

Mechanistic modelling of cropland and grassland ecosystems: focus on the water cycle and on cattle grazing

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Appendices

Appendix A

Existing models

Table A.1: Models cited in this thesis with the meaning of the acronyms and the sources used.

Acronym	Meaning	Source
Anthro-BGC	Anthro BioGeochemical cycles	Ma et al. (2011)
APSIM	Agricultural Production Systems sIMulator	McCown et al. (1996)
ASPECTS	Atmosphere-Soil-Plant Exchanges of Carbon in Temperate Sylvae	Rasse et al. (2001)
CERES-EGC	Crop Environment Resource Synthesis - Environnement et Grande Cultures	Gabrielle et al. (2006)
CERES-Maize	Crop Environment Resource Synthesis - Maize	Ritchie & Otter (1985)
CERES-Wheat	Crop Environment Resource Synthesis - Wheat	Ritchie & Otter (1985)
ChinaAgrosys	China Agrosystems	Wang et al. (2007)
CQESTR	Pronounced as "sequester"	Gollany et al. (2012)
DayCent	-	Necpálová et al. (2015)
DNDC	DeNitrification DeComposition	Li et al. (1992)
DSSAT	Decision Support System for Agrotechnology Transfer	Jones et al. (2003)
EPIC	Environmental Policy Integrated Climate	Williams et al. (1989)
ORCHIDEE	Organising Carbon and Hydrology in Dynamic Ecosystems	Krinner et al. (2005)
ORCHIDEE-STICS	Association of ORCHIDEE and STICS	de Noblet-Ducoudré et al. (2004)
PaSim	Pasture Simulation	Riedo et al. (1998)
RothC	Rothamsted Carbon	Coleman & Jenkinson (2014)
SPA	Soil Plant Atmosphere	Williams et al. (1996)
STICS	Simulateur mulTidisciplinaire pour les Cultures Standard	Brisson et al. (2003)

Appendix B

Additional modules of the TADA model

B.1 Soil temperature

Soil temperature is considered as a reservoir and is modelled in every soil layer. The evolution of this physical quantity is a result of heat conduction between soil layers:

$$c_{s,i}\Delta z_i \frac{dT_i}{dt} = F_{T,i-1} - F_{T,i} \quad (\text{B.1})$$

where $c_{s,i}$ is the volumetric heat capacity [$\text{J m}^{-3} \text{ kg}^{-1}$], depending on the proportion of solid and water phases in soil, T_i is the soil temperature in layer i and $F_{T,i-1}$ and $F_{T,i}$ are the heat fluxes due to conduction from layer $i-1$ and to layer $i+1$ respectively [K day^{-1}].

Heat conductive fluxes are obtained with the same soil discretization as for water fluxes:

$$F_{T,i} = D_{T\text{moy},i,i+1} \frac{T_{i+1} - T_i}{\frac{1}{2}(\Delta z_i + \Delta z_{i+1})} \quad (\text{B.2})$$

This flux is proportional to the gradient of temperature between two adjacent soil layers and to a mean soil heat conductivity $D_{T\text{moy},i,i+1}$ taking into account both layers heat conductivities [$\text{J m}^{-1} \text{ K}^{-1} \text{ day}^{-1}$], which are expressed as an empirical function of soil water content.

The two boundary conditions regulating heat transfer in soil are the following ones:

- At the top of the soil profile, the soil temperature is equal to the air temperature as no energy balance is included in TADA;
- At the bottom of the soil profile, the temperature does not evolve with time, and is equal to the annual mean air temperature. This hypothesis is acceptable at a certain depth, the soil profile has a higher thermal inertia than the air.

B.2 Root development

In ASPECTS, two kinds of roots were considered: coarse roots and fine roots, which had different development patterns and different roles. In TADA, this distinction is not made as winter wheat and ryegrass do not produce roots as coarse as trees do. Therefore, only one type of root is considered, and its elongation is modelled through time. Root development is of great importance as the presence of roots in soil horizons defines the amount of nitrogen and water that can be consumed.

The development of **winter wheat** roots is based on Jones et al. (1991). Right after seeding, the depth of winter wheat roots is equal to the depth of planting dpt_{sow} [m]. After that, root depth is computed every time step, as the sum of the previous root depth and the potential increase in root depth, weighted by a stress factor:

$$dpt_t = dpt_{t-1} + pot_{incr} * str_{rt} \quad (B.3)$$

where t stands for the time, pot_{incr} is the potential increase of root depth per time step [m] and str_{rt} is a stress factor, computed in the soil horizon where the root tip is growing. This factor ranges from 0 to 1, and is taken as the minimum value between a temperature stress, a soil strength stress, a soil aeration stress and an acidity stress, all ranging from 0 to 1 and computed according to Jones et al. (1991).

The potential increase of root depth pot_{incr} is calculated every time step, considering that roots grow from the sowing depth to the maximum root depth as a linear function of winter wheat development stage:

$$pot_{incr} = rt_{dpt,max} \frac{GS_t - GS_{t-1}}{GS_{dpt,max}}, \quad GS < GS_{dpt,max} \quad (B.4)$$

where $rt_{dpt,max}$ is the maximum root depth [m] which is a genotype-dependent parameter and GS_t and GS_{t-1} are the growth stages of time steps t and $t-1$. The growth stage GS ranges from 0 (seed) to 1 (maturity) and is computed from the development units ($UPVT$) in the phenological module. $GS_{dpt,max}$ is the growth stage at which the root system ceases to increase in depth in soils without rooting constraints. Cereals usually stop developing their root system during grain filling ($GS_{dpt,max}=0.6$ to 0.9), and root depth does not increase any more after that stage.

