Enregistrement scientifique n° : 883
Symposium n° : 7
Présentation : poster

A process-based model for carbon and nitrogen transfers in soil organic matter.
Un modèle mécaniste des flux de carbone et d'azote dans la matière organique du sol

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The MOMOS (MOdélisation de la Matière Organique des Sols) model was built using data from a laboratory incubation experiment of ^{14}C- and ^{15}N-labelled plant material in soils. The carbon model describes five compartments (Fig. 1) : labile (V_L) and resistant (V_R) initial plant material, microbial biomass (B), labile (A) and stable (H) humified compounds. The decrease of each compartment *i* is described by a first order kinetics with k_i as rate constant.
The nitrogen model (Fig. 1) uses the same compartments and parameters as the C model, with a rate constant multiplying factor f_n, indicating that the N turnover is faster than the C turnover. Nitrogen is directly transferred between the organic compartments (1 in Fig. 1) or indirectly by NH_4-N immobilisation (3). Ammonification (2) results from the difference between the output and the input of the organic compartments. Ammonium is immobilised (3/4 in microbial biomass; ¼ directly in the stable humified compartment) or nitrified (4), with a possible N loss by volatilisation (5). The nitrification process is described by a microbial growth function.
Built from ^{14}C and ^{15}N experimental data, the model was validated from the corresponding total C and total N data. The predictions were in agreement with 16 data series, including different forms of organic ^{14}C, total C, organic and inorganic ^{15}N, and total N.

Keywords : modelling, carbon, nitrogen, organic matter, microbial biomass, inorganic nitrogen, stable organic pools, labile organic pools, plant debris.

Mots clés : modélisation, carbone, azote, matière organique, biomasse microbienne, azote minéral, compartiment organique stable, compartiment organique labile, matériel végétal.

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1. Introduction

The aim was to develop the most simple and suitable model to describe carbon and nitrogen transfers in soils, using data from laboratory experiments.
Pansu and Sidi (1987) proposed two models with two and three compartments, to describe the mineralisation and humification kinetics in soil amended with wheat straw under controlled conditions.
Sallih and Bottner (1988) and Bottner *et al.* (1988) carried out laboratory controlled soil incubation experiments with ^{14}C and ^{15}N labelled wheat straw. The ^{14}C data (total-, plant debris- and microbial biomass-^{14}C) were used to develop a five compartment C-model (Sallih and Pansu, 1993) based on the same conceptual formulation as in the model of Pansu and Sidi (1987). The model (MOMOS-C) was validated with corresponding total C data and allowed to explain the field total organic C content and the plant fragment-C of the two studied soils (Pansu *et al.*, 1996).
More recently, the data from the same experiment (total-, plant debris-, microbial biomass-, NH_4- and NO_3-^{15}N) were used to built a MOMOS-N version which was validated with corresponding total-N data (Pansu *et al.*, 1998). This paper presents the combined MOMOS C and N model.

2. Materials and methods

2.1. Data acquisition

Data were collected from incubation experiments under controlled conditions, with two Mediterranean soils: a fersiallitic calcic soil (soil 1; 7% coarse sand, 29% clay) and, a typical brown soil (soil 2; 45% coarse sand, 11% clay) (CPCS, 1967) incubated with ^{14}C and ^{15}N labelled mature wheat straw. The soil characteristics and the experimental procedure have been previously described by Sallih and Bottner (1988), Bottner *et al.* (1988), Sallih and Pansu (1993) and Pansu *et al.* (1998). Following data were collected over two years:

- C and ^{14}C in (1) the whole soil, (2) the plant debris separated from the soil by physical fractionation, and (3) the microbial biomass (fumigation-incubation method, Jenkinson and Powlson, 1976),
- N and ^{15}N in (1) the whole soil, (2) the plant debris, (3) the microbial biomass, (4) K_2SO_4 extractable-ammonium and (5) extractable-nitrate.

2.2. Mathematical model

The flow diagram of MOMOS C and N model is presented in Fig. 1. The following abbreviations are used in the fig.1, in the equations and in the text:

oC, *oN*, *aN*, *nN* = organic C, organic N, ammonium N, and nitrate N respectively.

The state variables *oC* and *oN* (Fig.1) represent the 5 organic compartments as subscripts: V_L = labile plant material, V_R = resistant plant material, A = labile soil organic matter, B = microbial biomass, and H stable humified organic matter.

