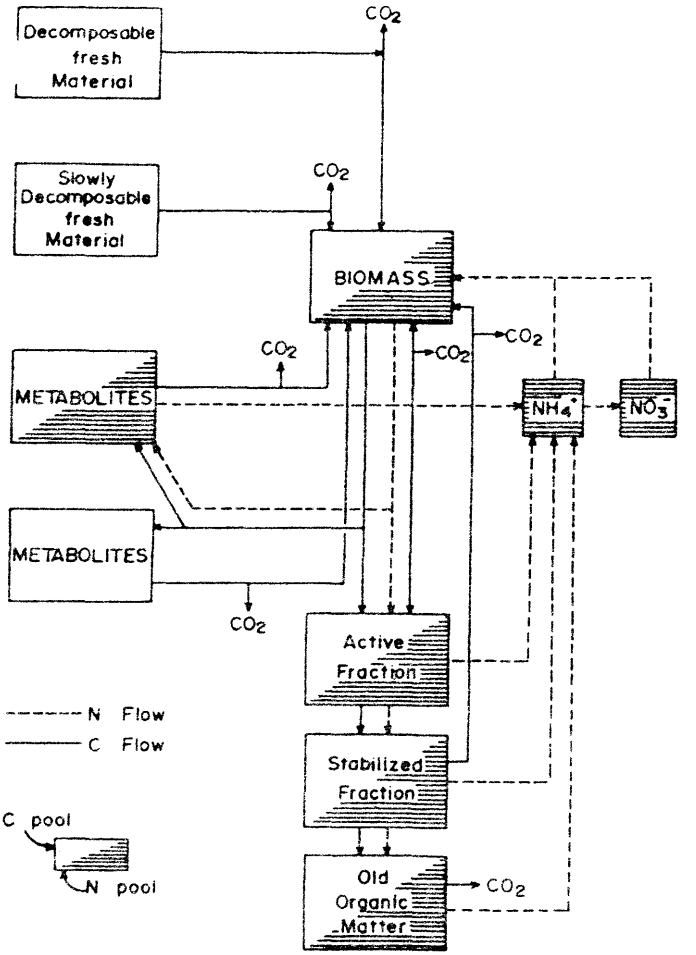

Fig. 1. Flow chart for transfer of C and N involved in the mineralization and immobilization processes.

strates added to soil can be adequately divided into the following categories: (1) decomposable fresh materials consisting of simple carbohydrates; (2) slowly decomposable fresh materials such as cellulose and hemicellulose; (3) materials containing C and N such as proteins, amino sugars, and other nitrogenous compounds; and (4) complex materials such as lignin. In the model, the soil C and N substrates were divided into active-(C+N), stabilized-(C+N) and old-(C+N) (Fig. 1). The techniques and assumptions used to determine the pool sizes are described elsewhere (Paul and Juma, 1980) and are summarized in Table 1.

The concept of an active and a passive organic N phase (Jansson, 1958) was incorporated into the model. The active organic N phase was divided into three components: biomass, active-(C+N) and metabolite-(C+N). This was possible as the biomass and active N can be

Table 1. Initial values of N pools and techniques used for pool size determination.

Pool	^{14}N	^{15}N	Technique
	($\mu g\ g^{-1}$ soil)		
Biomass	167	0.072	Fumigation incubation
Active fraction and metabolites	389	0.169	Isotopic dilution and curve peeling
Old fraction	2073	0	Associated with old carbon (carbon dating)
Stabilized fraction	1496	0	By difference

measured using the techniques summarized in Table 1. The passive organic N phase was divided into two components: stabilized N with a half life of ~35 years and old N with a half life of ~600 years. The dynamics of the mineralization processes are presented below:

a. *Microbial growth and N immobilization*

The dynamics of microbial growth and N immobilization were described by first-order kinetics. In most cases, the decomposition of C substrates is independent of microbial biomass size. In the model, the decomposition of C from any pool occurred if C was present in that pool and mineral N was not equal to zero. Thus,

$$dCX/dt = KX \cdot CX \cdot WCOF \cdot TCOF \quad (1)$$

where

dCX/dt = the rate of substrate decomposition (mg g^{-1} soil d^{-1})
KX = the decomposition rate constant for substrate CX (d^{-1})
CX = the substrate C pool size (mg C g^{-1} soil)
WCOF and TCOF = moisture and temperature reduction factors for sub-optimal conditions. The values of these reduction factors ranged from 0 to 1 depending upon the physical conditions prevailing in soil (Van Veen, 1977).

