Modelling water, carbon and nitrogen dynamics in soil covered with decomposing mulch

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Summary

A decomposing mulch of residues on the soil affects strongly the water, carbon and nitrogen cycling in the soil. The mulch generates complex and interacting effects that remain difficult to quantify and model. An original mulch module was developed and implemented in the PASTIS model to account for the main biological and physical effects of decomposing mulch. In the extended model, PASTIS$_{mulch}$, the formalism splits the mulch into a decomposable layer in contact with the soil and an overlying not decomposable layer that 'feeds' the former. The model was calibrated on laboratory data derived from mulched soil columns experiments. Two types of residues were tested: rape residues made of large elemental particles (length, 10 mm; width, 3–10 mm; thickness, 0.1–8 mm) with a C:N ratio of 29, and rye residues consisting of smaller particles (length, 10 mm; width, 2 mm; thickness, 0.1 mm) with a smaller C:N ratio of 16. Calibration showed that mulch parameters were dependent on the type of residue. The model run with calibrated parameters provided good simulations of the water, carbon and nitrogen dynamics, with global efficiencies greater than 0.8. The sensitivity analysis carried out on seven key parameters showed that the total mulch dry mass and the proportion of this dry mass in contact with the soil are decisive parameters. PASTIS$_{mulch}$ highlighted that mulch decomposition was not a continuous process but occurred in the form of successive pulses that correspond to favourable hydric conditions.

Introduction

In the context of global warming, agricultural management practices have been proposed as one way to mitigate CO_2 emissions by increasing C storage in agricultural soils (Paustian *et al.*, 1997). Conservation tillage changes C distribution into the soil, soil physical and chemical properties and the associated microbial activities (Coppens *et al.*, 2006). It has been suggested that the beneficial effect of soil C storage with conservation tillage could be counterbalanced by other impacts, such as an increase in N_2O emissions or NO_3^- leaching associated with changes in dynamics and distribution of water, C and N in soil (Ball *et al.*, 1999; Six *et al.*, 2002). Therefore the development of models that enable simultaneous prediction of the transformations of organic matter and the flows of heat and mass in soils is crucial to the assessment of various environmental impacts of soil management.

Many models have been developed to describe the effect of a surface residue mulch on the dynamics of water and temperature in the soil-plant-atmosphere system: SiSPAT (Gonzalez Sosa *et al.*, 1999), TEC$_{mulch}$ (Findeling *et al.*, 2003a), NTRM (Shaffer & Larson, 1987) and others (Bussière & Cellier, 1994; Findeling *et al.*, 2003b). These models were mainly used to assess the impact of the mulch on physical processes such as water runoff, soil thermal regime, erosion and evaporation. They do not account for the biological processes involved in the decomposition of the mulch.

Other models have been developed to simulate the decomposition of a litter of crop residues under various conditions. Amongst them, a first group of models has been designed to address the long-term effects of residue management on the C storage and the N leaching in soils: CENTURY (Parton *et al.*, 1987), GENDEC (Moorhead & Reynolds, 1991), and ROTHC (Coleman & Jenkinson, 1996). Moorhead *et al.* (1999) showed that they predict fairly well the fate of C and N as controlled by litter quality, nitrogen availability and abiotic factors. However, these models work with time steps too large

(typically 1 day or more) to account satisfactorily for the strong interaction between the mulch decomposition and the water, nitrogen and temperature regime in the soil-atmosphere system.

A second group of models has been developed to simulate the decomposition of a surface residue mulch and the associated C and N dynamics at the shorter time-scale of a crop cycle: CERES-N (Quemada *et al.*, 1997), STICS (Brisson *et al.*, 1998), NCSOIL (Molina *et al.*, 1983), APSIM (Thorburn *et al.*, 2001), and EXPERT-N (Berkenkamp *et al.*, 2002). APSIM and EXPERT-N have in common a specific *mulch module* that splits the mulch into two layers, one being in close contact with the soil while the upper layer is 'feeding' the former as a function of external factors (management, climatic events, etc.). Although these models proved efficient in simulating mulch decay, there is general agreement about a lack of knowledge of the mechanisms that drive mulch decomposition (Guérif *et al.*, 2001). The effect of abiotic factors (mulch temperature, mulch water content, nitrogen limitations and contact between mulch and soil) on the dynamics of decomposing microorganisms is poorly documented. Consequently, modelling mulch decomposition remains a challenging issue.

The main objective of this work is to propose a new modelling approach to mulch decomposition in interaction with its biochemical quality and physical properties, at the crop cycle scale. A module that takes the mulch into account was developed and implemented in the PASTIS model (Garnier *et al.*, 2003; Lafolie, 1991), which simulates water, heat and solute transport, and C and N cycling in soil. The subsequent model is referred to as PASTIS$_{mulch}$. Its originality lies in a coupling between the biological processes that drive mulch decomposition and the mass and heat flows in the soil-mulch-atmosphere continuum. It includes a description of abiotic factors by laws currently used for incorporated residues and adapted to the mulch by taking into account the specific water regime of the mulch. Two types of mulch were tested: a mulch of rape residues collected at maturity of the crop and having a high C:N ratio, and a mulch of rye residues collected during the vegetative phase and having a lower C:N ratio. The experiments were conducted under laboratory conditions for both residues. The strategy adopted relied on three steps: (i) developing the mulch module of PASTIS$_{mulch}$ to simulate the effect of the mulch on the water, carbon and nitrogen dynamics, (ii) calibrating the model for both residues with the experimental data collected by Coppens *et al.* (2006) in soil columns, and (iii) evaluating the model and assessing its sensitivity to some key parameters of the mulch.

Materials and methods

The PASTIS model

The one-dimensional mechanistic model PASTIS (Prediction of Agricultural Solute Transfer In Soils), described by Lafolie

(1991), Garnier *et al.* (2001) and Garnier *et al.* (2003), simulates the transport of water, solutes and heat using classical equations, i.e. Richard's equation for water flow, the convection-dispersion equation for solute transport and the convection-diffusion equation for heat flow.

