**Scientific Description of LPJ-GUESS developments**

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# Biogenic volatile organic compounds (BVOC)

*Guy Schurgers, October/November 2011, updated January 2013 (GS) & July 2016 (Stijn Hantson)*

## Introduction

Emissions of two (groups of) terpenoids, isoprene (C5H8) and monoterpenes (C10H16), were incorporated in LPJ-GUESS because of their role in atmospheric chemistry and aerosol formation. Terpenoid production is closely linked to photosynthesis.

## Calculation of terpenoid production

The description of terpenoid production in LPJ-GUESS is based on the algorithms in Niinemets et al. (1999, 2002), and is described in Arneth et al. (2007a, isoprene) and Schurgers et al. (2009a, monoterpenes). Production of isoprene and monoterpenes is calculated by assigning a fraction of the electron flux generated for photosynthesis to terpenoid synthesis. Terpenoid production is calculated as

where *J* is the rate of photosynthetic electron transport, *ε* is the fraction of this rate that is attributed to terpenoid production, and *α* is the yield of terpenoids per unit of electron flux. The latter is calculated as (Niinemets et al., 1999)

where *Ci* is the leaf-internal CO­2 concentration without water stress, and *Γ*\* is the CO2 compensation point, both obtained from the photosynthesis calculations. Because of the large temperature sensitivity of terpenoid production, *J* is recalculated from the photosynthesis scheme (Haxeltine and Prentice, 1996) applying a daytime leaf temperature rather than a daily average air temperature (see below). The fraction *ε* is based on a species-specific standard fraction *εs* (see initialization below), which is adjusted as a function of temperature, seasonality (in case of isoprene) and atmospheric CO2 concentration:

The temperature function *f(T)* provides a correction for the enhanced temperature optimum of terpenoid production compared to photosynthesis, and is calculated with an exponential function (Arneth et al., 2007a):

where *Ts* is a standard temperature (usually 30°C) and *a* defines the temperature sensitivity (0.1; Arneth et al., 2007a).

The seasonality for isoprene, *f(σ)*, is calculated based on a degree-day method in spring (degree-day requirement for isoprene is assumed to be twice as large as the requirement for phenology), and a decrease in autumn based on temperature and daylength (Schurgers et al., in press). This seasonality function is applied for deciduous PFTs only, evergreen PFTs are assumed to exhibit no seasonal changes in terpenoid synthesis.

The atmospheric CO2 concentration has been shown to affect terpenoid synthesis (e.g. Possell et al., 2005), enhancing emissions at CO2 concentrations lower than ambient, and reducing emissions at CO2 concentrations higher than ambient. This has been attributed (Wilkinson et al., 2009) to changes in the distribution of phosphoenol pyruvate (PEP) between cytosol and chloroplast, but the mechanisms behind this have not been fully unraveled yet (Wilkinson et al., 2009). The model uses a rather empirical function, scaling emissions with the ratio of a reference ambient CO2 concentration (370 ppm) and the actual CO2 concentration (Arneth et al., 2007a):

Because of the similarity in the synthesis pathways of isoprene and monoterpenes, the same CO2 sensitivity was applied for both, despite the fact that the sensitivity of monoterpenes to CO2 in the literature is less obvious.

For monoterpenes, multiple compounds can be represented, each of them following the computations above, but with different parameterizations. For the trunk version, 9 monoterpene compounds are separated in the code, which are subsequently divided in two main groups for the output, namely “endocyclic monoterpenes” being monoterpenes with an endocyclic double bond (outputted as TM1) and “others” including both acyclic monoterpenes and exocyclic monoterpenes (outputted as TM2). This separation is chosen because of its relevance for atmospheric chemistry models, and is used in e.g. EC-Earth.

## Calculation of emissions

Produced monoterpenes in plants have the potential to be (partially) stored, hence the often-observed light-independence of monoterpene emissions. However, this storage does not take place in all plants, and can be done in specific storage pools (e.g. resin ducts) or in non-specific storage. For the European PFTs, specific storage is implemented for all coniferous and herbaceous PFTs, because these species have been shown to emit monoterpenes independently of the availability of light. Monoterpene emissions for many broadleaf species have been reported to respond to light in a similar manner as isoprene (e.g. *Quercus ilex*, Staudt and Seufert, 1995; or *Fagus sylvatica*, Schuh et al., 1997), indicating that storage is not playing a role here. For the global PFT´s, storage was made dependent on the monoterpene species emitted.

Long-term storage is implemented as a single storage pool, which is filled by transferring part of the produced monoterpenes to this pool. Currently, half of the produced monoterpenes is transferred here for all storing PFTs, because this resulted in the best fit with observations of the annual cycle of emissions for Pinus ponderosa (Schurgers et al., 2009a). However, if new data become available, this fraction can be assigned to each PFT individually.

Release from this storage pool is implemented with a temperature-dependent time constant *τ*:

where *m* is the monoterpene storage pool size, and *Memis* is the rate of monoterpene emission from storage. The temperature dependence of *τ* is governed by a *Q*10 relationship:

The parameterization for this function was derived in Schurgers et al. (2009a): *τs*=80 d at a standard temperature *Ts* =30°C , and the temperature dependence *Q*10=1.9.

A short-term (~hours) storage of monoterpenes can occur as well in the mesophyll, but because of the time scales involved in this, it is not considered here.

## Initialization of standard fractions

The standard fractions *εs* of the PFTs used in the model are calculated by conversion from the reported leaf-level emission capacities *Is* (expressed in μg g-1 DW h-1), which are emissions standardized to 30°C and 1000 μmol PAR m-2 s-1. By calculating the photosynthesis rate for these standard conditions, the fraction *εs* necessary to support an emission of *Is* can be determined.

## Parameterization of BVOC production and emission

Emission capacities for PFTs were determined from recommendations for global modelling (global PFT set) or from leaf-level observations (European PFT set). Current values applied in the benchmark set are described in Arneth et al. (2007b, supplementary material, global PFT set) and Schurgers et al. (2009b, European PFT set). For monoterpenes, the original total emissions are maintained as in Schurgers et al. (2009), but separated into 9 different groups (listed in Table A2) (thereafter merged together in endocyclic (TM1) and other (TM2) groups) This relative abundance of each monoterpene species was derived from Messina al. (2015; table 4) for the global Pfts. For the European PFT’s, only endocyclic monoterpenes and other monoterpenes were separated (applied in the code as α-pinene and β-pinene, respectively), and relative abundances were derived from Öström *et al.*, in prep. and if not present, the global values were used. All parameters are listed in Appendix A.

For parameterization of new PFTs, literature values for emission capacities (measured at standard conditions and expressed in μg g-1 h-1) can be used.

For monoterpene emission capacities that are based on a temperature dependence only, a multiplication with 2 is recommended to correct for the synthesis taking place during daytime only (see Schurgers et al., 2009a).

## Temperature corrections

Because of the sensitivity of terpenoid production to temperature, corrections were implemented to convert the daily average air temperature to a daytime average leaf temperature.

For calculating the average daytime temperature from the daily value, the diurnal cycle is assumed to follow a sine wave with average temperature *Tav* and temperature amplitude *Tamp*, with the maximum temperature reached at noon. This sine wave is integrated over daylength *d* (in hours) centered around noon:

which can be solved analytically to

This daytime air temperature is used in the calculation of leaf temperatures. This calculation is made by computing the energy balance of the canopy, which can be written as

The fluxes of sensible heat and longwave radiation depend on the leaf temperature, and this is used to make the total of all fluxes balance. Net shortwave radiation is computed already for the downward radiation flux following Prentice et al. (1993). Latent heat is computed from the actual evapotranspiration multiplied with the vapourization energy λ.

Incoming and outgoing longwave radiation are computed from the air temperature and the leaf temperature, respectively, using Stefan-Boltzmann law:

A first order Taylor expansion is used as approximation to express the leaf temperature contribution εlσ*T*l4 as a function of *T*a, and atmosphere and leaf emissivities are assumed equal, which makes the net longwave radiation a linear function of the difference between leaf temperature and air temperature:

Similarly, the flux of sensible heat can be expressed as a linear function of the temperature difference, using PFT-specific values for the aerodynamic resistance *r*b,h:

in which ρ and *C*p are the density and the specific heat capacity of air, respectively. The temperature difference can then be computed from the energy balance, resulting in

or

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## Appendix A. PFT parameters used for global and European benchmarks.