The rate of C incorporation into the microbial biomass (CXINC; mg C g^{-1} soil d^{-1}) was

$$CXINC = (YCOFX/100) \cdot dCX/dt \quad (2)$$

where YCOFX is the efficiency of utilization of CX. The rate of CO_2-C evolution ($CXCO_2$, mg C g^{-1} soil d^{-1}) during the decomposition of CX was:

$$CXCO_2 = (1 - (YCOFX/100)) \cdot dCX/dt \quad (3)$$

The rate of N incorporation into the microbial biomass (CNINC, mg N g^{-1} soil d^{-1}) was

$$CNINC = (dCX/dt)/CNB \quad (4)$$

where CNB is the C:N ratio of the microbial biomass. Thus, the rate of N uptake during microbial growth was equal to the gross immobilization rate.

b. *Microbial biomass decay*

The decay of the biomass was described by first-order kinetics, i.e. the amount of biomass that decayed per unit time was proportional to its size. The decay C and N products were transferred into the active (C+N) and metabolite pools. The metabolites were divided into two classes: those containing C and N (proteins, amino sugars) and those containing C only (polysaccharides).

In the model, 50% of C and N of the microbial decay products were channelled into the active (C+N) pool. The remainder of the N was channelled into the metabolite (C+N) pool. The amounts of the C entering the metabolite (C+N) and metabolite C pools were calculated as follows:

Assuming a C:N ratio of three, the amount of C transferred to metabolite (C+N) pool was three times the amount of N transferred into it. The remainder of the C [50% of the total microbial C decay products minus C transferred into metabolite (C+N)] was channelled into metabolite-C pool.

c. *Mineralization of N*

Mineralization of N occurred during the decomposition of substrates containing C and N. The rate of N mineralization was calculated by multiplying the rate of C decomposition by the C:N ratio of the pool. Alternately, the rate of N mineralization was calculated by multiplying the decay rate constant (d^{-1}) for the (C+N) pool by the N content of the pool (mg N g^{-1} soil). The gross N mineralization rate was equal to the sum of the rates of N ineralization from various (C+N) pools.

d. *Stabilization of C and N*

Part of the active-(C+N) is transformed physically or chemically into the stabilized-(C+N). Further transformation of the stabilized-(C+N) results in the formation of recalcitrant organic matter. The amounts transferred from one pool to another were described by first-order kinetics.

8. INPUT PARAMETERS

The initial values, decay and transfer rate constants, efficiency of utilization of C substrates and C:N ratios of various (C+N) integrals needed in the model are summarized in Table 2.

Temperature and moisture content were time-dependent variables.

9. OUTPUT VARIABLES

The basic version of TRAMIN evaluates the following variables that are experimentally verifiable: biomass C and N, mineral N and CO_2-C released during incubation. When tracer ^{15}N is used, the following additional variables are verifiable: biomass ^{15}N, mineral ^{15}N,

Table 2. Initial values, decay and transfer rate constants, efficiency of utilization of C substrates and C:N ratios of various (C+N) integrals used in the model.

Pool	C	^{14}N	^{15}N	Decay rate constant	Efficiency of utilization of C	C:N ratio
	($\mu g\ g^{-1}$ soil)		($ng\ g^{-1}$ soil)	(d^{-1})	(%)	
Biomass	1,000	167	72	0.0143	-	6
Active fraction[1]	2,302	384	167	0.0037	40	6
Metabolite-C	15	-	-	1.0	60	-
Metabolite-(C+N)	15	5	2	1.0	60	3
Stabilized-(C+N)[2]	17,542	1,496	0	$6.0 \cdot 10^{-4}$	40	11
Old-(C+N)	24,455	2,073	0	$3.0 \cdot 10^{-6}$	-	11.8
Decomposable C	2	-	-	1.0	60	-
Slowly decomposable C	50	-	-	0.1	60	-
Mineral N	-	21	9	-	-	-

1. Transfer rate constant of active material to stabilized fraction = $0.5 \cdot 10^{-3}$ (d^{-1}).
2. Transfer rate constant of stabilized fraction to old fraction = $3.0 \cdot 10^{-6}$ (d^{-1}).

active ^{15}N and active ^{14}N. The model calculates the size of N integrals and their atom % abundances.