Once the assimilated carbon has been allocated to the distinct plant organs, it is important to know which quantity is allocated to the roots present in the different soil horizons. The potential allocation of carbon to layer i is computed as:

$$pot_{alloc,i} = \frac{5 \frac{rt_{dens,i}}{0.025 + rt_{dens,i}} str_{rt,i} * rt_{pres,i} * z_i}{LW_{ratio,i}} \quad (B.5)$$

where $rt_{dens,i}$ is the root length density [cm cm^{-3} of roots] for each soil layer (values gathered from Asseng, 1997; Hoad et al., 2004; Hodgkinson et al., 2017), $str_{rt,i}$ is a stress factor to root development (the same as for root depth increase), $rt_{pres,i}$ is a factor describing the tendency of a plant to distribute its roots in layer i (computed according to a genotype-dependent factor), z_i is the depth of the middle of layer i and $LW_{ratio,i}$ is the length to weight ratio of roots in layer i [km kg^{-1}], expressed as a function of the growth stage, of the root depth and of a stress factor.

Once the potential carbon allocation has been computed for each soil layer, the real carbon allocation is computed as:

$$alloc_{C,rt,i} = alloc_{C,rt} \frac{pot_{alloc,i}}{\sum_{i=1}^{nhz} pot_{alloc,i}} \quad (B.6)$$

where $alloc_{C,rt,i}$ is the carbon allocated to roots in layer i [$\text{gC m}^{-2} \text{ day}^{-1}$] and $alloc_{C,rt}$ is the assimilated carbon allocated to all roots, computed in the allocation module [$\text{gC m}^{-2} \text{ day}^{-1}$].

Modelling the root system of **ryegrass** is different from winter wheat, in the way that at the beginning of the simulation, ryegrass already has developed its root system which is going to fluctuate along the year, according to environmental factors. The implemented new module of root development is based on Arora & Boer (2003) that improved the exponential root density profile proposed by Jackson et al. (1996). The potential root depth [m] is calculated at a given time t as:

$$dpt_{pot,t} = 3 \frac{(W_{rt})^{\alpha_{rt}}}{\beta_{rt}} \quad (B.7)$$

where W_{rt} is the total root biomass expressed in units of dry matter [gDM m^{-2}], and α_{rt} and β_{rt} are parameters depending on the type of vegetation. For $\alpha_{rt}=0$, roots grow horizontally, as $dpt_{pot,n}$ does not change with an

increase of root biomass. For $\alpha_{rt}=1$, roots mainly grow vertically. Therefore, the value of α_{rt} , between 0 and 1, defines whether roots grow preferentially horizontally or vertically. Similarly, β_{rt} determines if, for a given root dry matter content, the root system will rather be shallow or deep.

To take the effect of environmental factors into account, the actual root depth is not taken equal to the one computed with equation B.7, but a potential increase of root depth is computed every time step, which is then weighted by a stress factor, formulated in the same way as for winter wheat:

$$dpt_t = \begin{cases} dpt_{t-1} + str_{rt}(dpt_{pot,t} - dpt_{t-1}) & \text{if } dpt_{pot,t} - dpt_{t-1} > 0 \\ dpt_{t-1} + (dpt_{pot,t} - dpt_{t-1}) & \text{if } dpt_{pot,t} - dpt_{t-1} \leq 0 \end{cases} \quad (B.8)$$

where dpt_t is the actual root depth a time t and dpt_{t-1} at the previous time step. If $(dpt_{pot,t} - dpt_t)$ is positive, it means that roots should theoretically grow. Therefore, a stress factor is applied to make sure that root growth is limited under adverse conditions. On the contrary, if roots are supposed to shrink, mainly due to a decrease of root biomass, no stress factor is applied in equation B.8.

The root density profile proposed by Arora & Boer (2003) has an exponential form, as many root segments are expected to be encountered in soil surface and much fewer in deeper soil horizons. The root density [kg m^{-2}] at a given depth is given by:

$$\rho_i = \beta_{rt}(W_{rt})^{(1-\alpha_{rt})} e^{-z_i \frac{\beta_{rt}}{(W_{rt})^{\alpha_{rt}}}} \quad (B.9)$$

where z_i is the depth of the middle of soil layer i [m]. In order to maintain a certain root density profile, carbon is allocated to the roots of each soil layer proportionally to their theoretical root density:

$$alloc_{C,rt,i} = alloc_{C,rt} \frac{\rho_i}{\sum_{i=1}^{nhz} \rho_i} \quad (B.10)$$

where $alloc_{C,rt,i}$ is the carbon allocated to roots in layer i [$\text{gC m}^{-2} \text{ day}^{-1}$] and $alloc_{C,rt}$ is the assimilated carbon allocated to all roots, computed in the allocation module [$\text{gC m}^{-2} \text{ day}^{-1}$].