*Table A1. BVOC-related PFT parameters in the global benchmark setup. Values originate from Arneth et al. (2007b, supplementary material) and Schurgers et al. (2009a).*

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **PFT** | ***Is***  **(μg g-1 h-1)** | **Isoprene seasonality** | ***Ms***  **(μg g-1 h-1)** | ***fstor***  **(-)** | ***ga***  **(m s-1)** |
| BNE | 8 | 0 | 4.8 | 0.5 | 0.14 |
| BINE | 8 | 0 | 4.8 | 0.5 | 0.14 |
| BNS | 8 | 1 | 4.8 | 0.5 | 0.14 |
| TeNE | 8 | 0 | 4.8 | 0.5 | 0.14 |
| TeBS | 45 | 1 | 1.6 | 0 | 0.04 |
| IBS | 45 | 1 | 1.6 | 0 | 0.04 |
| TeBE | 24 | 0 | 1.6 | 0 | 0.04 |
| TrBE | 24 | 0 | 0.8 | 0 | 0.04 |
| TrIBE | 24 | 0 | 0.8 | 0 | 0.04 |
| TrBR | 45 | 0 | 2.4 | 0 | 0.04 |
| C3G | 16 | 1 | 1.6 | 0.5 | 0.03 |
| C4G | 8 | 0 | 2.4 | 0.5 | 0.03 |
| C3crop | 16 | 1 | 1.6 | 0.5 | 0.03 |
| C4crop | 8 | 0 | 2.4 | 0.5 | 0.03 |

*Table A2.* Percentage of speciated monoterpene EFs with respect to the PFT bulk monoterpenes, adapted from Messina et al. (2015; table 4). α-pinene, limonene and 3-carene are grouped in TM1, the rest in TM2.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | α-pinene | β-pinene | limonene | myrcene | sabinene | camphene | 3-carene | t-β-ocimene | others |
| BNE | 35.4 | 14.6 | 8.3 | 5 | 5 | 4.2 | 17.5 | 5.4 | 4.6 |
| BINE | 35.4 | 14.6 | 8.3 | 5 | 5 | 4.2 | 17.5 | 5.4 | 4.6 |
| BNS | 66.2 | 15 | 3.7 | 2.5 | 3 | 2.3 | 4.2 | 2.8 | 0.3 |
| TeNE | 35.4 | 14.6 | 8.3 | 5 | 5 | 4.2 | 17.5 | 5.4 | 4.6 |
| TeBS | 32.6 | 8.7 | 6.1 | 2.8 | 30.4 | 0.4 | 2.4 | 11.3 | 5.3 |
| IBS | 32.6 | 8.7 | 6.1 | 2.8 | 30.4 | 0.4 | 2.4 | 11.3 | 5.3 |
| TeBE | 46.3 | 12.2 | 12.2 | 5.4 | 8.3 | 4.9 | 1 | 4.4 | 5.3 |
| trBrEv | 39.5 | 11 | 9.2 | 7.3 | 7.3 | 5.5 | 4.8 | 9.2 | 6.2 |
| trBrEv | 39.5 | 11 | 9.2 | 7.3 | 7.3 | 5.5 | 4.8 | 9.2 | 6.2 |
| TrBrDe | 39.5 | 11 | 9.2 | 7.3 | 7.3 | 5.5 | 4.8 | 9.2 | 6.2 |
| C3G | 23.1 | 12.3 | 14.6 | 6.2 | 6.5 | 5.4 | 6.5 | 13.8 | 11.6 |
| C4G | 20 | 8 | 28 | 5.7 | 5 | 5.3 | 5.7 | 12 | 10.3 |
| C3crop | 27.7 | 15.4 | 9.2 | 4.6 | 6.2 | 3.1 | 20 | 3.1 | 10.7 |
| C4crop | 27.7 | 15.4 | 9.2 | 4.6 | 6.2 | 3.1 | 20 | 3.1 | 10.7 |

*Table A3. BVOC-related PFT parameters in the European benchmark setup. Values originate from Schurgers et al. (2009b), where the emission factor are separated from TM1 and TM2 monoterpene groups, based on Öström et al. (in prep) and when not available Messina et al. (2015).*

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **PFT** | ***Is***  **(μg g-1 h-1)** | **Isoprene seasonality** | ***Ms TM1***  **(μg g-1 h-1)** | ***Ms TM2***  **(μg g-1 h-1)** | ***fstor***  **(-)** | ***ga***  **(m s-1)** |
| Abi\_alb | 0.05 | 0 | 1.1 | 0.7 | 0.5 | 0.14 |
| BES | 2.0 | 0 | 2.4 | 1.6 | 0.5 | 0.04 |
| Bet\_pen | 0.2 | 1 | 2.1 | 3.9 | 0 | 0.04 |
| Bet\_pub | 0 | 1 | 0.1 | 0.9 | 0 | 0.04 |
| Car\_bet | 0 | 1 | 0.06 | 0.02 | 0 | 0.04 |
| Cor\_ave | 0 | 1 | 0 | 0 | 0 | 0.04 |
| Fag\_syl | 0 | 1 | 3.5 | 6.5 | 0 | 0.04 |
| Fra\_exc | 0 | 1 | 0 | 0 | 0 | 0.04 |
| Jun\_oxy | 0 | 0 | 1.2 | 0.8 | 0.5 | 0.14 |
| MRS | 2.0 | 0 | 2.4 | 1.6 | 0.5 | 0.04 |
| Pic\_abi | 0.5 | 0 | 3.9 | 2.1 | 0.5 | 0.14 |
| Pin\_syl | 0 | 0 | 3.2 | 0.8 | 0.5 | 0.14 |
| Pin\_hal | 0 | 0 | 6.1 | 3.9 | 0.5 | 0.14 |
| Pop\_tre | 20. | 1 | 2.4 | 1.6 | 0 | 0.04 |
| Que\_coc | 0.1 | 0 | 6. | 4. | 0 | 0.04 |
| Que\_ile | 0.05 | 0 | 9.6 | 6.4 | 0 | 0.04 |
| Que\_pub | 50. | 1 | 0 | 0 | 0 | 0.04 |
| Que\_rob | 40. | 1 | 0 | 0 | 0 | 0.04 |
| Til\_cor | 0 | 1 | 0 | 0 | 0 | 0.04 |
| Ulm\_gla | 0 | 1 | 0 | 0 | 0 | 0.04 |
| C3\_gr | 0 | 1 | 0.45 | 0.55 | 0.5 | 0.03 |
| C4\_gr | 0 | 1 | 0.55 | 0.45 | 0.5 | 0.03 |

## Appendix B. List of symbols and their abbreviations in the model code

|  |  |  |  |
| --- | --- | --- | --- |
| **symbol** | **code abbrev.** | **description** | **unit** |
| *Ci* | pi\_co2\_opt | leaf-internal CO2 concentration | ppm |
| *Cp* | cp | specific heat capacity of air | J kg-1 K-1 |
| *H* | - | sensible heat flux | W m-2 |
| *I* | iso  mon  indiv.iso  indiv.mon | isoprene /monoterpene production | g C m-2 d-1 |
| *J* | J\_opt | electron flux | mol m-2 h-1 |
| *L* | lai | leaf area index | m2 m-2 |
| *Lnet* | - | net longwave radiation | W m-2 |
| *Memis* | - | monoterpene emission from storage | mg C m-2 d-1 |
| *Q10* | q10\_mstor | temperature dependence | - |
| *Snet* | rsnet | net shortwave radiation | W m-2 |
| *T* | temp | temperature | °C |
| *Ta* | temp | air temperature | °C |
| *Tamp* | tempamp | temperature amplitude | °C |
| *Tav* | temp | average temperature | °C |
| *Tcanopy,av* | temp  temp\_leaf\_daytime | average canopy temperature | °C |
| *Tdaytime* | temp  temp\_leaf\_daytime | daytime temperature | °C |
| *Ts* | Tstand | standard temperature | °C |
| *a* | a | temperature sensitivity | - |
| *d* | daylength | daylength | h |
| *k* | LAMBERTBEER\_K | light extinction coefficient | - |
| *m* | indiv.monstor | monoterpene storage pool | mg C m-2 |
| *p*CO2 | co2 | atmospheric CO2 concentration | ppm |
| 1/*rb* | gc | boundary layer conductance | mm s-1 |
| *t* | - | hour of day | h |
| *z* | - | relative height in the canopy | - |
| *Γ\** | gammastar | CO2 compensation point | ppm |
| *α* | a\_Y\_opt | photon content of light | - |
| *ε* | eps\_eff\_iso  eps\_eff\_mon | fraction of electron flux allocated to terpenoid production | - |
| *εl* | emiss\_leaf | leaf emissivity | - |
| *εs* | pft.Y\_eps\_iso  pft.Y\_eps\_mon | fraction of electron flux allocated to terpenoid production under standardized conditions | - |
| *λE* | lhloss | latent heat flux | W m-2 |
| *ρ* | rhoair | density of air | kg m-3 |
| *σ* | sigma | Stephan-Boltzmann constant | W m-2 K-4 |
| *τ* | tcstor | time constant | d |
| *τs* | tcstor\_s | time constant under standardized conditions | d |

# Synchronised hydrology

*Michael Mischurow, November 2011*

## Issue

In the trunk version of LPJ-GUESS (revision 833 and earlier) there was a disconnect between calculations of water supply and demand, and as consequence, of water stress condition. Demand was calculated based on the today’s value of precipitation, whereas supply was based on soil water content that wasn’t updated with the same precipitation. This likely was due to the fact that the function interception() was included into the canopy\_exchange() call and therefore it wasn’t possible to update soil water content between calls to interception() and aet\_water\_stress().