When ^{14}C is used, the following variables are verifiable: biomass ^{14}C, $^{14}CO_2$-C, active ^{14}C (sum of active (C+N), metabolite C and metabolite (C+N)). The model calculates the size of C integrals and their specific activities.

When ^{14}C and ^{15}N are used all the above mentioned variables are verifiable.

10. OBSERVATIONS

Enriched ^{15}N soil samples were obtained from a field experiment conducted on Weirdale loam, a Gray-Black Chernozemic soil. These surface samples were incubated in the laboratory for 12 weeks at field capacity moisture content and 28±1 °C. During the incubation, total N, biomass N, active N and mineral N and their atom % ^{15}N abundances were determined. Also, biomass-C and CO_2-C evolved were measured. Detailed experimental procedures are summarized elsewhere (Paul and Juma, 1980).

The TRAMIN programme was used to simulate the ^{14}N, ^{15}N and C transformations.

11. COMPARISON OF RESULTS

The predicted values of total organic ^{15}N remaining in soil and cumulative CO_2-C evolved were slightly higher than the experimental values (Table 3); the mineral ^{15}N level predicted was lower than the actual value. The other outputs were similar indicating that the gross, transfer rate constants and pool sizes used (Table 2) were of proper magnitude.

The dynamics of various ^{14}N and ^{15}N pools as predicted by the model are shown in Table 4. During the 12 weeks incubation, when no exogenous C was supplied, the biomass with an initial size of 72 ($ng\ g^{-1}$) immobilized 56 ng $^{15}N\ g^{-1}$ soil and decayed by 76 ng^{-1} resulting in a final size of 53 $ng\ g^{-1}$ (Fig. 2). The metabolite N mineralized rapidly and constituted

Table 3. Comparison of experimental data with simulation model outputs at the end of 12 weeks incubation.

Pool	Experimental	Simulated
	(μg g^{-1} soil)	
Total organic ^{15}N remaining in soil	0.203	0.211
Biomass-^{15}N	0.052	0.053
Active fraction + metabolite-^{15}N	0.152	0.150
Stabilized-^{15}N fraction	-	0.007
Mineral-^{15}N	0.045	0.039
Mineral-^{14}N	115	121
Cumulative CO_2-C evolved	938	1153

Table 4. Dynamics of various N fractions in soil during 12 weeks incubation.

Fraction	Simulated values				Experimental value at end of 12 weeks
	Inital size	Inputs	Outputs	Size at end of 12 weeks	
^{15}N (ng g^{-1} soil)					
Biomass-N	72	56	76	53	52
Metabolite-N	2	38	39	1	152
Active-N	166	38	54	150	-
Stabilized-N	0	7	0.1	7	-
Old-N	0	0	0	0	-
Mineral-N	9	86	56	39	45
^{14}N (μg g^{-1} soil)					
Biomass-N	167	163	187	143	152
Metabolite-N	5	94	98	1	-
Active-N	384	94	125	352	-
Stabilized-N	1496	15	55	1456	-
Old-N	2073	0.1	0.4	2073	-
Mineral-N	21	263	163	121	115

only a small pool at any time. The active N with an initial size of 166 ng ^{15}N g^{-1} increased by 38 ng g^{-1} and released 54 ng resulting in a final size of 150 ng g^{-1}. A small portion (7 ng g^{-1}) of the ^{15}N released from active-N was transferred to the stabilized fraction while the rest was mineralized. At the end of the 12 weeks incubation, the ^{15}N content of the stabilized-N showed a net increase while the ^{15}N content of biomass and active N showed a net decrease. During the 12 weeks incubation, the model predicted a net mineralization of 30 ng g^{-1} ^{15}N. The relative net changes of the ^{15}N pools expressed as a fraction of ^{15}N mineralized were biomass (-63%), active-N (-53%), metabolite-N (-3%), stabilized-N (+23%), old-N (0%). At present, it is not possible to measure the ^{15}N in stabilized-N and old-N.