B.3 OM mineralization and humification

The mineralization encompasses the fluxes coming from soil litter and SOM to CO_2 and NH_4 . The humification corresponds to the carbon and the nitrogen transfer from litter to SOM. Those fluxes are calculated with the same equations than in ASPECTS (see Bureau n.d.) except that woody litter is not represented for the grassland and cropland (because there are no woody materials in the vegetation). The carbon mineralization of litter or SOM (x) for an horizon i is calculated as:

$$miner_{C,x,i} = x_{c,i} * f_{\theta,i} * f_{T,i} * f_{aera,i} / lifespan_x \quad (B.11)$$

with $x_{c,i}$ the carbon content of the litter or SOM reservoir [gC m^{-2}], $lifespan_x$ the lifespan of the specific pool [day], $f_{\theta,i}$, $f_{T,i}$ and $f_{aera,i}$ the water, temperature and aeration factor, calculated with the following equations:

$$f_{water,i} = 0.5 + 0.5 * \cos(\pi + \frac{5.2358 * (\theta_i - \theta_{wp})}{\theta_{fc} - \theta_{wp}}) \quad (B.12)$$

$$f_{temp,i} = 2 * e^{\gamma_{temp} * (\frac{1}{56.02} - \frac{1}{T_{soil,i} - 227.13})} \quad (B.13)$$

$$f_{aera} = \frac{1 - \frac{\theta_i}{\theta_{sat}}}{1 - poro_{crit}} \quad (B.14)$$

with $poro_{crit}$ a critical porosity value calculated with a parameter and the clay content of the horizon and γ_{temp} the soil temperature parameter. The mineralized nitrogen is calculated as:

$$miner_{N,x,i} = \frac{miner_{C,x,i} * \beta_x}{CN_{x,i}^2} \quad (B.15)$$

with β_x a nitrogen mineralization parameter and $CN_{x,i}$ the C/N ratio. The humification is calculated as a ratio of the litter mineralization with:

$$hum_{N,i} = \gamma_{hum} * miner_{N,litter,i} \quad \text{and} \quad hum_{C,i} = hum_{N,i} * CN_{SOM,i} \quad (\text{B.16})$$

with γ_{hum} the fraction of the mineralized nitrogen which is humified and $CN_{SOM,i}$ the C/N ratio of the SOM. No movements of the litter and the SOM are taken in account in the model.

B.4 Nitrogen cycle

Nitrogen deposition and symbiotic fixation

Nitrogen deposition covers the dry and wet depositions of NH_4 and NO_3 , which are calculated as:

$$dep_{NO_3} = dep_{NO_3,an} * \frac{prc}{prc_{an}} \quad \text{and} \quad dep_{NH_4} = dep_{NH_4,an} * \frac{prc}{prc_{an}} \quad (\text{B.17})$$

with $dep_{NO_3,an}$ $dep_{NH_4,an}$ the annual depositions of NO_3 and NH_4 in an open field measured by ICP (2010) ($0.63 \text{ gN m}^{-2} \text{ yr}^{-1}$ for NH_4 and 0.54 for NO_3), prc and prc_{an} the precipitation during the time step and the year respectively. Equation B.17 illustrates that N depositions will gradually occur when precipitations are encountered. To simplify this phenomenon, the assumption is made that dry deposition are also incorporated in the soil profile with the incoming precipitations.

In TADA, unlike for forests, no symbiotic and non-symbiotic fixation is considered for grasslands and croplands, due to a lack of converging information in the literature.

Nitrification and denitrification

The nitrification is a chemical reaction converting NH_4 into NO_3 which occurs with a release of N_2O . The rate of this reaction in soil layer i is calculated with the following equation:

$$nitr_{NO_3,i} = NH_{4,i} * \min(\beta_{ph} * stress_{ph,i}, \beta_{\theta} * stress_{\theta,i}, \beta_T * stress_{T,i}) * rate_{nitr} \quad (\text{B.18})$$

with $NH_{4,i}$ the ammonium content of soil layer i [gN m^{-2}], $rate_{nitr}$ the basal rate of nitrification [day^{-1}], β_{ph} , β_{θ} , β_T the coefficients traducing the importance of the stress factors $stress_{ph,i}$, $stress_{\theta,i}$ and $stress_{T,i}$ respectively. The calculation of these stress factors comes from ASPECTS and is fully described in Bureau (n.d.). The N_2O produced during this process is calculated as:

$$nitr_{N_2O,i} = nitr_{NO_3,i} * (rate_{N_2O} + rate_{stress} * (f_{nitr,\theta,i} + f_{nitr,T,i})) \quad (\text{B.19})$$

where $nitr_{NO_3}$ is the NO_3 produced by nitrification, $rate_{N_2O}$ the minimal fraction of nitrification that create N_2O , $rate_{stress}$ the varying rate in function of the stress, $f_{nitr,\theta,i}$ is a factor introducing the influence of water availability. It is equal to 0 when the soil water content (SWC) is below the wilting point, grow linearly and is equal to 1 if SWC exceeds the saturation point. $f_{nitr,T,i}$ is a temperature factor equal to 0 when soil temperature is below 0°C , grow linearly and is equal to 1 if soil temperature is greater than 25°C .

The denitrification converts NO_3 into N_2 and N_2O . The total flux is calculated with the next equation:

$$denit_{tot,i} = \min\left(\frac{rate_{denit} * NO_{3,i}}{step}, \beta_{denit} * f_{denit,T,i} * f_{denit,\theta,i} * \min(\beta_{NO_3} * f_{NO_3}, \beta_{resp} * f_{resp})\right) \quad (\text{B.20})$$

rate of denitrification [-], $NO_{3,i}$ the nitrate content in the soil [gN m^{-2}], $step$ the time step of the simulation [day], β_{denit} the denitrification factor, $f_{nitr,T}$, $f_{nitr,\theta}$, β_{NO_3} , f_{NO_3} , β_{resp} and f_{resp} are temperature, water, NO_3 content and respiration parameters and factors respectively. Refer to Bureau (n.d.) for the calculation of these factors. The fraction of N_2 and N_2O produced by denitrification is calculated according to the following equations:

$$denit_{N_2O,i} = \frac{denit_{tot,i}}{1 + (\min(f_{NO_3,i,bis}, f_{resp,i,bis}) * f_{WFPS,i})} \quad (\text{B.21})$$