The CANTIS submodel (Carbon and Nitrogen Transformations In Soil) simulates the transformations of carbon and nitrogen (Garnier *et al.*, 2003). Soil organic matter is divided into three non-living organic pools: fresh, soluble and humified organic matter (FOM, SOL, HOM, respectively) and two living pools. The microbial population is split into an autochthonous biomass (AUB) that decomposes humified organic matter and a zymogenous biomass (ZYB) that decomposes fresh and soluble organic matter. The meanings of the parameters are listed in Table 1.

Adaptation of the PASTIS model

PASTIS was originally designed for incorporated residues. In this work, the model is adapted to the case of a surface residue mulch to take into account the physical effects of the mulch on rain interception and evaporation (Findeling, 2001), and the specific dynamics of decomposition of the latter. The new model is referred to as PASTIS$_{mulch}$ and the introduced parameters are listed in Table 2.

For rain interception, the mulch as a porous medium can intercept rainfall up to a maximum value $R_{m,max}$ (m) defined as:

$$R_{m,max}(t) = \frac{\theta_{mp,max}}{\rho_{mp}} DM_m(t), \qquad (1)$$

where $\theta_{mp,max}$ is the maximum volumetric water content of mulch particles (m^3 m^{-3}), ρ_{mp} is the density of mulch particles (g m^{-3}) (both assumed constant during decomposition), DM_m is the mulch dry mass (g m^{-2}), and t is time (days). Mulch water storage, R_m (m), is calculated as:

$$\Delta R_m = \begin{cases} \Delta R \exp\left(-\alpha_m \frac{R_{m,max} - R_{m,res}}{R_{m,max} - R_m}\right) & \text{if } R_m < R_{m,max}, \\ 0 & \text{if } R_m = R_{m,max}, \end{cases} \qquad (2)$$

Table 1 Estimated biological parameters used in the CANTIS (Carbon and Nitrogen Transformations In Soil) submodel

Symbol	Parameter	Rape	Rye
k_Z	Decomposition rate of zymogenous biomass (ZYB)/d^{-1}	0.0206	0.0490
k_A	Decomposition rate of autochthonous biomass (AUB)/d^{-1}	4.89×10^{-3}	4.89×10^{-3}
k_H	Decomposition rate of humified organic matter (HOM)/d^{-1}	2.50×10^{-4}	2.50×10^{-4}
h_Z	Humification coefficient by ZYB	0.1403	0.2629
h_A	Humification coefficient by AUB	0.3761	0.3761

Table 2 Mulch parameters used in the mulch module of PASTIS$_{mulch}$ (Prediction of Agricultural Solute Transfer In mulched Soils) model

Symbol	Parameter	Rape	Rye
$DM_m(0)$	Initial dry mass /g m^{-2}	552.8	417.4
$DM_{m,c}(0)$	Initial dry mass in contact/g m^{-2}	To be calibrated	
z_m	Mulch thickness/cm	1	2†
α_{feed}	Mulch feeding rate/day^{-1}	To be calibrated	
$\theta_{mp,max}$	Maximal volumetric water content of mulch particles/m^3 m^{-3}	0.212	0.700
$w_{mp,max}$	Maximal gravimetric water content of mulch particles/g g^{-1}	2.078	2.000
$R_{m,max}$	Maximal mulch water storage/m	0.0013	0.0010
$\theta_{mp,res}$	Residual volumetric water content of mulch particles/m^3 m^{-3}	0.030	0.105
α_m	Mulch propensity to water recharge	0.25	0.25
ρ_{mp}	Density of mulch particles/g m^{-3}	102 000	350 000
$z_{m,zyb}$	Maximum extension depth of zymogenous biomass in the soil/cm	To be calibrated	

†Thickness of the rye mulch decreased continuously from 2 cm to 0.5 cm along the experiment.

where R is the cumulative rainfall (m), α_m is the mulch propensity to water recharge (–), and $R_{m,res}$ is the residual mulch water content (m) calculated from the residual volumetric water content of mulch particles, $\theta_{mp,res}$ (m^3 m^{-3}), as in Equation (1). The amount of rain that is not intercepted by the mulch is transmitted to the soil. When the flux of water reaching the soil exceeds the Darcy's infiltration flux, ponding water is stored and infiltrated later on into the soil.

For evaporation, the mulch acts as a physical barrier to convective and diffusive vapour fluxes between the soil and the atmosphere (Findeling *et al.*, 2003a). As a consequence, the total potential evaporation rate, E^{pot} (kg m^2 s^{-1}), is split into the potential evaporation rate of the mulch, E_m^{pot} (kg m^2 s^{-1}), and the soil, E_s^{pot} (kg m^2 s^{-1}):

$$E_m^{pot} = \xi E^{pot}$$
$$E_s^{pot} = (1 - \xi)E^{pot}, \tag{3}$$

where $\xi = 0.352$ is the propensity of the mulch to reduce soil evaporation demand (Findeling, 2001). E_s^{pot} is applied to the soil. E_m^{pot} is applied to the mulch to evaporate its water storage:

$$\Delta R_m = -\min(E_m^{pot}\Delta t; R_m). \tag{4}$$

For decomposition, residue decomposition is highly dependent on the contact with microorganisms and the available mineral nitrogen resource (Garnier *et al.*, 2003; Henriksen & Breland, 2002). In the case of mulch, the residue particles that are closely in contact with the soil will decompose more easily because microorganisms from the soil can colonize them and fungi can use their hyphae to absorb mineral nitrogen in the soil to decompose the residue. On the contrary, the upper particles that are not in contact with the soil will hardly decom-

pose because of water limitation that hinders microorganism activity. Based on an approach similar to that of Thorburn *et al.* (2001) in the APSIM-Residue model, we define two compartments for the mulch (Figure 1):

$$DM_m(t) = DM_{m,c}(t) + DM_{m,nc}(t), \tag{5}$$

where $DM_{m,c}$ is the mulch dry mass in contact with the soil (kg m^{-2}) and $DM_{m,nc}$ is the mulch dry mass not in contact with the soil (kg m^{-2}). The former can decompose whereas the latter is assumed unavailable for decomposition. $DM_{m,nc}$ is set to an initial value and then decreases exponentially with time to account for the progressive rearrangement of the mulch due to climatic action (rain and wind). This decrease corresponds to an equivalent increase in $DM_{m,c}$:

$$\Delta DM_{m,c}(t) = \alpha_{feed}DM_{m,nc}(t)\Delta t, \tag{6}$$

where α_{feed} (d^{-1}) is the extinction coefficient of $DM_{m,nc}$ and called the feeding rate of the decomposable mulch compartment by the non-decomposable mulch compartment. Decomposition of $DM_{m,c}$ is based on the CANTIS model (above). $DM_{m,c}$ is split into fresh and soluble organic matter as done by Garnier *et al.* (2003) for incorporated organic matter in PASTIS. Mulch decomposition is controlled by the temperature, water and nitrogen abiotic functions (respectively: f_T, f_W and f_N) defined for the incorporated soil organic matter decomposition in Garnier *et al.* (2001). However, these functions are calculated by using mulch variables instead of soil variables. The mulch particle temperature ($T_{mp} = 20°C$, constant in this experiment) and the mulch particle volumetric water content, θ_{mp} (m^3 m^{-3}), are used to calculate, respectively, the abiotic functions f_T and f_W in the mulch. Also, only a limited topsoil layer can be involved in mulch decomposition because the influence of the zymogenous biomass, which decomposes the mulch, is limited by the maximum length of the fungal hyphae (Figure 1). The thickness of this topsoil layer is defined by the maximum extension depth of the zymogenous biomass, $z_{m,zyb}$ (m). Nitrogen immobilization for mulch decomposition is restricted to the amount of mineral N contained in the topsoil layer of thickness $z_{m,zyb}$. Thus, for the mulch, f_N is calculated from the available amount of mineral N in this layer. Finally, mineralized N from the mulch is assumed to be produced in the same topsoil layer.

Experimental data used to evaluate the model

The experimental design is thoroughly described in Coppens *et al.* (2006). Two types of crop residues were used to form the mulch: (i) a moderately decomposable residue, namely mature oilseed rape (*Brassica napus* L.) with a C:N ratio of 29, and (ii) an easily decomposable residue, namely young rye (*Secale cereale*) with a C:N ratio of 16 (Table 3). For the rape, the residues consisted of a mixture of leaves (25%), stalks (41%), branches (8%) and pods (26%). For the rye residue, the
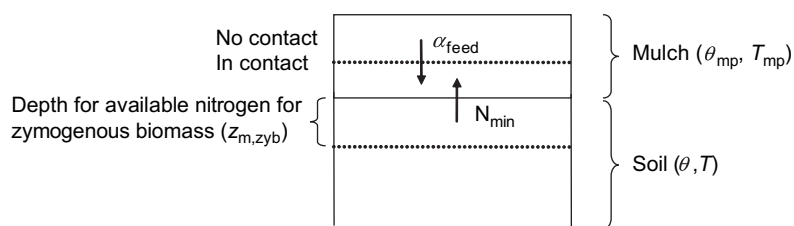
Figure 1 Conceptual diagram of mulch decomposition processes based on a two mulch compartments approach (for variables, see text).

sample consisted only of green leaves. Both residues were chopped into 10-mm long particles with scissors, before application onto the soil. The rape particles were 3–10 mm wide and 0.1–8 mm thick. The rye particles were smaller, with typical width and thickness of 2 mm and 0.1 mm, respectively. For both residues, the soluble fraction (SOL) was determined by water extraction and the rapidly decomposable material (RDM), the hemicelluloses (HEM), the cellulose (CEL), and the lignin (LIG) fractions of the fresh organic matter (FOM) were determined by proximate analysis (Van Soest & Wine, 1967). Initial water contents were 0.03 and 0.11 m^3 m^{-3}, respectively, for the rape and the rye mulches.

The soil was a silt loam, Typic Hapludalf (Orthic Luvisol), of the experimental site of INRA, Mons-en-Chaussée, northern France (49°80′N, 3°60′E) (Table 3). The soil was 2-mm sieved at field moisture content (0.217 and 0.176 m^3 m^{-3} for the rape and the rye experiment, respectively). Plastic cylinders (15.4 cm diameter and 30 cm length) were used to pack the soil to 25 cm depth at 1.3 g cm^{-3} (6.022 kg of dry soil per column). For each residue experiment, a dry mass of 13.78 g (equivalent to 7.4 t ha^{-1}) was applied at the surface of each cylinder as mulch (Coppens *et al.*, 2006). The experiment lasted 9 weeks and included three rain applications followed by three drying periods (Table 4). Artificial rain was applied to the columns with a rain simulator (12 mm $hour^{-1}$) at day 0 (30 mm), day 21 (10.5 mm) and day 42 (11 mm). The amount of water applied as the second and third rain was calculated to offset the water depletion during the current evaporation period. During the drying periods, the columns were kept in a climate chamber at 20°C and 70% relative air humidity to allow evaporation.

CO_2 flux from the soil surface to the atmosphere was calculated from the accumulation rate of CO_2 in the headspace of the columns. Soil volumetric water content (by TDR) and soil water potential (by tensiometer) were measured at 6 and 14 cm depth. Mass loss of the columns was used to calculate daily evaporation. Mulch water content was measured on three specific columns equipped with detachable mulch placed on a 1-mm aperture mesh. These data were used to calculate the water content of the mulch, after correction of the mass for leached and mineralized C as described by Coppens *et al.* (2006).

Soil solution was sampled at 2-cm depth for mineral nitrogen measurement (NO_3^- and NH_4^+) by colorimetry, 12 hours after each rain. Destructive measurements were carried out on specific columns (three for each residue) after 3, 6 and 9 weeks. Mulch dry mass was measured after oven drying (70°C, 72 hours). Mineral nitrogen content in the 0–5 cm topsoil was KCl-extracted before each rain and measured by colorimetry (NO_3^- and NH_4^+). The total C content of the soil and the recovered plant residues was determined using an elemental analyser. The microbial biomass carbon was determined by a modified fumigation-extraction method proposed by Vance *et al.* (1987).