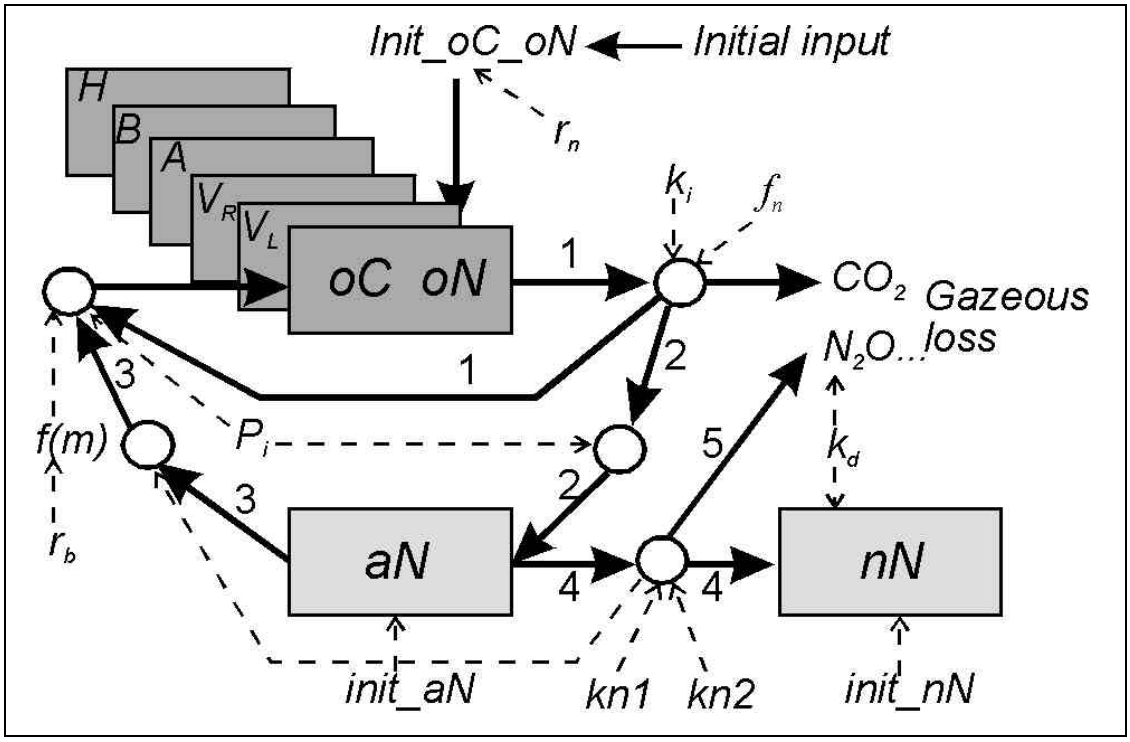

Fig. 1 - The MOMOS C and N model.
oC oN : organic C and N pools (V_L, V_R, A, B, H)
aN : NH_4-N
nN : NO_3-N

1 : *oN* reorganisation
2 : ammonification
3 : NH_4-N immobilisation
4 : nitrification
5 : volatilisation

Organic carbon (*oC*) dynamic *versus* time *t* is fitted according to a system of five first order differential equations. For any compartment *m* among *i* compartments, the dynamic is directed by :

$$\frac{d\ oC_m}{dt} = -\ k_m\ oC_m + \ P_m \sum_i k_i\ oC_i \qquad (1)$$

where k_m, k_i (time^{-1}) are kinetic constants of *m* and *i* compartments (with $k_A = k_{VL}$) and P_m (dimensionless) is the input proportion entering into the compartment *m* (with $P_{VL} = P_{VR} = 0$).

MOMOS describes the N transformations using the structure and parameters defined in the C model, with additional N specific parameters. The input into a given organic-compartment *m* (oN_m) includes a part P_m (defined above) which originates directly from the organic compartments (oN_i) and a part which results from the immobilisation of ammonium (*aN*). This is directed by:

$$\frac{d\ oN_m}{dt} = f_n\left(-k_m\ oN_m + P_m \sum_i k_i\ oN_i\right) + f(m)\left(aN\left(1-k_{n1}\left(k_{n2}-aN\right)\right)\right) \qquad (2)$$