During the 12 weeks incubation, the biomass with an initial size of 167 μg ^{14}N g^{-1} soil immobilized 163 μg g^{-1} and decayed by 187 μg g^{-1} resulting in a net decrease of 24 μg g^{-1} (Fig. 3). The metabolite-N and active-N with equal inputs also declined. The stabilized-N showed a net mineralization of 40 μg g^{-1} while the old N contributed 0.3 μg g^{-1}. Gross

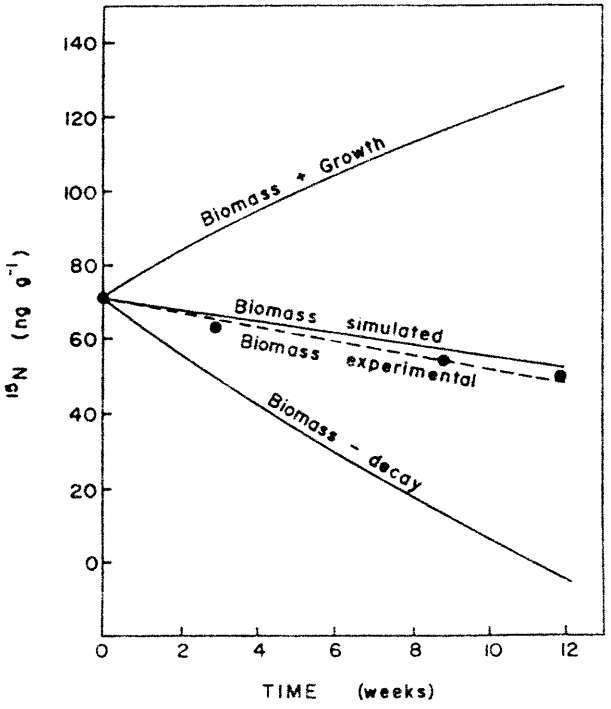

Fig. 2. Biomass-^{15}N: cumulative growth and decay rates.

mineralization during this period amounted to 263 µg g^{-1}, while the net mineralization was 100 µg N g^{-1}. The relative net contribution of N fractions to mineral ^{14}N were biomass (24%), metabolites (4%), active-N (32%), stabilized-N (40%), old-N (0.3%). At present, it not possible to determine the sizes of metabolite-N, active-N, stabilized-N and old-N.

The turnover time of any pool can be calculated from the tracer data provided the system is in steady state conditions. The soil system generally is not in a steady state condition on a short term basis. Therefore, it is necessary to use simulation techniques to get a good estimate of the fluxes in and out of various pools. In the present version of the TRAMIN model, the C, ^{14}N and ^{15}N transformations were simulated. The major advantage of simulating the N isotopes separately is that it helps to quantify these fluxes accurately. For any pool, the ^{14}N is a good indication of changes in size while the ^{15}N is an excellent index of the activity within the pool. Sensitivity analysis showed that the decay or transfer rate constants used in the model had a very narrow range of values.

Jansson (1958) showed that mineralization and immobilization of N were continuous processes and demonstrated the internal cycling of N. The model predicted that ^{15}N in soil undergoes rapid turnover. During the 12 weeks incubation, 36% (86 ng g^{-1}) of the ^{15}N initially present in soil was mineralized while 23% (56 ng g^{-1}) was reimmobilized. The net change of 30 ng g^{-1} was ~13% of the total ^{15}N at the beginning of the experiment. Thus,

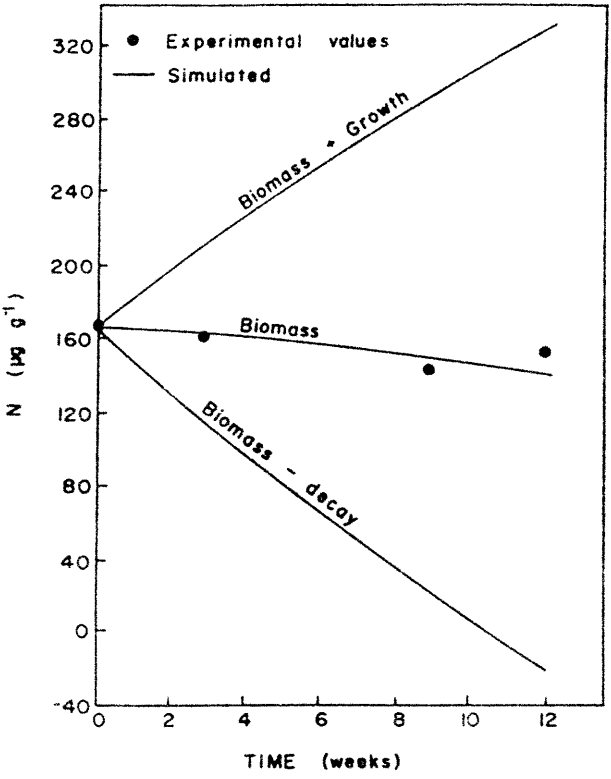

Fig. 3. Total microbial biomass-N: cumulative growth and decay rates.