Modelling conditions and parameters

$PASTIS_{mulch}$ was applied to the 25-cm soil columns covered by the mulch of rye and rape of constant thickness, z_m (m). Depth was set to zero at the soil–mulch interface. Rain intensity and actual evaporation were imposed on the model as the

Table 3 Characteristics of the soil, the rape residues and the rye residues

Parameter	Soil	Rape residues	Rye residues
Mulch particle size:			
Length/mm	/	10	10
Width/mm	/	3–10	2
Thickness/mm	/	0.1–8	0.1
Specific surface/cm^2 g^{-1}	/	152	329
C content/%	0.85	42.2	43.4
N content/%	0.09	1.45	2.70
C:N ratio	9.47	29.1	16.1
Clay/%	13.4	/	/
Silt/%	81.6	/	/
Sand/%	5.0	/	/
pH H_2O	8.2	/	/

Table 4 Description of experimental conditions for the rape and rye experiments

Parameter	Rape experiment	Rye experiment
Amount of soil†/kg $column^{-1}$	6.022	6.022
Initial N-NO_3^- in soil/mg kg^{-1} soil	9.80	29.85
Amount of residues† added/g $column^{-1}$	13.78	13.78
N added by residue/g $column^{-1}$	0.20	0.37
C added by residue/g $column^{-1}$	5.82	5.98
Temperature/°C	20	20
Duration/days	64	64
Days of rain application/days	0 (30 mm), 21 (10.5 mm), and 42 (11 mm)	

†Amount expressed in dry mass.

surface boundary condition for water. At the bottom of each column, the water boundary condition was a Neumann zero flux condition. Temperature was constant and set to 20°C in the whole system. The equations of PASTIS$_{mulch}$ were solved by using a finite differences technique with regular node spacing of 0.5 cm and a time step between 0.001 and 360 s.

Initial conditions. The initial conditions were derived from measurements for each experiment. The initial water condition of PASTIS$_{mulch}$ was given by a constant volumetric water content profile: $\theta = 0.217$ m^3 m^{-3} for the rape experiment and $\theta = 0.176$ m^3 m^{-3} for the rye experiment. Solutes in the soil were initialized with constant concentration profiles: $[NO_3^-] = 0.257$ mg cm^{-3} for the rape experiment, $[NO_3^-] = 0.783$ mg cm^{-3} for the rye experiment.

Water flow input parameters. The soil water retention curve, $h(\theta)$, was obtained for each residue mulch experiment by TDR and tensiometer measurements in the column (matric potential in the range –5 to –20 kPa) and the pressure extractor method for lower matric potentials (in the range –50 to –150 kPa). The experimental data were fitted with the Van Genuchten model:

$$S_e(h) = \frac{\theta - \theta_r}{\theta_s - \theta_r} = [1 + (\alpha h)^n]^{-\left(1 - \frac{1}{n}\right)}, \tag{7}$$

where $S_e(h)$ is the effective saturation (–), θ_r and θ_s are, respectively, the residual and saturated volumetric water contents (m^3 m^{-3}), α is the scaling factor of matric potential (m^{-1}), and n is an empirical shape parameter (–).

The Van Genuchten model was selected for the hydraulic conductivity curve $K(\theta)$:

$$K(\theta) = K_s S_e^l \left[1 - \left(1 - S_e^{1/m}\right)^m\right]^2, \tag{8}$$

where K_s is the saturated soil hydraulic conductivity (m s^{-1}), m is an empirical shape parameter (–), and l is the tortuosity parameter set to 0.5. These parameters were determined by non-linear fitting on the simulated soil matric potentials at 6 and 14 cm depth compared with the corresponding tensiometric measurements. All the parameters of Equation (7) and Equation (8) are given in Table 5 for both experiments.

Biological input parameters. We estimated the biological parameters of the CANTIS submodel (Table 1) by fitting the model to the data of independent soil incubations (C and N mineralization curves). Standard incubations were carried out following the experimental layout described in Mary *et al.* (1993). The incubation data obtained in the soil *without* residue were used to estimate three parameters for the decomposition of humified organic matter: the decomposition rates, k_A and k_H, and the humification coefficient h_A (Table 1). The incubation data obtained in the soil *with* incorporated residues

(1–3 mm particles) were used to calculate three parameters concerning the decomposition of fresh organic matter: the decomposition rate k_Z, the humification rate h_Z, and the C:N ratio of the zymogenous biomass (Table 1). The other generic parameters (not presented here) were set to default values described in Garnier *et al.* (2003).

Model calibration, evaluation and sensitivity analysis

Calibration. The PASTIS$_{mulch}$ model was calibrated on three parameters that were introduced in the formalism of mulch decomposition and were difficult to assess by direct measurement or observation: the initial amount of mulch dry mass in contact with the soil, $DM_{m,c}(0)$ (g m^{-2}), the mulch feeding rate, α_{feed} (day^{-1}), and the maximum extension depth of zymogenous biomass in the soil, $z_{m,zyb}$ (cm). The Nash efficiency, E_f (–), was used to assess model performance:

$$E_f = \frac{\sum_{i=1}^{n} (m_i - \overline{m})^2 - \sum_{i=1}^{n} (m_i - s_i)^2}{\sum_{i=1}^{n} (m_i - \overline{m})^2}, \tag{9}$$

where m_i and s_i are the measured and simulated values for a given state variable, and $\overline{m}$ is the average of the n measured values. For each residue, the efficiency was calculated for the amount of carbon remaining in the mulch and for the nitrate content of the 0–5 cm topsoil layer. The arithmetical average of these efficiencies, $\overline{E}_f$ (–), was used to identify the best simulation for the rape and the rye experiments. For both experiments the tested values for calibrated parameters were 0, 20, 40, 60, 80 and 100% of $DM_m(0)$ for $DM_{m,c}(0)$, 10^{-1}, 10^{-2} and 10^{-3} day^{-1} for α_{feed}, and 1, 3, 5, 7 and 10 cm for $z_{m,zyb}$.

Evaluation. The model was evaluated with the calibrated mulch parameters for both mulch experiments. The simulations of the water, nitrogen and carbon dynamics were analysed and discussed for the soil and the mulch.