$$denit_{N2,i} = \frac{denit_{tot,i}}{1 + 1/(\min(f_{NO3,i,bis}, f_{resp,i,bis}) * f_{WFPS,i})} \quad (B.22)$$

where $f_{NO3,i,bis}$, $f_{resp,i,bis}$ and $f_{WFPS,i}$ are factors related to the NO_3 availability, the soil respiration and the water-filled pore space (WFPS). These three factors are calculated as follows:

$$f_{NO3,i,bis} = 12.5 - 25 * \tan(\pi * 0.01 * (NO_{3,i} - 190)/\pi) \quad (B.23)$$

$$f_{resp,i,bis} = 13 + 30.78 * \tan(\pi * 0.07 * (resp_i - 13.)/\pi) \quad (B.24)$$

$$f_{WFPS,i} = \frac{1.4}{13^{17/13^{2.2 * WFPS_i}}} \quad (B.25)$$

with $NO_{3,i}$ the total soil nitrate content of the horizon in $\mu gN \text{ g(soil)}^{-1}$, $resp_i$ the heterotrophic respiration of the previous time step and $WFPS_i$ the water filled pore space of the soil horizon of interest.

Nitrogen uptake

The nitrogen uptake subroutine does not change compared to ASPECTS and is completely detailed in Bureau (n.d.). Briefly, this process is based on the principle of supply from soil nitrogen and demand of the plant reserve. Firstly, TADA computes the maximum absorption rate of NO_3 and NH_4 either by diffusion or by mass flow transport (i.e. by water transport). Secondly, this maximum absorption rate is compared to the demand of the plant nitrogen reserve. If the supply exceeds the demand, the maximum amount of nitrogen is absorbed, until filling the reserve. Otherwise, the available nitrogen is entirely absorbed. The unique difference between forest and grassland or cropland ecosystems is the upper limit of the reserve. The maximum reserve of cropland is equal to a quarter of the total nitrogen content of plant organs while grassland species are assumed to store a tenth of their total nitrogen content.

Nitrogen allocation and translocation

As for nitrogen uptake, nitrogen allocation also follows the supply and demand principle. However, the supply now comes from the nitrogen reserve and the demand comes from the different plant organs. In order to compute the demand of these organs, their C/N ratios are compared to their optimal C/N ratios using the following equation:

$$dem_x = \frac{C_x * (\frac{1}{CN_{opt_x}} - \frac{1}{CN_x})}{step} \quad (B.26)$$

with C_x the carbon content of a given organ x , CN_{opt_x} the optimal C/N ratio and CN_x the actual C/N ratio of this organ. The optimal C/N ratios come from the literature for ryegrass organs (data gathered from Li et al., 1994; Jongen et al., 1995; Thornley, 1998; Abdelgawad et al., 2014; Jiang et al., 2016; Wang et al., 2016; Roche et al., 2017), and are modelled as a function of the growth stage for winter wheat (Kröbel et al., 2011). The total demand is then compared to the available nitrogen in the reserve (res_{disp}) which is estimated as follows:

$$res_{disp} = \frac{0.1 * res}{step} \quad (B.27)$$

with res the nitrogen content in the reserve computed into the nitrogen uptake module. The role of equation B.27 is to prevent the N reserve from being consumed in one time step, which would not stick to the reality. If res meets the demand of the organs, the amount of allocated nitrogen is dictated by the equation B.26 and is equal to the demand. If the total demand is greater than the value of res_{disp} , the allocation pattern is defined as:

$$alloc_x = \frac{dem_x}{\sum_{x=1}^{n_{org}} dem_x} * res_{disp} \quad (B.28)$$

with x corresponding to a given organ and n_{org} the total number of plant organs. According to this equation, each organ receives a fraction of the available nitrogen proportional to its demand.

As TADA has a more complex set of plant reservoirs for croplands, the allocation pattern shows some specificities. From the beginning of grain filling to the harvest of winter wheat, nitrogen is exclusively allocated to the grain and can be translocated from non-reproductive organs to the reproductive ones. The translocation occurs if the actual C/N ratio of an organ is lower than the optimal C/N ratio of this organ. If this is the case, the maximum translocation flux (i.e. supply from plant organs) is equal to the opposite value of dem_x calculated in equation B.26 ($offer_x = -dem_x$). If this supply exceeds the grain demand (dem_{grain}), the translocation flux from each organ is computed with:

$$trans_x = \frac{offer_x}{\sum_{x=1}^{n_{org}} offer_x} * dem_{grain} \quad (B.29)$$

Otherwise, if the demand exceeds the supply, all the nitrogen necessary and available in the reserve is allocated to the grain.

Nitrogen leaching

The nitrogen leaching module also follows the approach proposed by ASPECTS and is detailed in Bureau (n.d.). The NH_4 and NO_3 concentrations in soil solution are calculated from their total quantity and their solute buffer power, which is the ratio between ions adsorbed on the solid phase and ions in solution. These solute molecules follow the water movement which can be divided into a vertical and a horizontal component. The amount of leached NH_4 and NO_3 is therefore divided into a horizontal leaching flux and a vertical leaching flux. However, these dynamics do not occur if the NH_4 and NO_3 concentrations are below a given threshold defined by $azom_i$ and calculated as follows:

$$azom_i = azom_{min} * (\theta_{sat,i} - \theta_{fc,i}) * thick_i \quad (B.30)$$

with $thick_i$ the thickness of the soil horizon i , $azom_{min}$ the soil nitrogen content below which plants can no longer extract ($4.889 \text{ gN m(micropore)}^{-3}$). If the NH_4 or NO_3 concentration in a given soil layer is below this threshold, the leaching transport of the concerned molecule is null.