## Solution

However, interception, while a canopy process is not related to the canopy\_exchange() in other ways. Hence, it is possible by exposing interception() to the framework to add a soilwater module function that would deal with distribution of the daily rainfall. It seems reasonable to only deal with the top layer moisture (provided top layer is of reasonable depth) and to keep this new function neat and simple. Such new function, named initial\_infiltration() is now added to the soil water module. There, rainmelt (rainfall + snowmelt) is added to the top soil layer up to the water holding capacity (wcont = 1), any remaining rainmelt is redistributed in the normal fashion in function soilwater() called after canopy\_exhange().

## Physical rationale

Rainfall is typically a much faster process than soil water transport and it is therefore highly unlikely that the rain water available to the canopy won’t be available to the roots in the top soil layer. By the same logic water availability in the lower level(s) would be lagging behind the top layer’s one and thus water transport shall have bearing on plant development. Slight reduction in runoff and increase in growth can be predicted and were confirmed according to the benchmarks.

## Remaining issue

In interception() there is no distinction made with regard to the type of precipitation, so the snow is also deemed to incur evaporation costs, that doesn’t seem correct, but someone more experienced with this question should weigh in.

# Diurnal canopy-exchange processes

*Michael Mischurow, July 2012*

Implementation a diurnal cycle processes in canopy exchange module cover the following processes (functions): demand, aet\_water\_stress, water\_scalar and npp (and bvoc).

## Assumptions

This part of canopy exchange module is dealing mainly with calculation of the amount of carbon assimilated by the vegetation, depending on the water-stress conditions. The two major assumptions were incorporated in the code:

* Supply remains constant throughout the day, while demand changes are driven by the canopy conductance; the water stress is therefore changes throughout the day too.
* Vmax is calculated on a daily scale and therefore daily averages are used for this.

An example of diurnal I/O is available in benchmark watch\_diurnal code.

The reasonable duration for the sub-daily periods is probably from about 15 minutes up to 6 hours: at too high a resolution simulations could become computationally expensive; at too low resolution averaging doesn’t make much sense.

## Miscellaneous

### Monthly mode

Monthly mode (ifdailynpp equals 1) contradicts diurnal mode, therefore in case such a contradiction encountered the model should exit without performing any calculations.

### Sub-daily root respiration

Currently, soil temperature is calculated analytically as a dampened and lagged air temperature. The analytical formulation based on an annual cycle and it produces daily values. Such approach is not suitable to the sub-daily mode, as the soil temperature follows diurnal cycle (additionally dampened and lagged).This is the reason for using daily values of soil root respiration (based on daily soil gtemp). Additionally, while the value of soil temperature is calculated at 25 cm depth, we have information about PFT-specific fine root distribution between the two soil layers. Simple weighted average root depth would always be lower than 25 cm, as long as root fraction in the lower soil layer is different from zero.

# Nitrogen cycle with new SOM scheme

*David Wårlind, Ben Smith, Thomas Hickler, April 2013*

## Introduction

Nutrients, and then most often nitrogen, is a limiting factor for plant growth. To account for this the N cycle has been implemented in LPJ-GUESS. The main objective of this work has been to get a stable plant interaction with soil available mineral N. To achieve this, three main areas have been developed; i) new structure for soil organic matter, where it is possible to represent the N dynamics in both the inorganic and organics soil system (Comins and McMurtrie 1993; Parton et al. 1993; Friend et al. 1997; Parton et al. 2010) ii) establish a scheme for plant N allocation, demand, uptake, stress etc (Haxeltine and Prentice 1996; Friend et al. 1997; Zaehle and Friend 2010) iii) ecosystem N fluxes (Cleveland et al. 1999; Lamarque et al. 2011, 2013)

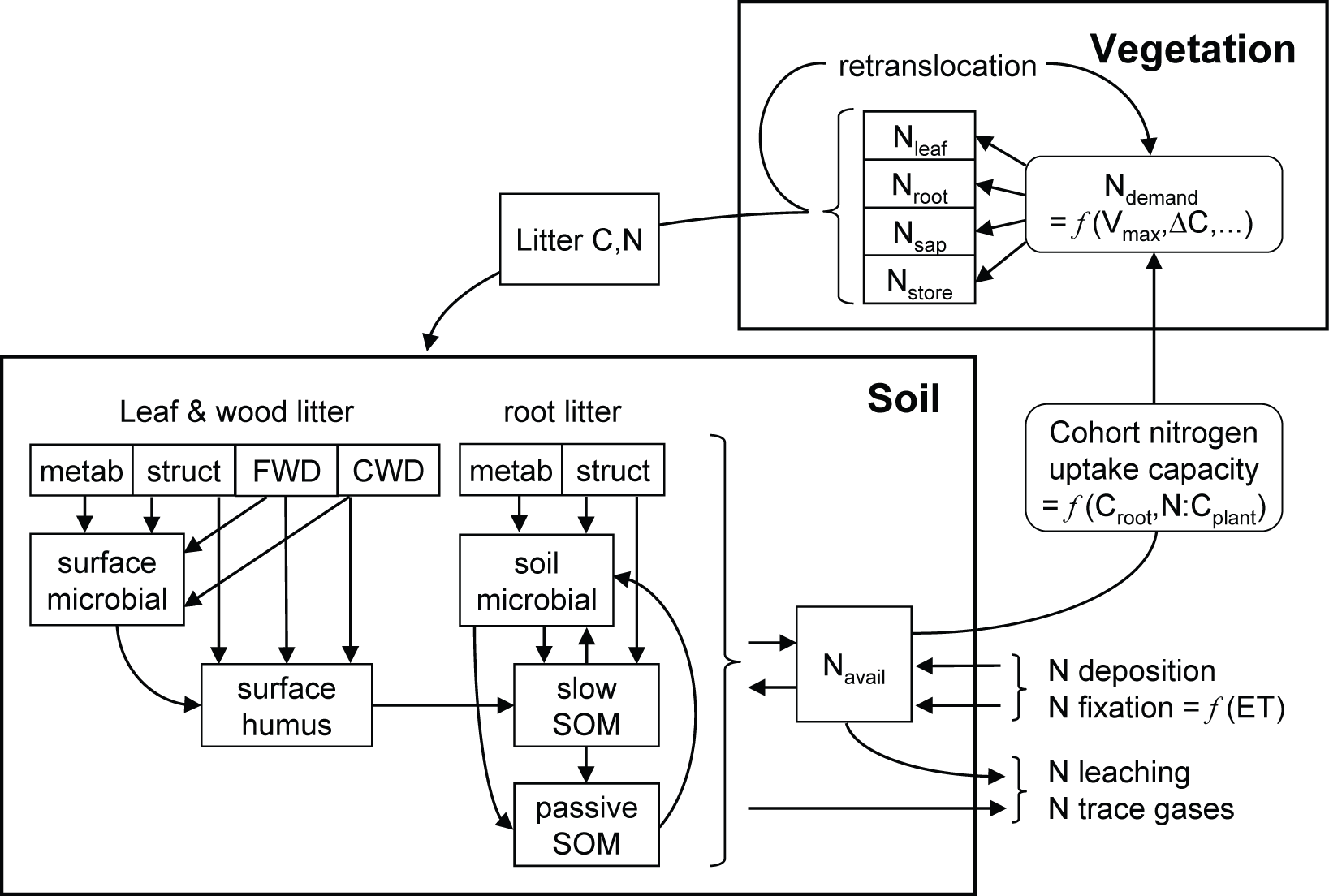


Figure 1. Schematic overview of N cycle in LPJ-GUESS. Abbreviations: FWD=fine woody debris; CWD=coarse woody debris; Navail=soil mineral N pool; Nleaf=leaf N mass; Nroot=fine root N mass; Nsap=sapwood N mass; Nstore=plant labile N store; Ndemand=daily plant N demand; Vmax=canopy rubisco capacity; ∆C=daily biomass increment; N:Cplant=aggregate N:C mass ratio for leaves and fine roots; ET=actual evapotranspiration. See text for further details.