Sensitivity analysis. A one-at-a-time analysis of sensitivity of PASTIS$_{mulch}$ was carried out on the three calibration parameters plus four additional mulch parameters: the initial dry mass, $DM_m(0)$, the maximal and residual volumetric water content of mulch particles, $\theta_{mp,max}$ and $\theta_{mp,res}$, respectively, and the mulch propensity to water recharge, α_m. The relative variation of the parameters, $\Delta X_i(j)$ (–), was defined as:

$$\Delta X_i(j) = \frac{X_i^j - X_i^*}{X_i^*}, \tag{10}$$

where $X_{1 \leq i \leq 7} \in \{DM_m; DM_{m,c}; \alpha_{feed}; z_{m,zyb}; \theta_{mp,max}; \theta_{mp,res}; \alpha_m\}$ stands for the tested parameter, and X_i^* and X_i^j are the optimum value and current value j of parameter X_i, respectively. Model sensitivity was studied through two significant output variables related to mulch effects: the final carbon amount

Table 5 Hydraulic parameters of soil retention and soil conductivity curves for the rape and the rye experiments

Symbol	Parameter	Rape experiment	Rye experiment
Retention curve $h(\theta)$			
θ_s	Saturated volumetric water content/$m^3\,m^{-3}$	0.535	0.500
θ_r	Residual volumetric water content/$m^3\,m^{-3}$	0.000	0.000
α	Scaling factor of matric potential/m^{-1}	25.9	10.7
n	Empirical shape parameter	1.185	1.228
Conductivity curve $K(\theta)$			
K_s	Saturated water conductivity/$m\,s^{-1}$	1.67×10^{-5}	4.17×10^{-5}
m	Empirical shape parameter	0.225	0.200

remaining in the mulch, $C_{m,fin}$ (mg C m^{-2}), and the final nitrate content in the 0–5 cm topsoil layer, $NO_{3,fin}^-$ (kg N ha^{-1}). The sensitivity, ζ (–), was expressed for each parameter and each variable as:

$$\zeta(X_i, j, Y_k) = \frac{1}{2}\left\{\left[\frac{Y_k^{rape}\left(X_1^*, \ldots, X_i^j, \ldots, X_7^*\right)}{Y_k^{rape}\left(X_1^*, \ldots, X_i^*, \ldots, X_7^*\right)} - 1\right] + \left[\frac{Y_k^{rye}\left(X_1^*, \ldots, X_i^j, \ldots, X_7^*\right)}{Y_k^{rye}\left(X_1^*, \ldots, X_i^*, \ldots, X_7^*\right)} - 1\right]\right\}, \quad (11)$$

where $Y_{1 \leq k \leq 2} \in \{C_{m,fin}; NO_{3,fin}^-\}$ is the type of simulated variable.

Results and discussion

Model calibration

The values of calibrated parameters (Table 6) show two different patterns for the rape and the rye experiments. For the rape, the optimal value of the initial mulch dry mass in soil contact ($DM_{m,c}(0)$) was only 20% of total initial mulch dry mass. The larger size of the rape mulch particles (Table 3) impeded close contact between the soil and the mulch particles, especially those from the upper part of the mulch. For the rye, we found an optimal value of $DM_{m,c}(0)$ of 80% of total initial mulch dry mass. This result can be explained by the smaller size and the greater specific surface of the elemental particles of rye residue compared with rape residue. According to the calculation proposed by Angers & Recous (1997), the specific area was 329 $cm^2\,g^{-1}$ for the rye residues and only 152 $cm^2\,g^{-1}$ for the rape residues (Table 3). The mulch feeding rate, α_{feed}, took the largest value of the calibration range and was the same for both kinds of residue. This parameter had little influence on simulation, which will be discussed in the sensitivity analysis section. The maximum extension depth of zymogenous biomass in the soil, $z_{m,zyb}$, revealed another difference between the residues. For the rape this parameter took a large value of 5 cm. This suggests that fungi

Table 6 Optimal value of the parameters and statistical performance of the calibrated model for the rape and the rye experiments

Symbol	Parameter, variable	Rape	Rye
$DM_{m,c}(0)$	Initial mulch dry mass in soil contact/$g\,m^{-2}$	110.6	333.9
$\frac{DM_{m,c}(0)}{DM_m(0)}$	Initial proportion of mulch dry mass in soil contact/%	20	80
α_{feed}	Mulch feeding rate/day^{-1}	0.1	0.1
$z_{m,zyb}$	Depth for available N for mulch decomposition/cm	5	1
Global performance			
E_f	Average model efficiency	0.804	0.825
Carbon in mulch			
E_f	Model efficiency for carbon	0.813	0.924
Slope	Slope of linear regression	0.711	0.876
Origin	Origin of linear regression/$mg\,C\,m^{-2}$	80.5	34.1
σ_{res}	Residual standard deviation/$mg\,C\,m^{-2}$	6.1	6.7
R^2	Coefficient of determination	0.832	0.955
B	Bias/$mg\,C\,m^{-2}$	0.8	5.1
Nitrate in soil (0–5 cm)			
E_f	Model efficiency for nitrate	0.795	0.725
Slope	Slope of linear regression	0.914	0.579
Origin	Origin of linear regression/$kg\,N\,ha^{-1}$	0.8	6.6
σ_{res}	Residual standard deviation/$kg\,N\,ha^{-1}$	1.3	2.0
R^2	Coefficient of determination	0.813	0.930
Bias	Bias/$kg\,N\,ha^{-1}$	–0.2	–3.3

had an important role in rape mulch decomposition, which is in good agreement with the higher C:N ratio of this residue. The fungal hyphae probably facilitated the colonization of the poorly clumped mulch particles and allowed the deep absorption of nitrate into the soil as already observed by Frey *et al.* (2000). For the rye, $z_{m,zyb}$ took a small value of 1 cm. The close contact of this residue with the soil and its low C:N ratio made it easier for microorganisms to decompose and required less extra (soil) mineral nitrogen. Finally, no significant correlation was observed between parameters $DM_{m,c}(0)$ and $z_{m,zyb}$ for the rape or the rye experiment, which suggests that parameters were independent and specific to the decomposition processes they encompassed.

The simulations performed with the calibrated parameters were satisfactory (Table 6), with global efficiencies of 0.804 and 0.825 for the rape and the rye experiments, respectively. Carbon in mulch was well simulated for both residues with efficiencies greater than 0.8, with good regression statistics despite a small bias of 5.1 mg C m^{-2} for the rye. PASTIS$_{mulch}$ reproduced fairly well the nitrate dynamics in the 0–5 cm topsoil layer for the rape, which provided good values for all statistical criteria. The model performed satisfactorily for the rye in spite of a larger bias of –3.3 kg N ha^{-1}. The linear correlation

between simulation and observation was strong ($R^2 = 0.930$) but the regression was far from the 1:1 line.