Appendix C

Required data and parameters in TADA

C.1 Species and general parameters

Table C.1: Species parameters

Parameter	Description	Units	Forest	Crop	Pasture	Forest	Value	References	Pasture
<i>Main characteristics</i>									
SLA	Specific leaf area	$\text{m}^2 \text{gC}^{-1}$	0.045	0.0365	0.0445	Aspects		measured in Lonzée	Lazzarotto et al., 2009
SSA	Specific stem area	$\text{m}^2 \text{gC}^{-1}$	-	0.0067	-	-		Andrew & Storkey, 2016; Confalonieri et al., 2013	-
<i>Phenological parameters</i>									
A_p	Thermal semi-amplitude of the vernalizing effect	$^{\circ}\text{C}$	-	10	-	-		Brisson et al., 2008	-
B_p	Subsoil plantlet elongation curve parameter	$^{\circ}\text{C d}$	-	0.006	-	-		calibrated	-
C_p	Subsoil plantlet elongation curve parameter	-	-	3.8	-	-		calibrated	-
$\text{day}^{l_{fal}}$	Day length when leaf abscission starts	hr	10.5	-	-	Aspects		-	-
DS_{ear}	Developmental stage at ear emergence	-	-	-	0.55	-		-	Lazzarotto et al., 2009
DS_{veg}	Developmental stage at the start of vegetative growth	-	-	-	2	-		-	Lazzarotto et al., 2009
E_{max}	Maximum elongation of the coleoptile in darkness condition	cm	-	8	-	-		Brisson et al., 2008	-
f_{ear}	Shoot allocation coefficient after ear emergence	-	-	-	0.25	-		-	Lazzarotto et al., 2009
gdd_{bud}	Cumulative degree-days since FEB 10, over 5°C for budburst	$^{\circ}\text{C}$	75	-	-	Aspects		-	-
i_{perm}	Flag (0 = deciduous; 1 = evergreen)	-	0	-	-	Aspects		-	-
P_{base}	Base photoperiod for development	hr	-	6.3	-	-		Brisson et al., 2008	-
P_{sat}	Saturating photoperiod for development	hr	-	20	-	-		Brisson et al., 2008	-
S_p	Root sensitivity to drought (1=insensitive)	-	-	0.5	-	-		Brisson et al., 2008	-
S_v	Photoperiod sensitivity (1=insensitive)	-	-	0	-	-		Brisson et al., 2008	-

T_{base}	Minimum threshold temperature for development	°C	-	0	5	-	Brisson et al., 2008	Lazzarotto et al., 2009
T_{froid}	Optimum vernalization temperature	°C	-	6.5	-	-	Brisson et al., 2008	-
T_{stop}	High temperature stopping phasic development and leaf expansion	°C	-	35	-	-	Brisson et al., 2008	-
T_{rep}	Normalization factor for grass development	°C d	-	-	225	-	-	Lazzarotto et al., 2009
T_{max}	Maximum threshold temperature for development	°C	-	28	-	-	Brisson et al., 2008	-
$upvt_{germ}$	UPVT required to reach germination	°C d	-	50	-	-	Brisson et al., 2008	-
$upvt_{st3}$	UPVT required during stage 3 (germination to terminal spikelet)	°C d	-	275	-	-	Brisson et al., 2008	-
$upvt_{st4}$	UPVT required during stage 4 (terminal spikelet to flag leaf visible)	°C d	-	270	-	-	calibrated	-
$upvt_{st5}$	UPVT required during stage 5 (flag ligule visible to end of leaf growth)	°C d	-	105	-	-	calibrated	-
$upvt_{st7}$	UPVT required during stage 7 (grain filling to physiological maturity)	°C d	-	530	-	-	calibrated	-
$upvt_{veg}$	UPVT required during vegetative period	°C d	-	837	-	-	Brisson et al., 2008	-
VN	Number of vernalizing days required	d	-	55	-	-	Brisson et al., 2008	-
VN_{min}	Minimum vernalizing days required	d	-	7	-	-	Brisson et al., 2008	-
<i>Photosynthetic parameters</i>								
a_1	Stomatal resistance factor	-	20	2.3	7.1	Aspects	calibrated	calibrated
χ_n	Ratio of photosynthetic capacity to leaf nitrogen at 25°C	$\text{mmol mol}^{-1} \text{s}^{-1}$	0.4567	0.21	1.02	Aspects	calibrated	calibrated
N_b	Leaf nitrogen not associated with photosynthesis	$\text{mmol m}^{-2}(\text{leaf})$	1	25	25	Aspects	De Pury & Farquhar, 1997	De Pury & Farquhar, 1997
ibbl	Flag for Leuning (0) or Ball-Berry (1) stomatal resistance equation	-	0	0	0	-	-	-
θ_A	Curvature factor of response of canopy photosynthesis	-	1	0.8	0.8	Aspects	calibrated	calibrated
θ_J	Curvature factor of response of canopy photosynthesis to irradiance	-	0.7	0.7	0.7	Aspects	De Pury & Farquhar, 1997	De Pury & Farquhar, 1997
vpdo	Stomatal resistance factor	Pa	1000	1000	1000	Aspects	Aspects	Aspects
k_n	Coefficient of leaf nitrogen in a canopy	-	0.713	0.713	0.713	De Pury & Farquhar, 1997	De Pury & Farquhar, 1997	De Pury & Farquhar, 1997
<i>Radiation parameters</i>								
β_0	Boland-Ridley-Lauret model parameter	-	-2.4	-2.4	-2.4	calibrated on Lonzée data	calibrated	calibrated on Lonzée data
β_1	Boland-Ridley-Lauret model parameter	-	2.77	2.77	2.77	calibrated on Lonzée data	calibrated	calibrated on Lonzée data
β_2	Boland-Ridley-Lauret model parameter	-	0.033	0.033	0.033	calibrated on Lonzée data	calibrated	calibrated on Lonzée data
β_3	Boland-Ridley-Lauret model parameter	-	0.054	0.054	0.054	calibrated on Lonzée data	calibrated	calibrated on Lonzée data
β_4	Boland-Ridley-Lauret model parameter	-	1.03	1.03	1.03	calibrated on Lonzée data	calibrated	calibrated on Lonzée data
β_5	Boland-Ridley-Lauret model parameter	-	0.63	0.63	0.63	calibrated on Lonzée data	calibrated	calibrated on Lonzée data
<i>Carbon parameters</i>								