## Ecosystem N fluxes

### N input to ecosystem

N enters the ecosystem via N deposition (single bulk value encompassing wet and dry deposition) and biological N fixation (BNF, kgN ha–1 yr-1). N deposition is prescribed as monthly mean values from an external database (Lamarque et al. 2011, 2013), whereas BNF is computed prognostically based on an empirical dependency on ecosystem evapotranspiration (ET) from Cleveland et al. (1999). Among three alternatives proposed by Cleveland et al. (1999) we chose the lower-range “conservative” parameterisation, with 5-year average actual evapotranspiration (AET, mm yr–1), prognosed by the model, as the independent variable:



BNF is distributed equally throughout the year and added directly to the soil available mineral N pool, *N*avail (Fig 1), which is capped at a saturation level of 2 gN m–2 following Parton et al. (1993). BNF in excess of the saturation level is discarded (assumed not to have occurred). N deposition during periods of snow lie (finite snow pack) is stored in the snow pack and released to the soil in proportion to snow melt.

### N loss from ecosystem

N is lost from the ecosystem via leaching, computed daily as the sum of leached soluble organic N and leached mineral N, and through volatilisation by wildfires. In addition, 1% of daily N mineralisation is assumed to be lost as gaseous emissions from soils (Thomas et al. 2013). Leaching of soluble organic N and C is computed conjointly as a fraction (*LO*) of the soil microbial SOM N and C pool, dependent on percolation (*PH2O*, cm/month) and soil sand fraction (*TS*), following Parton et al. (1993), using updated parameters from the CENTURY 5 manual:



For mineral N, the leaching fraction (*LM*) depends on daily percolation as a fraction of available soil water content (*WTOT*, mm):



N lost due to wildfires is released to the atmosphere as NH3, NO, NO2, N2O and N2. The relative fractions are taken from Levine (1996).

## Soil organic matter dynamics

C and N dynamics of soils are simulated conjointly by an SOM scheme adopted from the CENTURY model (Parton et al. 1993), with modifications by Comins & McMurtrie (1993) and Kirschbaum & Paul (2002), and updates by Parton et al. (2010). Eleven pools differing in C:N stoichiometry and base decay rate are distinguished (Fig 1). Decomposition, computed daily for each pool, results in heterotrophic respiration (release of CO2) and transfer of C and N between pools, satisfying mass balance. Carbon entering the receiver pool drives N mineralisation or immobilisation. N is mineralised (added to the soil mineral N pool, *N*avail) when N transferred from a donor pool exceeds the corresponding increase dictated by the prescribed C:N ratio of a receiver pool (N “supply“ exceeds “demand“). Conversely, if the N flux from a donor pool is too small to satisfy the C:N ratio of the receiver pool (demand > supply), N immobilisation occurs, reducing *N*avail to satisfy the deficit. If *N*avail is insufficient to satisfy the N demand for immobilisation among all pools, decay rates are reduced proportionately so that net immobilisation matches *N*avail.

Pool C:N ratios are determined as follows. For the surface microbial pool, the C:N ratio varies between 10 and 20 depending on the bulk N content of current surface litter (determined prognostically by the growth and physiology of the vegetation providing the source of the litter; see below) (Parton et al. 1993; Fig 2). For the soil microbial, surface humus and soil slow pools, C:N ratio varies between upper and lower bounds depending on *N*avail (Parton et al. 2010; Fig 2). The soil passive pool has a fixed C:N ratio of 9 (Parton et al. 2010).

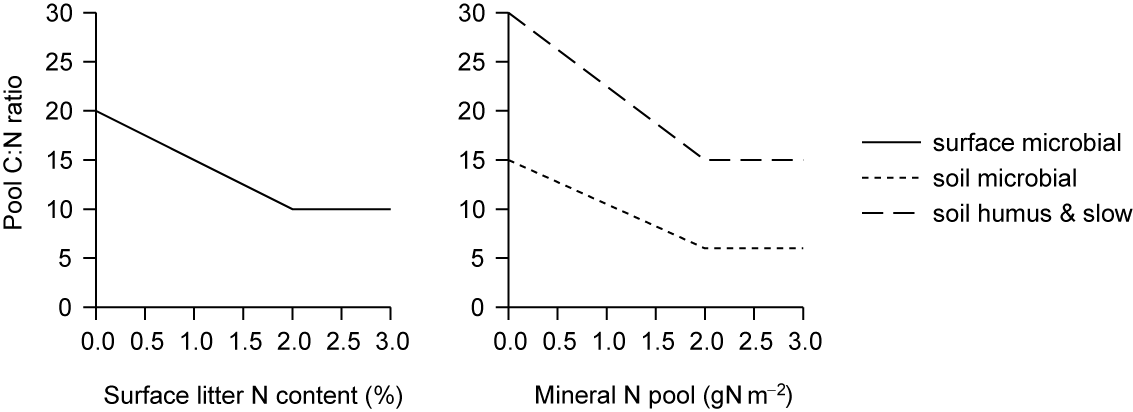


Figure 2. Determination of target C:N ratio of receiver pools in SOM flux transfer scheme (Parton et al. 1993, 2010).

Daily decay rates for each pool (C fraction: *Cj*, kgC m–2) are determined by a prescribed maximum (base) decay rate (*kj,max*; Parton et al. 2010; Table 1) and dependencies on temperature, soil moisture and soil texture:



where *f*(*T*soil) is a dimensionless scalar in the range 0-1 related to soil temperature (*T*soil, °C) by the relationship (Comins & McMurtrie 1993):



*f*(*W*) is a dimensionless scalar in the range 0-1 related to soil moisture following (Friend et al. 1997):



where σ is a proxy for percentage of water-filled pore spaces in the soil, given by:



where *θ* is current soil water content and *θ*max is soil water saturation capacity as a proportion of soil column depth, calculated from soil texture following Cosby et al. (1984).

*f*(*S*) is a dimensionless scalar in the range 0-1 determined from soil fractional silt plus clay content (*S*) following Parton et al. (1993):



Litter resulting from vegetation turnover (mortality or phenology), effected in the model on the last day of a given year, is transferred to the litter SOM pools on the first day of the following year. Leaf and root litter is partitioned into structural (resistant to decomposition) and metabolic (readily decomposable) fractions based on the estimated lignin:N ratio (Parton et al. 1993):



where *F*m and (1–*F*m) are the metabolic and structural litter fractions, respectively; λ is assumed lignin content as a fraction of total C mass (leaves: 20%; fine roots: 16%), and *cn* is the prognostic C:N ratio of the incoming material.

Sapwood and heartwood biomass lost due to mortality or disturbance enters the fine and coarse woody debris litter pools, respectively.

In the ins-file there is a switch, ifcentury, to change between the original, som\_dynamics\_lpj(), and CENTURY, som\_dynamics\_century(), SOM scheme. If N should be enabled then the CENTURY SOM scheme needs to be used.

## Vegetation N cycling

### Plant N demand and uptake

Plants obtain N for allocation to their biomass compartments leaves, fine roots and (for woody PFTs) sapwood through root uptake from the soil mineral N pool *N*avail. N uptake takes place daily and is the smaller of current supply, i.e. *N*avail, and demand, subject to a maximum constraint on total uptake.