Model evaluation

Mulch water content. Gravimetric measurements showed the successive mulch wetting-drying cycles (Figure 2a,b): the gravimetric water content of mulch particles, w_{mp} (g g^{-1}), quickly increased during the rain application and then decreased gradually during the evaporation stage. The initial maximal observed gravimetric water content was close to $w_{mp,max}$ for both residues (Table 2) and then increased slightly for the rape residues and more substantially for the rye residues. The observed increase in mulch retention after rain as decomposition proceeded can be attributed to the increase in the porosity of the plant cell walls (and consequently an increase in the bulk water retained in cell walls) associated with the degradation of cell wall polymers (Brett & Waldron, 1996). The much

greater effect with rye residue may result from the faster alteration of the cell wall components due to initial characteristics. Five or 6 days after rain application w_{mp} reached a minimal value of 0.3 g g^{-1} for both residues, which corresponded to the mulch residual water content $\theta_{mp,res}$ (Table 2). The time necessary to reach this minimal value decreased along mulch decomposition because the residue dry mass and thus the maximal mulch water storage decreased and because the increase in mulch porosity enhanced the rate of water loss of the mulch.

The model simulated well the water dynamics of the rape mulch ($E_f = 0.852$). The successive wetting and drying cycles were well reproduced. However, some discrepancies were observed for the rye mulch ($E_f = 0.529$), for which the model underestimated the maximal mulch water content and the time necessary for the mulch to dry. PASTIS$_{mulch}$ could not account for an increase in maximal gravimetric water content during simulation.
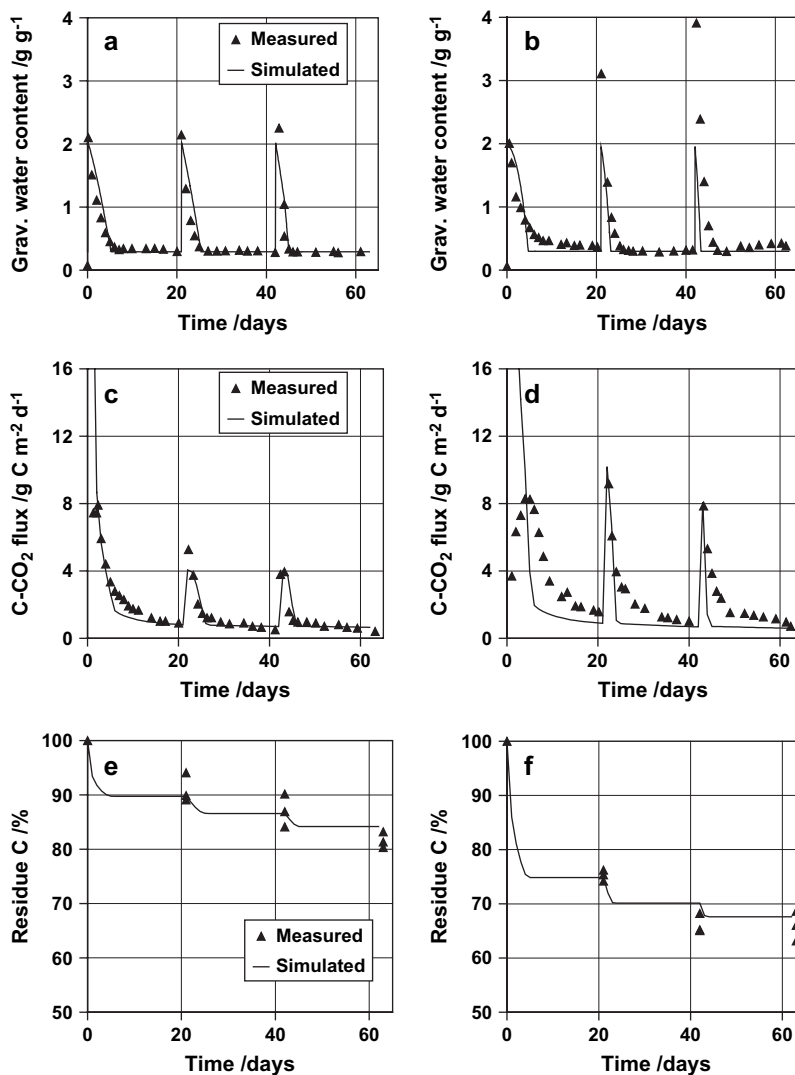
Figure 2 Simulated and measured gravimetric mulch water content: (a) rape experiment and (b) rye experiment. Simulated and measured total CO$_2$ fluxes (soil + mulch): (c) rape experiment and (d) rye experiment. Simulated and measured remaining carbon in mulch: (e) rape experiment and (f) rye experiment.

Total carbon mineralization. Measured and simulated total (soil and mulch) CO_2 fluxes are represented in Figure 2(c,d). Measured CO_2 fluxes were greater during and just after the rain application and then decreased during the evaporation period, for both residues. This trend was correlated to the evolution of gravimetric water content of the mulch. The CO_2 production was stimulated by a large water content of the mulch. For the rape experiment, the CO_2 peak tended to decrease over time (7.9, 5.3 and 4.0 g C m^{-2} day^{-1} for the first, second and third peaks, respectively), while the peaks for the rye experiment tended to remain constant over time, with a rate between 7.9 and 9.2 g C m^{-2} day^{-1}. This behaviour can be partly explained by the greater amount of soluble organic compounds of the rye mulch, which generated larger and more lasting CO_2 emissions. Also the greater water content of the rye mulch during the second and third rains (Figure 2a,b) facilitated mulch decomposition. No temperature effect was observed because temperature was maintained as constant during the whole experiment. However, in real conditions both temperature and moisture may change simultaneously and drive mineralization, which was not addressed in this work.