a_{sgm}	Sigmoid function parameter	-	-	-0.3	-	-	Fitting from Ehdaie et al., 2008	-
c_{sgm}	Sigmoid function parameter	-	-	15	-	-	Fitting from Ehdaie et al., 2008	-
dm_c	Carbon content of dry matter	$gC\ gDM^{-1}$	-	0.449	0.4271	-	Measured in Lonée	Measured in Dorinne
cvf_{cst}	Constant carbon assimilation efficiency	-	-	-	0.74	-	-	Choudbury, 2000
DG_0	CO ₂ gas diffusion coefficient in the air at 273.16K and 101.3kPa	$m^2\ s^{-1}$	-	$1.39e^{-5}$	$1.39e^{-5}$	Fang & Moncrieff, 1999	Fang & Moncrieff, 1999	Fang & Moncrieff, 1999
$percent_{left}$	Percentage of C left in the reserve pool after grain remobilization	-	-	0.2	-	-	Ehdaie et al., 2008	-
$remob_{eff}$	Carbon remobilization efficiency	-	-	0.75	-	-	Ehdaie et al., 2006	-
$time_{remob}$	Sigmoid function parameter	-	-	40	-	-	Ehdaie et al., 2008; Pheloung & Siddique, 1991	-
tns_c	Percentage of non structural carbohydrates in dry matter	$gC\ gDM^{-1}$	-	-	0.15	-	-	Downing & Gamroth, 2007

Respiration parameters

a_k	Teleonomic partitioning constant for grassland	$gN\ gDM^{-1}$	-	-	0.35	-	-	Lazzarotto et al., 2009
r_k	Maintenance respiration constant	$gC\ gDM^{-1}$	-	-	0.03	-	-	Lazzarotto et al., 2009
c_k	Teleonomic partitioning constant for grassland	$gC\ gDM^{-1}$	-	-	1	-	-	Lazzarotto et al., 2009
Q_{10}	Maintenance respiration factor	-	2.7	2	2	Aspects	Spitters et al., 1989	Lazzarotto et al., 2009
rm	Maintenance respiration weighting coefficient	-	-	-	0.7	-	-	Lazzarotto et al., 2009
rm_0	Reference maintenance respiration rate at 20°C	$gC\ gDM^{-1}\ day^{-1}$	-	-	0.012	-	-	Lazzarotto et al., 2009

Temperature-dependent parameters

T_{low}	Lower temperature for temperature function	C	-	0	0	-	Lazzarotto et al., 2009	Lazzarotto et al., 2009
T_{ref}	Reference temperature for temperature function	C	-	20	20	-	Lazzarotto et al., 2009	Lazzarotto et al., 2009
T_{up}	Upper temperature for temperature function	C	-	45	45	-	Lazzarotto et al., 2009	Lazzarotto et al., 2009

Nitrogen parameters

$azomin$	Soil N content below which plant can not extract NO ₃	$gN\ m^{-3}$	0.44	0.44	0.44	Gego, 1993	Gego, 1993	Gego, 1993
β_{lit}	Litter nitrogen mineralization	$gC\ gN^{-1}$	20	22	22	Aspects	calibrated on Dorinne data	calibrated
β_{som}	SOM nitrogen mineralization	$gC\ gN^{-1}$	15	16.5	16.5	Aspects	calibrated on Dorinne data	calibrated
dm_n	Nitrogen content of dry matter	$gN\ gDM^{-1}$	-	-	0.0275	-	-	Measured in Dorinne
$fresN_{max}$	Fraction of plant nitrogen defining the maximum nitrogen reserve	-	0.25	0.25	0.25	Aspects	Aspects	Aspects
$frNH_4c$	NH ₄ concentration on the root surface	$molN\ cm^{-3}$	$2e^{-8}$	$2e^{-8}$	$2e^{-8}$	Aspects	Robinson et al., 1991	Robinson et al., 1991
$frNO_3c$	NO ₃ concentration on the root surface	$molN\ cm^{-3}$	$2e^{-8}$	$2e^{-8}$	$2e^{-8}$	Aspects	Robinson et al., 1991	Robinson et al., 1991
$rate_{nitr}$	Optimum nitrification rate (ratio of NH ₄ content)	-	0.4	0.1432	0.1432	Aspects	calibrated on Dorinne data	calibrated