Vegetation N demand is based on a solution of the carboxylation capacity of rubisco (*V*max) that maximises net assimilation at the canopy level given current temperature, light interception and intercellular [CO2], the latter affected by ambient [CO2] but also by the influence of soil moisture and boundary layer humidity on stomatal conductance (Haxeltine & Prentice 1996a,b; Sitch et al. 2003). Following Haxeltine & Prentice (1996a), leaf N content (*N*leaf, gN m–2) is related to *V*max (gC m–2) by the relationship:



where *T* is air temperature (°C), *L* is day length (s), *C*leaf is leaf C mass, accounting for canopy phenology (gC m–2) and *f*(LAI) is a modifier dependent on current leaf area index (LAI, m2 m–2) that accounts for the empirical finding that leaf N content declines more gradually with canopy depth compared to incoming sunlight (Lloyd et al. 2010; Peltoniemi et al. 2012):



Based on the *Nleaf* eqn, the target leaf C:N mass ratio may be calculated as *C*leaf*/N*leaf. Leaf C:N is, however, constrained to remain within prescribed boundaries [*CN*leaf*,*min, *CN*leaf*,*max] based on observations (Reich et al. 1992; White et al. 2000). C:N ratios for the further compartments fine roots and (for woody PFTs) sapwood are assumed to vary proportionately with leaf C:N, fine roots maintaining a C:N ratio 1.16 times higher, and sapwood 6.9 times higher than leaves (Friend et al. 1997). Since allocation of the current year’s NPP is effected only once per year in LPJ-GUESS, allocation ratios (proportion of biomass increment allocated to each respective compartment) from the previous year are assumed when computing daily demand for allocation to fine roots and sapwood.

Plants maintain a store of labile nitrogen, *N*store (kgN m–2), to buffer fluctuations in the balance between N demand and supply from the soil mineral N pool. Following Zaehle & Friend (2010), the maximum capacity of *N*store is related to current size as:



where *C*sap, *C*root, *C*leaf and *N*leaf denote sapwood C mass, fine root C mass, leaf C mass and leaf N mass, respectively, on allocation the previous year; *k* is set to 0.05 for evergreen woody, 0.15 for deciduous woody and 0.3 for herbaceous PFTs. The store is replenished by uptake from *N*avail.

Daily N demand for allocation to *N*store is computed as:



where *NPPa* and *NPPy–*1 are the current year’s accumulated and previous year’s NPP, respectively, and *N*turnover is the expected amount of N to be reallocated from turnover of leaves, fine roots and sapwood, based on tissue C:N ratios and biomass from the previous year.

Where the current day’s bulk N demand cannot be fulfilled by the present size of *N*avail, total uptake is reduced to *N*avail. Uptake may also be further reduced to a ceiling, *N*up, max, computed following Zaehle & Friend (2010) as:



Where *N*up,root is a linear scalar of the maximum N uptake per unit fine root biomass, *C*root, assuming a proportional increase in uptake capacity with root exploration volume, assigned the fixed values 2.8 and 5.51 gN kgC–1 day–1 for woody PFTs and grasses, respectively (Rothstein et al. 2000; Macduff et al. 2002). Modifiers account for the effects of the current mineral N pool, soil temperature (same as for decay rates) and plant N status on uptake capacity, as follows:



representing a combined linear and saturating effect of mineral N concentration on N uptake (Zaehle & Friend 2010), with *km*, the half-saturation concentration for N uptake, set to 1.48 gN m–3 for woody PFTs (Rothstein et al. 2000) and 1.19 gN m–3 for grasses (Macduff et al. 2002); *z*soil is the soil column depth (1.5 m).



representing a tendency for N uptake to increase as the concentration of relatively mobile N compounds within the plant, characterised by *NC*plant (below) declines. *CN*leaf*,*min and *CN*leaf*,*max are the prescribed minimum and maximum bounds for leaf C:N.



Vegetation N demand and uptake are computed each daily time step for each average individual plant (in practice, each age/size class in each replicate patch for woody PFTs, and once for the herbaceous ground layer in each patch). In the event that bulk demand cannot be met by the available N supply, the supply is partitioned among individuals in proportion to their relative uptake strength *fNup* which is related to estimated fine root surface area following:



where *X* (indiv m–2) is stem (cohort) density (included as a weighting factor for the most abundant cohorts) and *k*Nup, set to 1.6 for woody PFTs and 1.9 for grasses, weighs N uptake towards PFTs having shallower root distributions, coinciding with an assumed greater concentration of available N in the upper soil layer (Franzluebbers & Stuedemann 2009). It also implies that plants become more efficient at taking up N when their store of relatively mobile N approaches its lower limit, e.g. through physiological up-regulation of root uptake capacity (Raynaud & Leadley 2004); the existence of such a response is also suggested by studies of plant-mycorrhizal associations, which are often more developed in N-depleted habitats (Olsrud et al. 2004).

Where N uptake is insufficient to meet individual demand, individuals attempt to fulfil the deficit using their current labile N store. If demand is still not met after the N store is depleted, rubisco capacity and thereby leaf and whole-plant demand (as well as photosynthesis) are reduced to the maximum level that can be satisfied given the current supply plus storage, effecting N limitation. The N store is replenished, up to its maximum capacity (see above), on the last day of the year by retranslocation of up to 50% of the N mass of shed leaves, fine roots and sapwood on conversion to heartwood (Aerts 1996, Vergutz et al. 2012).

N demand and stress is modelled in a similar way as water demand and stress. First individual N demand and uptake capacity is calculated in ndemand(), if uptake capacity cannot meet demand then N stress on rubisco capacity (vmax) is determined in vmax\_nitrogen\_stress(), all resolved in canopy\_exchange() just as for water demand and stress.

### Plant growth and C and N allocation

Plant growth takes place on the last day of the simulation year by allocation of annual accrued NPP to the biomass compartments leaves, fine roots and (for woody PFTs) sapwood subject to allometric constraints. The only modification resulting from the incorporation of N cycling in the model to the allocation scheme is the addition of an N stress scalar (υ) in the functional balance constraint that governs the relative allocation of biomass to foliage versus fine roots:



where *lr*max is a PFT-specific constant (Table 2) and ω is a soil moisture stress scalar in the range 0-1, with smaller values reflecting increased soil moisture stress (Sitch et al. 2003). Where *N* stress exceeds soil moisture stress, this results in an increased allocation of biomass to fine roots at the expense of foliage:



where *CN*leaf,aopt is the leaf C:N ratio that would have been realised if plant *N* demand had been fulfilled by the available supply plus storage every day of the current year; *C*leaf and *N*leaf are realised C and N mass, accounting for N limitation.

## Additional updates

### α*a*

The incorporation of N limitation naturally results in a reduction in simulated NPP, regionally and globally, relative to the C-only version of the model, which lacks such limitation. To compensate for this nutrient effect on global C balance and fluxes, the quantum efficiency scalar α*a* was recalibrated to a value that resulted in simulated global C fluxes within the approximate range of observation-based estimates. For the C-only simulations of this study, which were performed with the C-N model, but with N limitation switched “off”, α*a* was likewise calibrated to the global fluxes. The resulting settings of this parameter were 0.70 and 0.55 with N limitation enabled and disabled, respectively. It may be postulated that the 15 percentage-point differential between these values corresponds to the global limitation of primary production attributable to N limitation, whereas the residual difference of 30% between realised and potential canopy quantum efficiency, obtained with N limitation enabled, more closely reflects the spectral factors traditionally invoked to explain this parameter.

### SLA

In conjunction with the incorporation of N cycling, an equation linking SLA to the PFT parameter leaf longevity (*a*leaf), originally adopted from Reich et al. (1997), was replaced with separate parameterisations of the same relationship for needleleaved and broadleaved PFTs, following Reich et al. (1992). The new equation has the form:



with SLA in m2 kgC−1and *a*leaf in yr. The regression coefficients {β0, β1}, fitted to a global dataset by Reich et al. (1992), are set to {2.41,−0.38} and {2.29,−0.40} for needleleaves and broadleaves, respectively.

As a consequence of this update, leaves are simulated to be generally thicker, with lower SLA and consequently reduced PAR per unit invested leaf C. The global data presented in both the 1992 and 1997 Reich et al. papers are, however, more faithfully reproduced, suggesting the presence of a unit conversion error in the original implementation. The resulting reduction in productivity per unit leaf C more strongly penalises species with short-lived leaves, particularly deciduous species and grasses, providing one explanation for an increased dominance by woody PFTs relative to grasses in simulations with the updated model, whether or not N limitations are enabled.

### Photosynthesis optimization

Before it has been possible to scale photosynthesis with fpar and only calculate it once per PFT, but now each individual have its own N status resulting in that this optimization is not possible anymore. Therefore, with enabled N cycle, photosynthesis has to be done on individual basis.

# Land cover and land use

*Mats Lindeskog and Stefan Olin, July 2015*

## Land cover representation

Land use and cropland representations are implemented in LPJ-GUESS based on LPJ-mL, (Bondeau et al., 2007), with a number of modifications and extentions (Lindeskog et al., 2013). Supported land cover types in addition to potential natural vegetaion (PNV) are cropland, pasture and managed forest (urban and barren land fraction input may be used also, but these have no vegetation implementation). Land cover change is based on net area fraction input data for the land cover types and stand types within a land cover type (e.g. different crops). Optionally, gross land cover transition input may be used together with the net area fraction input. A number of options how to treat transferred land (harvest, pooling/creation of new stands etc.) may be selected either in the instruction file or by settings in the code.