The peaks of CO_2 production were rather well described by the model, except at the beginning of simulation where the model strongly overestimated CO_2 flux during 1 day for the rape and 3 days for the rye experiment. Global efficiencies were poor for both experiments ($E_f < 0$), but became acceptable when removing the early overestimated simulation points from the calculation ($E_f = 0.9$ for the rape and $E_f = 0.4$ for the rye experiment). The model considered that no time lag was necessary for the zymogenous biomass to colonize the residues at the beginning of the experiment. This assumption is questionable and may partly explain the discrepancies between simulations and measurements at the beginning of the experiment, as already observed by Garnier *et al.* (2003) for incorporated residues. Also, the model was calibrated with incubation experiments using residue particles of 1–3 mm length although the mulch on the columns had particles of 10 mm length. Angers & Recous (1997) and Sims & Frederick (1970) showed that residue decomposition was greater at the beginning of incubation for small particles (mm) than for larger particles (cm).

Mulch decomposition. Observed carbon content of mulch decreased strongly during the first 3 weeks and then more slowly for both residues (Figure 2e,f). Decomposition of rye mulch was faster than decomposition of rape mulch. At day 64, measurement showed that on average only 66% of the added carbon remained in the rye residue mulch versus up to 83% in the rape residue mulch. As already observed for the CO_2 flux (Figure 2c,d), mulch decomposition occurred mainly after rain when the mulch was wet and was more intense after the first rain. The greater decomposition of rye can be explained by a lower total C:N ratio, a greater proportion of soluble

organic compounds and a larger specific surface of its elemental particles (Table 3), hence a closer contact between mulch and soil for this residue (Table 6), as discussed earlier.

PASTIS$_{mulch}$ reproduced well the two different decomposition dynamics, with efficiencies of 0.813 and 0.924 for the rape and the rye, respectively, and differences between simulation and observation always smaller than 5.1% (0.5 g C m^{-2}) in absolute terms.

Nitrogen dynamics. Measured N-NH$_4^+$ content in soil was always smaller than 1 mg N kg^{-1} soil, which was negligible compared with the N-NO$_3^-$ content. Consequently, we only considered nitrate as inorganic nitrogen. Measurements of N-NO$_3^-$ amounts in the topsoil layer (0–5 cm) are presented in Figure 3(a,b) for the end of each drying period. An increase in nitrate content over time was observed for both residues. This increase can result from mineralization of humified soil organic matter, nitrate leaching from the mulch, and convective transport of nitrate by capillary rise of water in the soil during evaporation stages. The increase in N-NO$_3^-$ over time was larger for the rye mulch than for the rape mulch. This was mainly due to a greater net release of N by the rye mulch, whose N content was greater (C:N of 16 for the rye versus 29 for the rape) and whose decomposition was more complete (Figure 2e,f).

Measured and simulated values were in good agreement for both experiments (Figure 3a,b), with efficiencies greater than 0.725. The main discrepancy was found for the amount of N-NO$_3^-$ of the rye experiment (Figure 3b). The model slightly underestimated the data at the end of the third evaporation period.

Figure 3(c,d) shows measured N-NO$_3^-$ concentration in the soil solution at 2 cm below the mulch just after the rain. Nitrate concentration stayed nearly constant over time under the rape mulch whereas it increased substantially under the rye mulch. This increase was in agreement with experimental data in Figure 3(b).

The model simulations overestimated nitrate concentration at 2-cm depth for both residues. This overestimation may partly be the consequence of gaseous losses by nitrification and denitrification (N$_2$, N$_2$O and NO) and/or a preferential downward convective transport of nitrate during the rain, which the model could not account for.

Simulation showed that nitrate concentration changed substantially over time for both residues. For each wetting-drying cycle, the simulated nitrate concentration decreased during rain application due to nitrate leaching and dilution effect and then increased during the evaporation period due to capillary rise, mineralization and concentration effect caused by water depletion. The nitrate dynamics was more marked when expressed in concentration (Figure 3c,d) than in quantity (Figure 3a,b) because concentration was sensitive to the changes in water content in addition to transport and mineralization/immobilization processes.
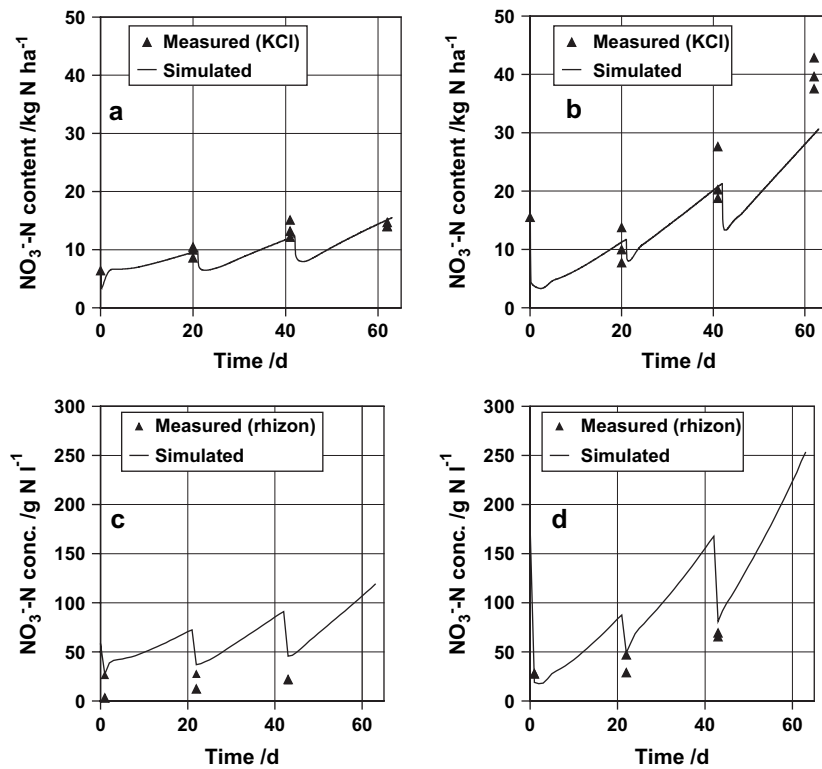
Figure 3 Simulated and measured nitrate content in the 0–5 cm topsoil layer: (a) rape experiment and (b) rye experiment. Simulated and measured nitrate concentration in soil solution at 2 cm below the mulch: (c) rape experiment and (d) rye experiment.