Animal parameters

DM_{cap}	Intake capacity of dry matter per LSU per day	$gDM\ LSU^{-1}\ day^{-1}$	-	-	8900	-	-	Gourlez de la Motte et al., 2019
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f_{meth}	Percentage of carbon intake lost as CH4 respiration	-	-	-	0.025	-	Gourlez de la Motte et al., 2019
f_{remove}	Percentage of shoot biomass removed by animal trampling	-	-	-	0.008	-	Vuichard et al., 2007
f_{resp}	Percentage of carbon intake lost as CO2 respiration	-	-	-	0.725	-	Gourlez de la Motte et al., 2019
$f_{ret,C}$	Percentage of carbon retained for milk or meat production	-	-	-	0	-	-
$f_{ret,N}$	Percentage of nitrogen retained for milk or meat production	-	-	-	0	-	-
f_{urine}	Percentage of urine present in excreta	-	-	-	0.6	-	Menzi et al., 1997 cited by Riedo et al., 2000; Oenema et al., 1997
f_{volat}	Percentage of nitrogen in excreta volatilized as ammonia	-	-	-	0.05	-	Menzi et al., 1997 cited by Riedo et al., 2000
h_{lim}	Grass minimum height under which animals can not graze	cm	-	-	3	-	Personal communication (J.Bindelle)

Root parameters

α_{rt}	Parameter for root development	-	-	-	5.86	-	Arora & Boer, 2003
bd_{coef}	Bulk density coefficient for root sensitivity to soil strength	-	-	1550	1600	Aspects	Jones et al., 1991
β_{rt}	Parameter for root development	-	-	-	7.67	-	Arora & Boer, 2003
$cr_{dpt,max}$	Maximum depth of the coarse root system	m	0.9	-	-	Aspects	-
fr_{dens}	Root carbon density	gC cm ⁻³ (root)	0.075	-	0.075	Aspects	Aspects
fr_{radius}	Root radius	cm	0.025	0.0077	0.0066	Aspects	Föhse et al., 1991
$LW_{ratio,harr}$	Root length to weight ratio at maturity	m g ⁻¹ (root)	-	175	-	-	Barracough & Leigh, 1984
ph_{max}	Maximum pH for root growth	-	9.25	9	8.4	Aspects	Hannaway et al., 1999
ph_{min}	Minimum pH for root growth	-	3.75	5	5.1	Aspects	Hannaway et al., 1999
$ph_{op,low}$	Lower pH for optimum root growth	-	4.25	5.4	5.5	Aspects	Hannaway et al., 1999
$ph_{op,up}$	Upper pH for optimum root growth	-	8.25	8	7.5	Aspects	Hannaway et al., 1999
$GS_{dpt,max}$	Growth stage at maximum root depth	-	-	0.9	-	-	Jones et al., 1991
$por_{h2o,crit}$	Critical water-filled porosity for root growth	-	0.4	0.4	0.4	Jones et al., 1991; Williams et al., 1989	Jones et al., 1991; Williams et al., 1989
rhizodep	Fraction of matter allocated to root going directly to the soil	-	-	-	0.134	-	Newman, 1978
$rt_{dpt,max}$	Maximum depth of the root system	m	-	2	-	-	Gregory et al., 1978; Kirkegaard & Lilley, 2007; Thorup-Kristensen, 2009
rt_{dens} (1-nhz)	Root length density in each soil layer	cm cm ⁻³ (root)	-	8; 8; 4; 1; 0.5	-	-	Asseng, 1997; Hodgkinson et al., 2017
$LW_{ratio,seed}$	Root length to weight ratio at seeding	m g ⁻¹ (root)	-	200	-	-	Barracough & Leigh, 1984
$Tp_{fr,base}$	Minimum soil temperature for root growth	C	5	2	0	Aspects	Porter & Gawith, 1999 Thornley, 1998

$T_{fr,op}$ wcg	Optimum soil temperature for root growth Coefficient for root distribution	C	20	16.3	20	Aspects	Porter & Gawith, 1999 Jones et al., 1991	Thornley, 1998
<i>Senescence parameters</i>								
f_{depl}	Depletion factor of the total available water	-	-	0.55	0.6	-	Allen et al., 1998	Allen et al., 1998
γ_{temp}	Mineralization temperature parameter	-	308.15	277.33	277.33	Lloyd & Taylor, 1994	calibrated	calibrated
τ_{ul}	Foliage lifespan at reference temperature (20°C)	d	219	70	83	Aspects	Van Heemst, 1988	Lazzarotto et al., 2009
τ_{fr}	Root lifespan at reference temperature (20°C)	d	-	58.97	100	-	Gibbs & Reid, 1992	Lazzarotto et al., 2009
τ_{w}	Woody biomass lifespan	d	54750	-	-	Aspects	-	-
$lifespan_{min}$	Litter lifespan	d	730	730	803	Aspects	Aspects	calibrated
$lifespan_{minc}$	Woody litter lifespan	d	7300	-	-	Aspects	-	-
$lifespan_{som}$	SOM lifespan	d	36500	36500	16100	Aspects	Aspects	calibrated