At the conversion of forest to cropland, by default 90 % of tree stems are harvested and the rest is oxidised the same year (burned). Part of the harvested wood (firewood) is oxidised the same year (67 %) and the rest moved to a pool with a 25-year turnover period, representing paper and timber. At cropland abandonment (conversion to natural vegetation), a new stand is created from bare ground, allowing the establishment of natural vegetation with a succession e.g. from grass to decidious trees and finally evergreen trees. An example of modelled carbon fluxes at cropland expansion and abandonment is shown for a moist tropical site in Africa in Figure 1.



Figure 1. Example of land use change modelling at a moist tropical site (9oW, 5.5oN) during the period 1901-. A. Carbon fluxes to the atmosphere associated with crop harvest and land use change (cropland expansion/deforestation). The ”slow C pool” represents the oxidation of carbon from the long-lived wood pool harvested at cropland expansion. B. Lifetime of natural vegetation stands. New stands are created at cropland abandonment and destroyed at subsequent cropland expansion. C. Cropland area fraction, showing the expansion and reduction of cropland area. D. NPP of three PFTs at one of the natural stands created at cropland abandonment, representing a typical plant successional sequence where an initial dominance of grass is followed by forest, dominated first by deciduous and later by evergreen trees.

When converting PNV to managed forest, the forest can either be clearcut or left standing, starting a cycle of simplified continuous cutting based on tree diameters (to be further developed).

Grazing of managed grassland is simulated by removing 50 % of the above-ground carbon. This is roughly in agreement with estimates of a 90 % removal in intensively grazed pastures and a 50 % re-entering of this carbon back to the litter pool as manure.

Fires are excluded by default from pasture, cropland and managed forest.

As for cropland (see below), stand managements for other land covers may be defined in stand types, or when using rotations, management types, in the instruction file, specifying “planting systems” (limiting PFTs that may establish, specified in the instruction file or by custom rules in the code), “harvest systems” (clearcut, continuous tree cutting), hydrology (irrigated/rain-fed), N fertilisation etc. Limiting establishment of natural PFTs may be specified for all land cover types in the stand type definition.

## Cropland representation

Separate crop phenology schemes on a daily time-step are present for simulations with and without N-limitation. Cropland without N-limitation is represented by eleven crop PFTs (temperate cereals, rapeseed, pulses, sugarbeet, maize, soybean, tropical cereals, sunflower, peanut, cassava and rice), simulated separately (without inter-PFT competition) and two grass PFTs (competing C3 and C4 grass) as cover crop between harvest and sowing. The same grass PFTs are used to represent pastures. Currently, two crop PFTs are defined for N-limited simulations (wheat and maize).

Irrigated crops are simulated separately. Irrigation water is added if atmospheric demand for transpiration exceeds plant water supply, but irrigated crops can still enter water stress if atmospheric demand exceeds a maximum evapotranspiration rate (5 mm/day).

In the *non-N-limited version*, there is a simple link between daily crop leaf carbon mass and LAI, while the the sum of heat units (degree days above a crop-specific base temperature, Tb) accumulated from the time of sowing mainly determines the allocation of photosynthates (Figure 2).



Figure 2. Non-N-limited crop phenology in LPJ-GUESS. The feedback between leaf area and leaf carbon mass via NPP is denoted by full-line arrrows and the heat unit sum control of the carbon allocation and leaf LAI is denoted by dotted arrows. \*HU sum: heat unit sum (dynamic potential HU adapted to local climate); LAI: leaf area index; HI: harvest index, NPP: net primary production.

Upon sowing, the initial carbon is set to 10 g m-2. Carbon allocation to crop roots, leaves and harvestable organs is done at a daily time-step. The development of the harvest index (HI), i.e. the fraction of above-ground carbon present in the harvestable organs, the root/shoot ratio and the onset of senescence and LAIdevelopment during senescence is dependent on accumulated heat units and calculated as in Bondeau et al. (2007). The PHU sum needed for full development of a crop, determining the time at which the crop is harvested, is calculated dynamically, using a 10-year running mean of heat unit sums accumulated from the sowing date to the end of a sampling period (ranging from 190 to 245 days) derived from default sowing and harvest limit dates as reported by Bondeau et al. (2007). The dynamic PHU calculation can be done either for an initial time period only, to calibrate for the local climate, or also for an extended period, to simulate adaptation to a changing climate by selecting suitable crop varieties/genotypes. A lower PHU limit of 900 degree days is used. Maintenance respiration of storage organs is set to zero. The non-N-limited modelled crop yield represents potential optimal yield, limited by climate and CO2 only.

***N-limited version, Olin et al. (2015):***

Below the updated version of LPJ-GUESS incorporating C-N interaction also for crops is described, for a more comprehensive description see Olin et al. (2015). The model allocates daily NPP based on the crop's development phase and allows for an adjustment of the allocation scheme based on the current nutrient and water status of the crop.

**Crop development**

Upon sowing, the development of a crop plant in LPJ-GUESS starts with a seedling that has an initial carbon mass in leaves and roots. The N content in the seedling is initiated with the highest N concentration ([N]) (the minimum C:Nleaf,min allowed in the model assuming a seed with a high N density.

**Development stage**

In most ecosystem and crop models, plant phenological development is modelled based on weather conditions often accumulated over a certain time period such as PHU (see above). Here we define development stage

(DS) as a number between 0 and 2 where: 0<DS<1 is the main vegetative phase, at DS=1 anthesis occurs and DS>1 represents the grain filling phase. Compared to the PHU implementation currently in the model, the use of DS facilitates a more detailed division of the growing period into the different crop phenological stages. Periods when the plant is more susceptible to heat and nitrogen stress can thus be represented in a more precise manner. DS at a given point in time (t) is a cumulative function of the maximal development rate dr (day-1) which differs between the vegetative phase and the reproductive phase. Following Wang & Engel (1998), DS is also modified using dimensionless scaling factors dependent on temperature (fT), vernalisation days (fvern) and photo-period (fphot):



**Daily carbon allocation**

For the allocation of the plant's daily assimilates, and their partitioning to the plant organs during the growing-season, we use the established allocation scheme from Penning de Vries et al. (1989). This scheme differs from the one described above for non N-limited in that the allocation of C to the different organs is related to the daily NPP and

to DS, as opposed to a function that meets a predefined target at the end of the growing-season. During the first part of the vegetative phase (DS<0.7 for winter wheat) most of the assimilates are used for root (R) and leaf (L) growth to maximise the uptake of water and nutrients and the absorption of radiation for photosynthesis, followed by a period when more of the assimilated C is allocated to the stem (St).

After anthesis, the grain-filling period starts, during which most assimilates are allocated to the storage organs. During this period, cereal crops reallocate some of their nutrients from the vegetative organs to the grains.

When a plant experiences water or nutrient deficit during the vegetative phase, it starts to invest a relatively larger fraction of the assimilates into roots to overcome the stress. It is thus important to be able to model the allocation to the roots separately from the other organs. The ratio between the allocation to leaves and stem (L:St), can be treated as constant during stress and thus a relationship between the allocation to R and that to the vegetative parts (V=St+L+R) that is also valid under stress can be established. This approach also gives an opportunity for future implementation of dynamic adjustments in the allocation during the vegetative phase, which is lacking in the current allocation model.

Relationships between allocation to L, St, R and grains (Y) from the original allocation model were established and fitted to a logistic growth function.

**Roots**

The allocation to R (gR) relative to the vegetative organs (gV) is shown in Fig. 3a:



**Leaves and stems**

Reflecting the shift from L (gL) to St (gSt) allocation during the initial part of the vegetative phase as outlined above, a relationship between the two organs was derived which is illustrated in Fig. 3a:

.