Sensitivity analysis

The model sensitivity, $\zeta(-)$, is presented for the final carbon amount remaining in the mulch and the final nitrate content in the 0–5 cm topsoil layer (Figure 4), for all parameters tested except the residual volumetric water content of mulch particles ($\theta_{mp,res}$) and the mulch propensity to water recharge (α_m). For these two parameters ζ was smaller than 4% for both model outputs and all relative variations of parameter from −100% up to + 200%. The greatest sensitivity was observed for the total initial dry mass of mulch ($\zeta(DM_m(0))$ up to 82%), the initial dry mass of mulch in contact with the soil ($\zeta(DM_{m,c}(0))$ up to 38%) and the maximal volumetric water content of mulch particles ($\zeta(\theta_{mp,max})$ up to 32%). ζ variation was moderate for the maximum extension depth of zymogenous biomass in the soil ($\zeta(z_{m,zyb})$ up to 16%), and limited for mulch feeding rate ($\zeta(\alpha_{feed})$ up to 4%).
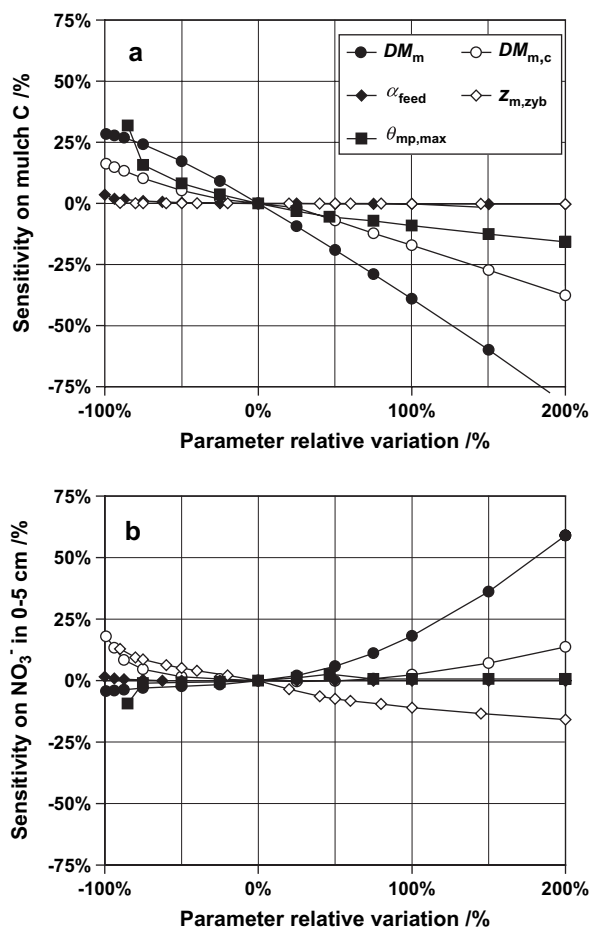
The parameters $DM_{m,c}(0)$ and $DM_m(0)$, which defined the amount of directly or indirectly available fresh organic matter for decomposition, had the greatest impact on model C output (up to 38 and 82%, respectively) (Figure 4a). The model C output was also very sensitive to $\theta_{mp,max}$ (up to 32%) that quantified the water storage capacity of the mulch and, consequently, the number of days during which the mulch was wet and could decompose. The parameter $z_{m,zyb}$ had logically little influence on the C cycle as it drove topsoil inorganic N dynamics.

For the N output variable (Figure 4b), the model sensitivity was moderate for $DM_{m,c}(0)$ and great for $DM_m(0)$, up to 18

and 59%, respectively, which emphasized the link between the carbon and nitrogen cycles in the mulch decomposition processes, and $z_{m,zyb}$ had a moderate impact (up to 16%). Nitrate content in the 0–5 cm topsoil layer decreased with this parameter because more nitrate was used by the zymogenous biomass for mulch decomposition. $\theta_{mp,max}$ had little effect on model sensitivity (up to 9%), partly because the extra mineralization caused by an increase in $\theta_{mp,max}$ was counterbalanced by a greater immobilization of the zymogenous biomass whose C:N ratio was less than that of residue. Finally, the tested N output of the model was almost insensitive to α_{feed} (less than 2%), which can be explained by the controlled laboratory conditions. In real *in situ* conditions this parameter could have more influence because weather conditions (wind drag force, heavy and variable rain events, freezing and thawing) and agricultural practices (tillage tools, cattle grazing and chopping) may influence strongly the structure of the mulch and, in turn, the amount of mulch in contact with soil.

Conclusions

This work emphasized the role of a mechanistic model in describing the simultaneous and complex processes in a soil covered with decomposing mulch, and providing C and N fluxes often not available by measurement. The assumption that only a fraction of the residues can decompose was tested successfully for both residues as mulch mineralization would be overestimated without fractionation. Also, the mulch module proved

Figure 4 Sensitivity analysis of the model outputs (final mulch residue carbon (a), and final nitrogen content in the 0–5 cm topsoil layer (b)) on five key parameters describing the mulch (for definition, see text).

and, in turn, abiotic hydric conditions for zymogenous biomass activity. Understanding and modelling this feedback still requires research on the mulch–soil interface and microbial colonization of mulch.

Acknowledgements

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robust by simulating the decomposition of two types of residues that differ significantly in biochemical quality and physical properties. The model PASTIS$_{mulch}$ was sensitive mainly to three parameters: the initial amount of mulch available for decomposition ($DM_{m,c}$), the maximal water content of mulch particles ($\theta_{mp,max}$), and the maximum extension depth of zymogenous biomass in the soil ($z_{m,zyb}$). The accurate estimation of these parameters is decisive. The parameter $\theta_{mp,max}$ can be measured directly. The parameter $z_{m,zyb}$ may be derived from a set of experiments where labelled ^{15}N is added to the soil at increasing depths below the mulch layer. The parameter $DM_{m,c}$ is more difficult to assess. However, future experiments with different types of mulch will help to correlate this parameter with physical properties such as mulch density, size and specific surface area of residue particles, and mulch geometry (standing stubble, lying leaves, etc.). Finally, we observed that decomposition associated with microbial activity could alter physical properties of the residues (e.g. porosity and hydrophobicity), which may change mulch water storage capacity

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