Table C.2: General parameters

Parameter	Description	Units			
<i>File names</i>					
initialfile	Name of the initial values file	-			
soilfile	Name of the soil characteristics file	-			
managementfile	Name of the management file	-			
pathres	Beginning of results file names	-			
<hr/>					
<i>Type of simulation</i>					
ecosyst	Type of ecosystem (1=forest;2=crop;3=grassland)	-			
nhd	Number of data per day	d-1			
nd	Numer of days in the one year	d			
nnh	Number of time steps per half hour	-			
nh	Number of time steps per day	d-1			
nhwk	Number of days for average of N uptake	d			
ifull	Flag to generate 1/2h results	-			
nyrstart	Starting year of simulation	yr			
nyrmax	Number of years to simulate	yr			
ident_simul	Variable to choose the simulation type	-			
ident_strs_n	Variable to choose to simulate nitrogen stress	-			
ident_mana	Forest management type	-			
ident_disease	Forest mortality due to disease	-			
isteady	Flag to start a steady-state simulation	-			
<hr/>					
<i>Numerical resolution</i>					
niter	Maximum number of correction iteration	-			
norder	Order of Runge-Kutta resolution	-			
thick_layer1	Thickness of the first fictive soil layer	m			
<hr/>					
<i>Environmental conditions</i>		Forest	Cropland	Grassland	Units
ico2	Atmospheric CO2 concentration	360	360	360	ppm
idepot	Annual nitrogen deposition for forest	28	28	28	gN 10-1 yr-1
sNH4_depos_an	Annual deposition of NH4 in open fields	-	0,63	0,63	gN-NH4 m-2 yr-1
sNO3_depos_an	Annual deposition of N03 in open fields	-	0,54	0,54	gN-N03 m-2 yr-1
<hr/>					
<i>Reservoirs information</i>					
nhz	Number of soil layers	6	5	3	-
ncp	Number of above-ground carbon pools	5	4	1	-
ncb	Number of below-ground carbon pools	6	4	4	-
nco	Number of carbon pools	41	24	13	-
nnp	Number of above-ground nitrogen pools	4	4	2	-
nmb	Number of below-ground nitrogen pools	7	5	5	-
nno	Number of nitrogen pools	46	29	17	-
nwp	Number of above-ground water pools	2	2	2	-
nwo	Number of water pools	8	7	5	-
ntp	Number of above-ground thermal pools	0	0	0	-
nto	Number of thermal pools	6	5	3	-
nres	Total number of pools	101	65	38	-
<hr/>					
<i>Site information</i>					
xlat	Latitude	50,3050	50,3123	50,3123	deg
xlong	Longitude	5,9980	4,7464	4,9678	deg

C.2 Initial reservoirs values

Table C.3: Initial reservoirs values used for the cropland ecosystem (Lonzée).

y	Reservoir	Unit	Above-ground or horizon 1	2	3	4	5	Method
1	storage organs (C)	g C m ⁻²	0					-
2	reserve (C)	g C m ⁻²	0					-
3	leaves (C)	g C m ⁻²	0					-
4	stems (C)	g C m ⁻²	0					-
5-9	root (C)	g C m ⁻²	0	0	0	0	0	-
10-14	litter (C)	g C m ⁻²	38.3481	76.8971	130.496	103.825	64.7867	†
15-19	SOM (C)	g C m ⁻²	619.424	1242.09	2107.86	1677.05	1046.48	†
20-24	CO ₂ (C)	g C m ⁻²	0.61	1.23	1.62	2.05	2.46	Aspects
25	storage organs (N)	g N m ⁻²	0					-
26	reserve (N)	g N m ⁻²	0					-
27	leaves (N)	g N m ⁻²	0					-
28	stems (N)	g N m ⁻²	0					-
29-33	root (N)	g N m ⁻²	0	0	0	0	0	-
34-38	litter (N)	g N m ⁻²	1.25916	2.54575	4.32951	4.07448	2.97388	*
39-43	SOM (N)	g N m ⁻²	62.9584	127.287	216.476	203.724	148.694	*
44-48	soil NO ₃	g N m ⁻²	0.42439	0.85801	1.45921	1.37325	1.00231	*
49-53	soil NH ₄	g N m ⁻²	0.30222	0.61101	1.03913	0.97792	0.71376	*
54	snow	mm H ₂ O	0					Measure
55	soil water TOP	m ³ m ⁻³	0.37781					Measure
56-60	soil water	m ³ m ⁻³	0.37781	0.38622	0.39909	0.4186	0.43964	Measure
61-65	soil temperature	K	273.628	274.645	276.614	281.016	290.057	Measure

†Total carbon measured, partitioned with calibration

*Measure of the total soil nitrogen, partitioned with Sharpley & Smith (1995) between NO₃, NH₄ and organic, calibration between litter and SOM.

Table C.4: Initial reservoirs values used for the grassland ecosystem (Dorinne).

y	Reservoir	Unit	Horizon			Method
			Above-ground or horizon 1	2	3	
1	shoot	g C m-2	27.4497			*
2-4	root (C)	g C m-2	70.159	25.161	4.3375	Jackson et al. (1996)
5-7	litter (C)	g C m-2	1820.99	43.5049	0.01709	†
8-10	SOM (C)	g C m-2	2916.54	5749.14	4846.52	†
11-13	co2 (C)	g C m-2	0.61	3	2.87	Aspects
14	shoot (N)	g N m-2	2.83027			*
15	vegetation reserves (N)	g N m-2	4.132			Optimum reserve calculated Jackson et al. (1996)
16-18	root (N)	g N m-2	2.71041	9.72013	1.67567	
19-21	litter (N)	g N m-2	9.10774	12.1584	11.5528	
22-24	SOM (N)	g N m-2	455.387	607.921	577.642	
25-27	soil NO3	g N m-2	2.71726	3.62742	3.44675	
28-30	soil NH4	g N m-2	1.4177	1.89257	1.7983	
31	snow	mm H2O	0			Measure
32	soil water TOP	m3 m-3	0.4984			Measure
33-35	soil water	m3 m-3	0.4984	0.4759	0.438	Measure
36-38	soil temperature	K	279.844	280.231	280.366	Measure

*Measure of herbage height the 26/11/2013, changed in carbon by means of allometric equation and dm_c/dm_n

†Total carbon measured, partitioned with calibration

‡Measure of the total soil nitrogen, partitioned with Sharpley & Smith (1995) between NO3, NH4 and organic, calibration between litter and SOM.