where k_i, k_m and P_m are the parameters defined in (1). The multiplying factor f_n increases the rate of N transformation, compared to the one of C. The flow of *aN* toward *oN* (arrow 3, Fig. 1) is distributed by *f(m)*: *f(m)* = 0 for $m \in \{V_L, V_R, A\}$, $f(m) = r_b$ for *m* = B (r_b is the proportion of NH_4-*N* which is immobilised into microbial biomass-N), *f(m)* = 1-r_b for *m* = H. The parameters k_{n1} and k_{n2} represent two nitrification rate constants. The ammonium-N (*aN*) balance is directed by:

$$\frac{d\ aN}{dt} = f_n\left(1-\sum_i P_i\right)\sum_i k_i\ oN_i - aN \qquad (3)$$

i.e. *aN* is nitrified or immobilised. Exchangeable ammonium represents the balance between ammonification and these outputs. Nitrate (*nN*) production is directed by:

$$\frac{d\ nN}{dt} = (1-k_d)\ k_{n1}\ aN\left(k_{n2}-aN\right)$$

$$\text{when } [aN \le k_{n2}], \text{ otherwise : } \frac{d\ nN}{dt} = 0. \qquad (4)$$

Equation 4 states that the nitrate production rate is proportional to the mass of depleted substrate (ammonium). Parameters k_{n1} and k_{n2} are the same as in eq.(2); k_d represents the fraction of N which is lost. Two alternatives for equation (4) using: i) enzyme kinetics or ii) the Monod's law (1941), were discussed by Pansu *et al.* (1998).

Calculation was performed according Press *et al.* (1992). The numerical integration was performed using Euler's method and the optimisation of the parameters using Powell's method, with the minimised criterion:

$$SSK = \sum_k p_k^2 \sum_j \left(y_{kj} - \hat{y}_{kj}\right)^2 \qquad (5)$$

where *j* identifies the number of sampling points; *k* is the number of data series and y_{kj} and $\hat{y}_{kj}$ are the measured and the predicted value of each data point respectively; p_k are weight coefficients for each data series.

3. Results and discussion

3.1. Mineralisation and humification processes

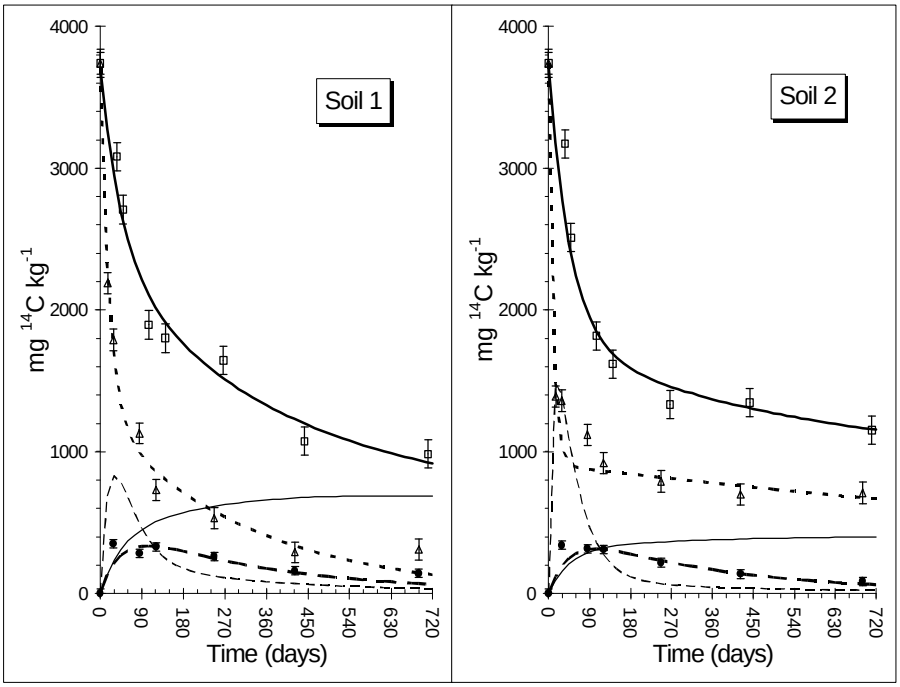

Fig.2. - Predicted and measured ^{14}C in the whole soil and in the organic compartments:

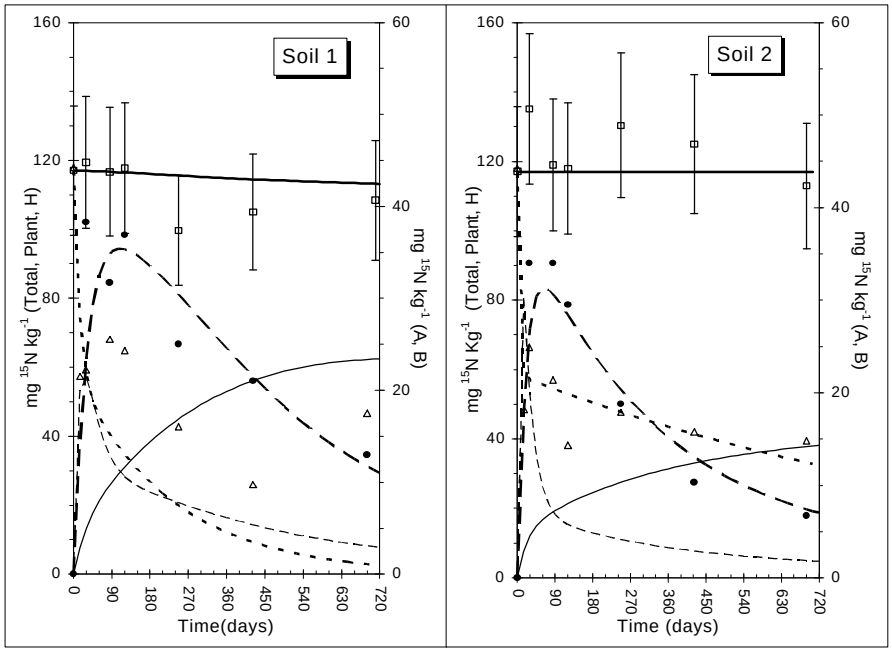

Fig.3. - Predicted and measured ^{15}N in the whole soil and in the organic compartments (for caption, see Fig. 2).

The variation of total ^{14}C and ^{15}N and of ^{14}C and ^{15}N in the organic compartments is shown in figures 2 and 3. Model fitting was in agreement with experimental data, except for plant debris-^{15}N in soil 1. In the experiment, the amount of coarse material-^{15}N was probably overestimated by incomplete dispersion of the fine particles in clayey soil (Pansu *et al*., 1998). Incomplete fractionation affected ^{15}N data (Fig.3) but not ^{14}C data (Fig.2), since nitrogen remained in the system, while most of ^{14}C was lost as CO_2.
The main difference between the two soils concerned the mineralisation and humification kinetics. Except at the beginning of the incubation, both processes were faster in soil 1 than in soil 2. After two years of incubation, the ^{14}C remaining in soil 1 and 2 was 25 % and 31 % of the initially added ^{14}C respectively (Fig.2), while the content of the stable humified compartment H was 18% and 11%.
Storage in the compartment H was more important for ^{15}N than for ^{14}C. At the end of incubation, H-^{15}N was 54% and 33% of added ^{15}N in soil 1 and 2 respectively (Fig. 3). After two years, the ratio "compartment H of soil 2 / compartment H of soil 1" was about 0.6 for both ^{14}C (Fig. 2) and ^{15}N (Fig. 3). Nitrogen was progressively incorporated into the stable humified compartment H. With a C-to-N ratio near 10 at the end of the experiment, this compartment appears to be the major ^{15}N long term storage reservoir.
After two years, 18% of added ^{14}C and 28 % of added ^{15}N remained in coarse material in soil 2, whereas these proportions were negligible in soil 1 (less than 3% of added ^{14}C).
The microbial biomass-^{14}C and -^{15}N amounts were similar for both soils, with a higher turnover rate in soil 1 compared to soil 2 for carbon (Bottner *et al*., 1988; Sallih et Pansu, 1993) and nitrogen (Pansu *et al*., 1998).
For both soils, nitrogen was quickly incorporated into microbial biomass. In agreement with the measured values, the predicted ^{14}C-to-^{15}N ratios of the compartment B was ≤ 10. In contrast, the variation of the ^{14}C-to-^{15}N ratio of the labile compartment A showed that ^{15}N of this fraction was quickly exhausted. The compartment A is the main energy source for micro-organisms.

