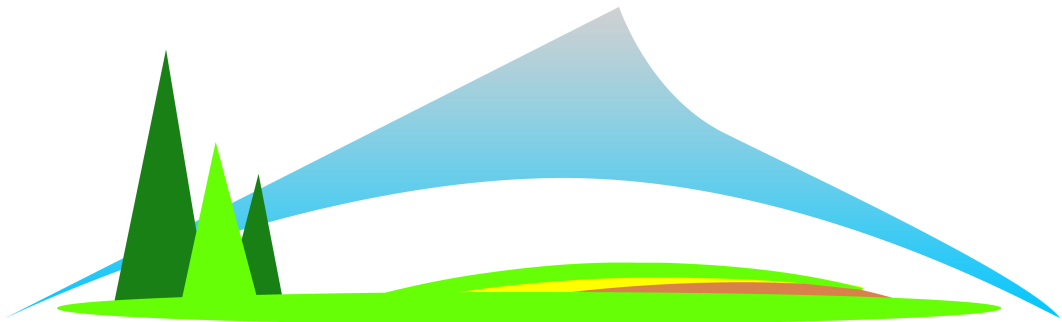


LandscapeDNDC v1.36.0

A process model for simulating
biosphere-atmosphere-hydrosphere exchange
processes

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Models Description

July 17, 2025

Institute of Meteorology and Climate Research – Atmospheric Environmental Research

Synopsis

LandscapeDNDC is a simulation framework for terrestrial ecosystem models on site and regional scales (Haas et al., 2013). LandscapeDNDC emerged from the site scale model MoBiLE (Grote et al., 2009), which was based on the Arable-DNDC and Forest-DNDC models (Li, 1992; Li et al., 1994; Stange et al., 2000).

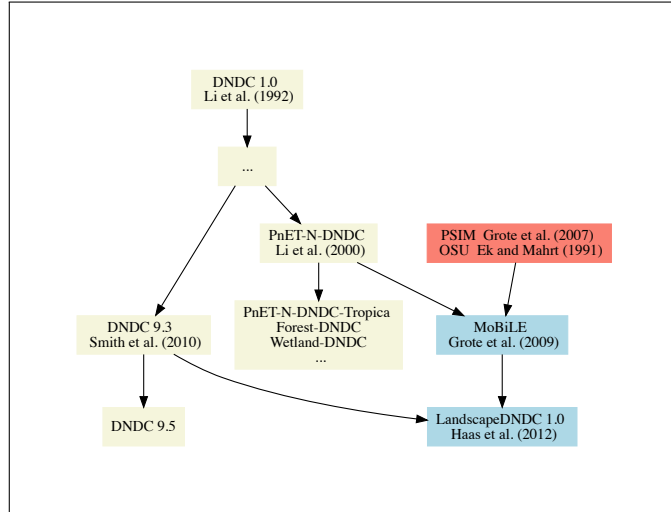


Figure 1: Schematic illustration of the history of the LandscapeDNDC development.

The modular design of LandscapeDNDC allows plugging in any choice of process descriptions for various parts of different natural ecosystems.

One important feature of LandscapeDNDC is its capability to handle more than one site, i.e., simulating many cells (e.g., regions) with a single program invocation. In contrast to other models, in LandscapeDNDC all cells are synchronized with respect to time, which is highly significant for model coupling by means of a model-independent communication infrastructure (Haas et al., 2013; Klatt et al., 2015).

Landscape is parallelized using MPI allowing the deployment on High Performance Computer (HPC) environments. LandscapeDNDC is written in C/C++ conforming to the standard known as C++ 11. It compiles and runs on:

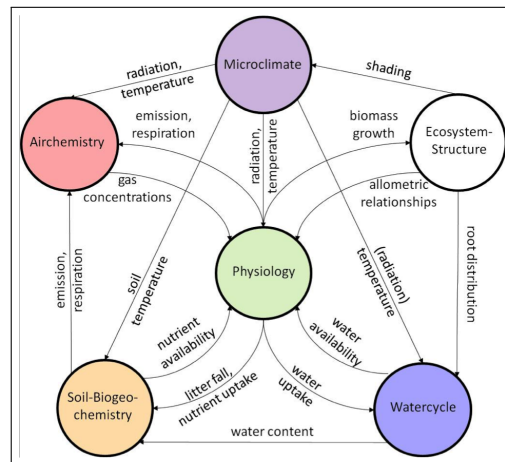


Figure 2: Schematic illustration of information flow between models representing different ecosystem domains.

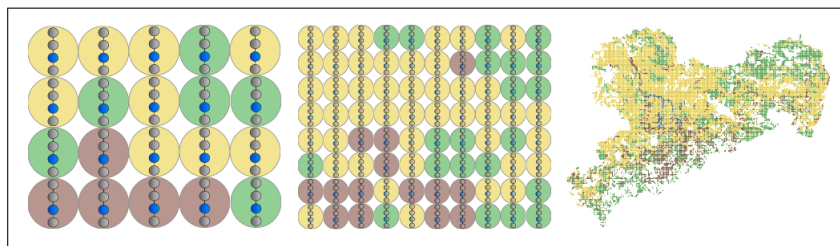


Figure 3: Schematic illustration of upscaling from site simulations to regional simulations.