**Harvestable organs, grains**

Finally a relationship of the allocation to grains (gY) as the fraction of the whole plant (gY+gV) allocation was derived:



**Dynamic allocation**

These relationships between the allocation to the different organs of the plant can be applied to favour allocation to one organ over others. Combining the equations for f1,f2 and f3 yields



which is illustrated for winter wheat in Fig. 3b

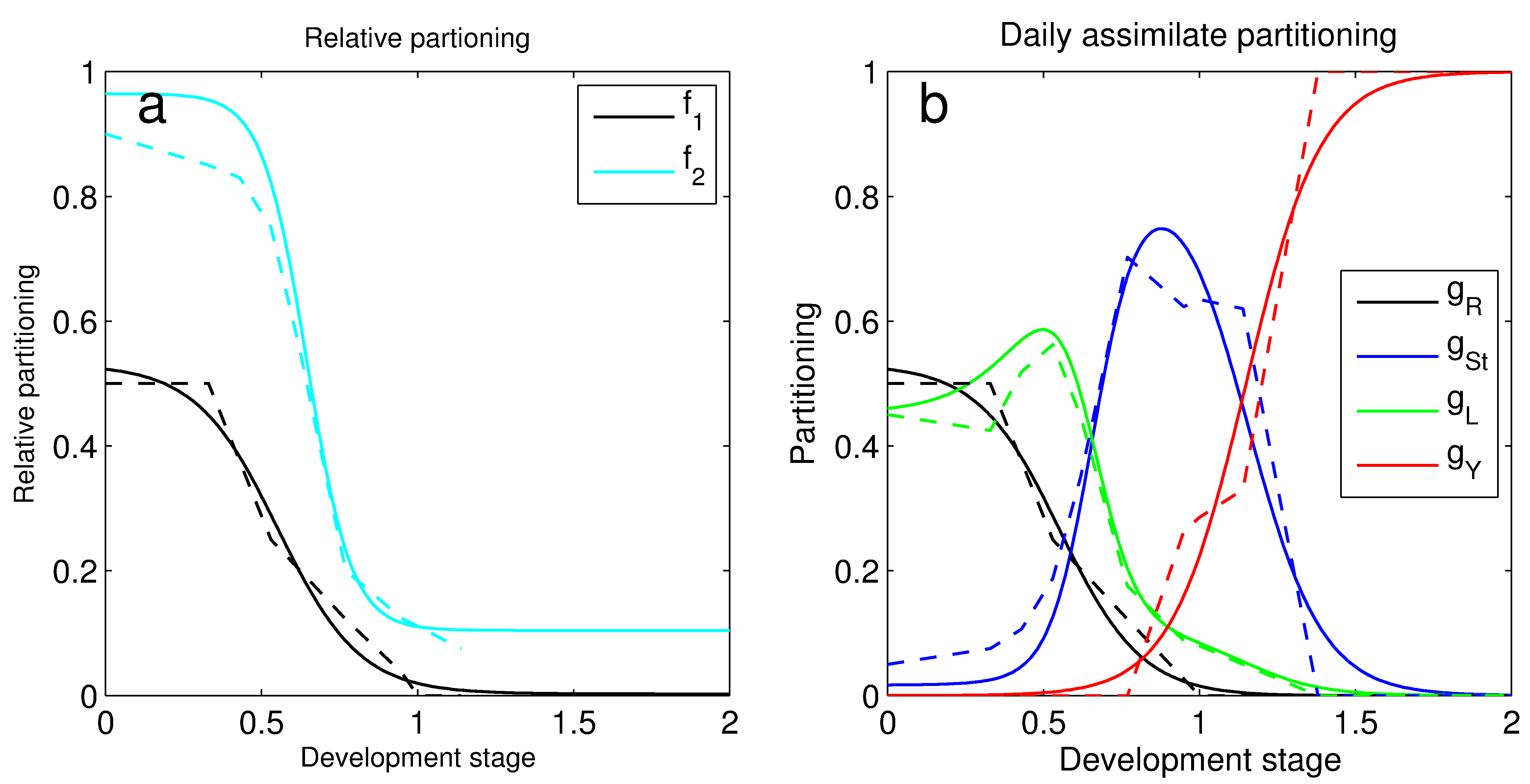


Figure 3: (a) The allocation to roots relative to vegetative organs (f1) and the allocation to leaves relative to leaves and stem (f2) for winter wheat. Dashed lines represent the allocation model from Penning de Vries (1989) and solid lines are the fitted equations. (b) The resulting allocation scheme to roots (gR), stem (gSt), leaves (gL) and grains (gY) (solid lines) compared to data from Penning de Vries (1989) (dashed lines).

**Carbohydrate retranslocation**

Crops store an easily mobilised reserve of carbohydrates in L, St and R (for some crops also tubers). To represent this in the model, a labile C pool is filled with a fraction of the daily assimilates directed to the stem (gSt), set here to 0.4 for wheat (Penning de Vries 1989). The labile C pool (MC,labile) is constrained between 0 and 0.4MC,St. During days when the daily assimilated C is lower than respiration costs (negative NPP), these sugars are used to compensate the loss. Additionally, during the grain-filling period the labile C pool is used to add to the grains and is reduced with a rate of 0.1 day-1 (Penning de Vries 1989).

**Daily nitrogen allocation**

During the vegetative phase in which the leaves and roots are expanding, the plant seeks to maximise photosynthetic gain by having a leaf N content that optimises the carboxylation capacity (Vmax).

**Leaf N content**

Nitrogen associated with Rubisco, the key enzyme in photosynthesis, makes up more than 20% of the total N in the leaves of wheat, but N is also important for plant structural tissues. However, the vertical distribution of N in the canopy is not even. Higher [N] is usually found in the upper part of the canopy, where leaves experience the highest levels of irradiance, compared to the more shaded leaves below. The decline in leaf [N] with the increase in cumulative leaf area index (LAI) from top to bottom typically follows an exponential decrease with a N extinction coefficient kN that is related to the light extinction coefficient (kL) as follows:

,

where b0 and b1 are regression coefficients taken from Yin (2003). From theory on optimal N distribution in a crop canopy, Yin (2000) derived a relationship between the LAI that can be supported given the amount of N that is currently in the leaves (LAIN) and kN:

,

where MN,L is the leaf N mass and Nb is the minimum N requirement for the leaf to function:

,

where C:NL,max reflects the minimum N required for photosynthesis and SLA is the specific leaf area. LAIN is then compared to LAI to determine the N status of the canopy, see section on Senescence below.

**Root N content**

In LPJ-GUESS, the N requirement of the root follows that of the leaves through the functional balance concept (described above in the N implementation section):

,

where MN,L denotes leaf N mass, MC,L leaf C mass, MN,R root N mass and MC,R root C mass. The theory behind the concept is that the activity of the roots (uptake and transport of water and nutrients) is proportional to that of the leaves (photosynthesis). A high photosynthesis rate in the leaves (high [N]L) implies a corresponding relative [N] in the roots to supply the demand of the leaves (Zaehle & Friend 2010).

**Plant N uptake**

For crops, we have expanded N uptake in the soil N module so that the N available for uptake by the plant (MN,avail) is related to the water content of the soil, as proposed by Xu-Ri (2008):

,

where φ is the fraction of projected leaf coverage by the plant (proportional to the fine root area), MN,soil is the mineral N mass of the soil and θ is the mean water content of the soil profile.

**Senescence**

Senescence, the killing of cells, can be either genetically programmed and age dependent, or induced by stresses or environmental factors. In the C-only original cropland version of LPJ-GUESS, leaf senescence is a function of PHU. We develop this further here with a dynamic response of plant senescence to its N status and age (DS).

**Leaf senescence**

If the N status of the leaves is suboptimal, the plant tries to maximise the leaf N in the canopy by redirecting some of it from the shaded leaves towards those that are more sunlit. This will eventually turn off the photosynthetic apparatus in the leaves from which all the non-structural N has been retranslocated. Senescence of part of the canopy in the model is induced when the N-determined leaf area index LAI (Yin 2000) is lower than the actual LAI. For plants, senescence of leaves is not an instantaneous process. The time for the acclimation of the N content in crop leaves is set to be 10 days. Implemented here is the proposed reduction of the leaf C mass as in (Yin 2000) but with an inertia of 0.1 day-1:



The leaf C mass is then updated MC,L' = MC,L - mC,sen and N accordingly using the minimum N content of the leaves, C:NL,max, MN,L' =MN,L - mC,sen (C:NL,max)-1. The senesced C and N is then transferred to a pool of dead leaves with a high C:N, currently set to 100 and the residual N is translocated to the labile N pool. In contrast to the labile C pool, N allocated to the labile pool is not determined as a fraction of the total allocation. The amount is constrained by the N translocated from senesced leaves and roots accordingly through the functional balance concept. The N that is translocated to the labile N pool due to senescence of the leaf is the leftover after maximising the C:NL status:



where C:NL,opt is the C:N below which a decrease has a small or no effect on photosynthesis which is estimated here as ¾ of the range between C:NL,max-1 and C:NL,min-1.