3.2. Nitrification, immobilisation and volatilisation processes

The variation of NH_4-^{15}N and NO_3-^{15}N is shown in Fig. 4. Model fittings were in agreement with experimental data. In soil 1, the exchangeable NH_4-^{15}N was lightly lower than the simulated *aN* compartment; a bias can result from a partial fixation of ^{15}N-NH_4 by clays (Pansu *et al*., 1998).
The MOMOS model does not need a specific parameter to simulate NH_4-N. A fraction of the output from the organic compartments, defined by P_i parameters (arrow 1 in Fig. 1), is directly reorganised (eq. 2). The remaining fraction is the input (2 in Fig. 1) into NH_4-N compartment (eq. 3). The output from NH_4-N compartment (3 and 4 in Fig. 1) at step *j*, is its whole content at step *j*-1 (eq. 3).
Nitrification (4 in Fig. 1) is the only process which cannot be simulated by a first order kinetics. MOMOS use a simple growth law (eq.4), according to which the nitrate production rate (growth rate) is proportional to the mass of depleted substrate (ammonium). Moreover, this equation allowed to simulate the delay, which was observed during the early weeks before the nitrification started. At this initial stage, the contents of compartments A and NH_4 were maximum. The C substrate as energy source (compartments A and V_L) is in excess and thus the microorganisms (compartment B) require nitrogen for their development. Nitrification is then delayed and all NH_4-N is

immobilised (3/4 in microbial compartment B, 1/4 directly in stable compartment H) until the content of the *aN* compartment falls under *kn2* (eq.4).
As generally described (Dommergues et Mangenot, 1970; Stevenson, 1986), MOMOS assumes that the microorganisms use NH_4^+ preferably to NO_3^- as inorganic N source. Gaseous N loss (5 in Fig. 1) during nitrification (N_2O release) and denitrification (N_2O and N_2) are regulated by k_d. The N loss (estimated by total ^{15}N balance) from soil 2 was not significant, thus $k_d = 0$. For soil 1, a loss of about 10% of the N-flux between NH_4^+ and NO_3^- ($k_d = 0.1$) occurred after the onset of nitrification.

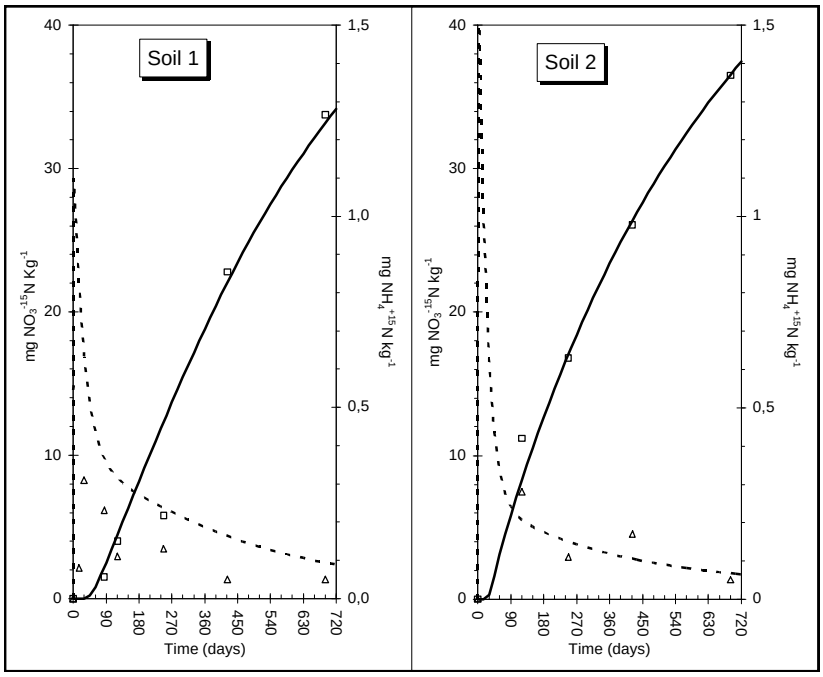

Fig. 4. - Predicted and observed inorganic ^{15}N: —— = NO_3 ^{15}N, - -Δ- - = NH_4 ^{15}N

3.3. Conclusion

The MOMOS formulation is relatively simple and based on data obtained under controlled conditions. The model was able to describe the transformation of labelled C and N as well as total C and N.
This model shows the conceptual difference between nitrification and the other biological processes in soils which are explained by first order kinetics, since they are associated with a wide range of diversified microbial species. In contrast, nitrification, which is associated principally with only two microbial genera, is described by a growth function. Exchangeable ammonium concentration results from the balance of all the other N fluxes. The equations allowed to simulate the observed delay of nitrification, when the energy source (carbon of compartment A) was in excess for microorganisms; during this initial phase, the whole exchangeable ammonium was immobilised.

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