net mineralization was 1/3 of the gross mineralization, i.e. of every 3 units of N that were mineralized, 2 were reimmobilized, resulting in a net mineralization of 1 unit. Therefore, the half life of ^{15}N in soil organic matter is very long due to the internal cycling of N.

Jansson (1958) suggested that the active organic N phase was the major source of mineralized N. Stanford and Smith (1972) used long term incubations and mathematical techniques to estimate the size and decay rate constant of the mineralizable N pool for 39 soils which were in net mineralization conditions. Thus, the decay rate constant they obtained was related to net mineralization only. The TRAMIN model after considering gross mineralization and immobilization rates predicted that all the N fractions in soil contributed to the mineral N. In this study the active organic N phase comprised of the biomass, active-N and metabolic-N and accounted for almost all of the ^{15}N mineralized, but contributed ~60% of the ^{14}N mineralized. The stabilized-N and old-N accounted for the rest of ^{14}N mineralized. The model predicted that various organic N pools are mineralizable and have different mineralization rate constants. Therefore, it is difficult to describe the soil processes involved in N mineralization by a single first-order decay equation, es-

pecially when a net mineralization rate constant is used in the equation.

12. LIMITS AND LIMITATIONS

The model assumes aerobic conditions at all the times and does not consider nitrification or N losses and gains. The N in soil was divided into biomass, active-N, metabolite-N, stabilized-N and old-N, although it is well known that the N compounds in soil form a continuum from simple soluble to recalcitrant compounds. These compounds were grouped into the above mentioned pools based on the decay rates of the pools as determined by tracer and isotopic dilution techniques. At present, it is not possible to measure the size and decay rate constants of the stabilized-N and old-N, however, a wealth of information exists in the literature which supports the concept that large pools or fractions with long half lives exist (Oades and Ladd, 1977).

The mineralization process described in the model assumes that when a substrate containing C and N is decomposed, the N is first converted to NH_4^+. Thus, compounds like simple amino acids and amino sugars are deaminated before being taken up by the biomass. The amount of N immobilized is governed by the amount of C incorporated into the biomass and by the C:N ratio of the biomass.

13. COMPUTER

IBM 360/370.

14. PROGRAMME LANGUAGE

CSMP III.

15. RUNNING TIME/COST

1.5 CPU minutes, cost $16.00 for simulating 84-day laboratory experiment.

USERS

The programme has been recently developed, however, the concepts developed could be applied to other soil systems where the role of micro-organisms is explicitly defined in the mineralization and immobilization of N.

17. DEVELOPERS AND PRINCIPAL CONTACT

Noorallah G. Juma and E.A. Paul
Department of Soil Science
University of Saskatchewan
Saskatoon, Saskatchewan
Canada S7N OWO

REFERENCES

Jansson, S.L., 1958. Tracer studies on nitrogen transformations in soil with special attention to mineralisation-immobilization relationships. Annals Royal Agricultural College

Sweden 24: 101-361.

Oades, J.M., and J.N. Ladd, 1977. Biochemical properties. In: J.S. Russell & E.L. Greacen (Eds): Soil factors in crop production. University of Queensland Press, St. Lucia. p. 127-160.

Paul, E.A., and N.G. Juma, 1980. Mineralization and immobilization of nitrogen by microorganisms. In: F.E. Clark and T. Rosswall (Eds): Terrestrial Nitrogen Cycles. Ecol. Bull. (Stockholm) (in press).

Paul, E.A., and J.A. van Veen, 1978. The use of tracers to determine the dynamic nature of organic matter. Transactions 11th International Congress Soil Science (Edmonton, Alberta) 3: 61-102.

Stanford, G., and S.J. Smith, 1972. Nitrogen mineralization potentials of soils. Soil Science Society of America Proceedings 36: 465-472.

Van Veen, J.A., 1977. The behaviour of nitrogen in soil. A computer simulation model. Ph.D. Thesis, Vrije Universiteit, Amsterdam.