In ageing leaves, observed enzyme efficiency is reduced. After anthesis, degradation of the enzyme Rubisco is higher than the de novo synthesis. To reflect this in the model, a reduction of the leaf N content at rate of 0.1 day-1 (Bertheloot 2008) starts at anthesis (DS>1).

In order to avoid excessive allocation of C to the leaves while the plant experiences leaf N deficit (mC,sen>0) during the vegetative phase, a rescaling of the factor that controls the flow of assimilates to the leaves was implemented:

.

**Root senescence**

Root senescence is still an relatively unexplored area. In the absence of a full mechanistic understanding, the dynamics of the root in the model are assumed to be coupled to those of the leaves through the functional balance concept (described above).

**Seed development**

During flowering and grain filling, a fraction of the assimilates is allocated to the grains, while the N transported to the grains comes primarily from the leaves. This is reflected in the model as a transport of N from the leaves, roots and the labile N pool. In the model the plant tries to meet the demand from the grain:

,

primarily by reducing the labile N pool, MN,labile.

**Nitrogen retranslocation**

If mN,Y,dem is larger than the labile N pool, the crop plant attempts to meet the unsatisfied N demand from the grains (mN,Y,dem' = mN,Y,dem - MN,labile) by a N transport from the donor organs (leaves and roots). These donor organs have a resistance to let go of their N, *r* , to account for the fact that N is needed for maintaining organ processes (e.g. photosynthesis and maintenance respiration):



where *j* denotes the organ, L or R. The actual transport of N (mN,retr) is calculated by summing the individual organs' relative portion of the total N demand from the grains after the labile pool has been emptied. If the demand on the organ is larger than the available N, it is reduced to its minimum N content (C:Nj,max):

.

During the initial part of the grain filling period, only leaves contribute to fulfilling the grain N demand. Once more than half of the assimilates goes to the grain (DS>1.15), the model can utilise part of the plant root N as well to fulfil the N requirements of the grains.

## Sowing and harvest (C-only and N-limited versions)

The relative degree of limitation by temperature and precipitation to the sowing dates—or the absence of such limitation in perennially moist areas (where incoming solar radiation generally limits plant production)—is determined based on the local climatology (Waha et al., 2011). Five main seasonality types to determine sowing date are specified as: TEMP (temperature seasonality); PREC (precipitation seasonality); TEMPPREC (both temperature and precipitation seasonality, minimum monthly temperature < 10oC), temperature determines sowing date; PRECTEMP (both temperature and precipitation seasonality, minimum monthly temperature >=10oC), precipitation determines sowing date; NONE (neither temperature nor precipitation seasonality), default sowing date used. For irrigated crops at PRECTEMP sites, temperature-dependent sowing is used by default. The temperature limits for temperature-dependent sowing are as in Waha et al. (2011).

Croplands are harvested each year. A PFT-specific fraction of the harvestable organs (the harvest efficiency, default value 0.9 for all crops) constitutes the yield (multiplied by 2.0 for deriving the total dry yield from carbon units, assuming a dry matter carbon content of 50 %) and is assumed to be oxidised within a year. Of the leaf carbon, a further fraction (the residue removal fraction) is removed (and oxidised within one year). This PFT parameter is set to 0.75 for all crops as default.

Different cropland managements are defined in stand types, or when using rotations, management types, in the instruction file with specified values for crop PFT, hydrology (irrigated/rain-fed), N fertilisation, fallow etc.

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## Appendix A. List of symbols and their abbreviations in the model code

|  |  |  |  |
| --- | --- | --- | --- |
| **symbol** | **code abbrev.** | **description** | **unit** |
| *BNF* | anfix | total annual nitrogen fixation | kgN ha-1 yr-1 |
| *Lo* | orgleachfrac | leaching from decayed organic carbon/nitrogen | - |
| *PH2O* | dperc | daily percolation | mm |
| *Ts* | sand\_frac | fraction of soil that is sand | - |
| *Lm* | minleachfrac | leaching from available nitrogen mineral pool | - |
| *WTOT* | - | total amount of water in the soil column | mm |
| *Navail* | nmass\_avail | mineral N in soil column | kgN m-2 |
| *Cj* | fracremain | daily decay rates for each pool | - |
| *kj,max* | K\_MAX | max exponential decay constants for each SOM pool | - |
| *σ* | wpfs | water filled pore spaces | - |
| *θmax* | wsats | saturation capacity | mm |
| *S* | clay\_frac | fraction of soil that is clay | - |
| *Fm* | fm | metabolic fraction of litter | - |
| *λ* | leaf\_lton / root\_lton | compartment litter lignin:N ratio | - |
| *cn* | - | C:N ratio of litter | kgC kgN-1 |
| *Nleaf* | leafoptn | optimal leaf N content | kgN m-2 |
| *L* | daylength | day length | s |
| *Nstore,max* | max\_n\_storage | maximum long-term N storage capacity | kgN m-2 |
| *k* | fnstorage | PFT specific storage constant | - |
| *Nstore* | nstore\_labile | labile N storage | kgN m-2 |
| *Nturnover* | retransn\_nextyear | expected amount of N to be retranslocated next year | kgN m-2 |
| *Nup.max* | maxnup | maximum N uptake capacity | kgN m-2 |
| *Nup,root* | nuptoroot | maximum N uptake capacity per fine root mass | kgN kgC-1 |
| *km* | km\_volume | half-saturation concentration for N uptake | kgN l-1 |
| *zsoil* | soildepth | soil column depth | m |
| *CNleaf,min* | cton\_leaf\_min | minimum C:N ratio of leaf | kgC kgN-1 |
| *CNleaf,max* | cton\_leaf\_max | maximum C:N ratio of leaf | kgC kgN-1 |
| *fNup* | strenght | relative N uptake strength | - |
| *X* | densindiv | average density of individuals | indiv m-2 |
| *kNup* | nupscoeff | weighting factor for root distribution | - |
| *lrmax* | ltor\_max | leaf to root mass ratio under non-stressed conditions | kgC kgC-1 |
| υ | nscal | N stress scalar | - |
| *CNleaf.aopt* | cton\_leaf\_aopt | annually optimal leaf C:N ratio | kgC kgN-1 |
| *aleaf* | leaflong | leaf longevity | year |

## Appendix B. C:N ratios and base decay rates for soil and litter organic matter pools.

|  |  |  |
| --- | --- | --- |
| **SOM pool** | **C:N ratio\*** | **Base decay rate, *k*max (day–1)** |
| surface metabolic litter | prognostic | 3.8 × 10–2 |
| surface structural litter | prognostic | 9.5 × 10–3 |
| fine woody debris | prognostic | 1.1 × 10–2 |
| coarse woody debris | prognostic | 2.2 × 10–3 |
| surface microbial | 10-20 | 2.7 × 10–2 |
| surface humus | 15-30 | 4.8 × 10–4 |
| soil metabolic litter | prognostic | 7.0 × 10–2 |
| soil structural litter | prognostic | 1.9 × 10–2 |
| soil microbial | 5-15 | 4.2 × 10–2 |
| slow SOM | 15-30 | 1.7 × 10–3 |
| passive SOM | 9 | 3.9 × 10–6 |
| \* prognostic = depends on growth and physiology of source plant material; see also Fig 2. | | |

## Appendix C. PFT parameter changes for BNS

|  |  |  |
| --- | --- | --- |
| **parameter** | **new** | **old** |
| gdd5min\_est | 350 | 500 |
| phengdd5ramp | 100 | 200 |

# C:N ratios of plant tissues

*Michael Mischurow, November 2015*

As implemented in C-N version of the model (Smith et al. 2014), nitrogen content of plant tissues can vary between minimum and maximum values of C:N. The relationship between the two was calculated based on White et al. (2000) and equal 2.78. As was acknowledged in the paper, these limits might be unreasonably wide, exaggerating biochemical plasticity of the real plants. The same issue was noted in the behaviour of other models with flexible stoichiometry, particularly related to the overestimation of the whole-plant nitrogen-use efficiency (Zaehle et al., 2014).

Recently, Meyerholt and Zaehle (2015) showed that fixing of C:N ratio for woody tissues can improve modelling performance. Here we going one step further and fixing both woody and root C:N ratios in a very narrow range. The ratio between minimum and maximum C:N values is, therefore, set to be 10/9 rather than 2.78 (i.e., minimum = 0.9 \* maximum). The choice of implementation approach was motivated, in part, by desire to keep changes to the existing framework (with the range of C:N values) to a minimum.

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