- GNU/Linux (GCC, CLang, Intel, PGI, MinGW/GCC Cross-compiling for Microsoft Windows)
- MacOS X (GCC, CLang)
- Microsoft Windows platforms (MinGW/GCC, MSVC 8, MSVC 11)

Here we present various model concepts and stand-alone models, which are currently implemented into LandscapeDNDC. Models are listed due to their ecosystem function:

- Microclimate
- Watercycle
- Vegetation
- Biogeochemistry

Please note that the model documentation is still in progress and at the moment neither guarantees completeness or correctness. Please consider also the LandscapeDNDC Users Guide for all questions regarding how to use LandscapeDNDC.

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Chapter 1

LandscapeDNDC MoBiLe

1.0.1 Overview

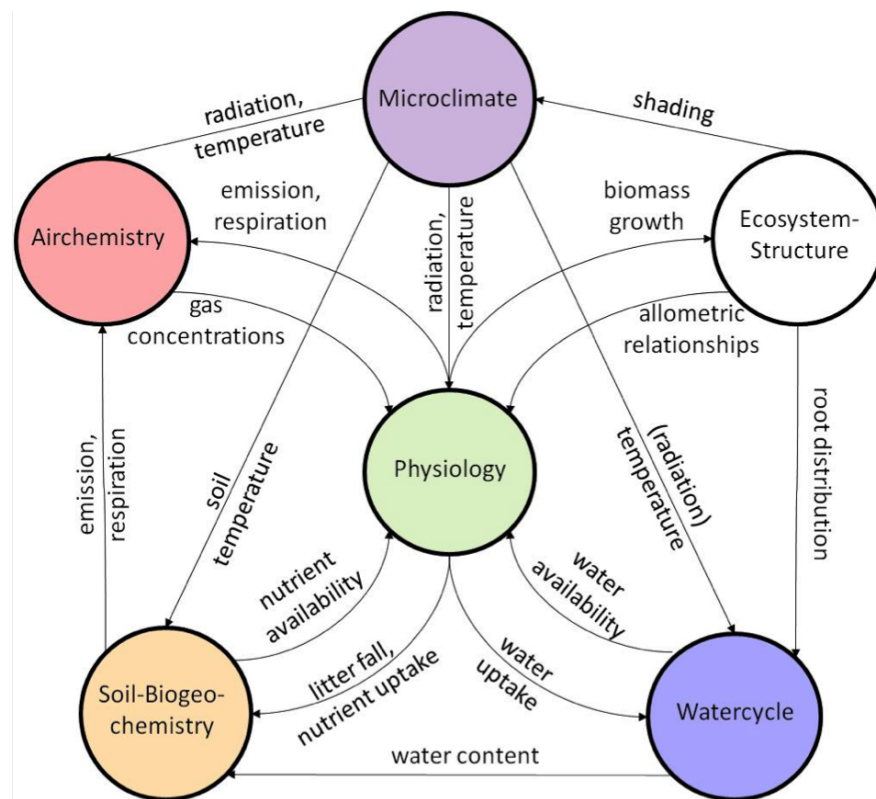


Figure 1.1: Models communication

Models are presented according to the respective ecosystem domain:

- Microclimate
- Watercycle
- Vegetation
- Soilchemistry
- Global State
- Standard outputs

1.0.2 Microclimate

- global_state_microclimate
- CanopyECM
- Microclimate libraries

1.0.2.1 global_state_microclimate

Initialisation

1.0.2.2 CanopyECM

User guide The microclimate model CanopyECM calculates:

- Radiation
- Temperature
- Wind velocity
- vapor pressure deficit (air humidity)
- Albedo

Model structure CanopyECM requires further models for:

- plant growth (e.g., distribution of leaf area)
- watercycle (e.g., soil water content)

Model options Available options: Default options are marked with bold letters.

- Soiltemperature (soiltemperature: **implicite** / explicite)
- Dirichlet boundary condition (annual average temperature) of bottom soil layer for soil temperature calculation (dirichletboundarycondition: **false** / true)
- Depth of lower boundary for soil temperature calculation (soilprofileextension: **0.0** / ...)
- Consider energy balance (energybalance: **false** / true)

Radiation Calculates radiation in each canopy layer and beneath the canopy and absorbed radiation in sunlit and shaded canopy fractions as well as the fraction of sunlit foliage area.

The basic algorithms are taken from Spitters 1986 Spitters (1986) and complemented by Thornley 2002 Thornley (2002).

In contrast to traditional approaches, light extinction is accounted for separately layer by layer, considering changes in crown shape.

Note that the procedure doesn't account for slope effects. A possible approach to address this might be that of Garnier and Ohmura 1968 Garnier and Ohmura (1968) also applied in Lexer & Hoenninger 2001 [**lexer_hoenninger:2001a**].

Vapor Pressure Deficit Calculates vapor pressure deficit (mbar, or hPa) for the ground and every foliage layer.

VPD is calculated based on the canopy layer temperature. It is assumed that the absolute water content throughout the canopy is , constant but the saturated vapor pressure and thus the pressure deficit changes with temperature in every layer.

Wind Speed Calculates wind speed decline throughout the canopy according to Lalic and Mihailovic (2009). However, the originally used dependency on leaf area has been replaced by one of plant area which also considers the impact of overall woody biomass.

Wind speed is calculated in each canopy layer (using cosh =Hyper Cosinus):

$$loc_win_{fl} = loc_win \cdot \frac{\cosh(ExtFac \frac{hCum - hBottom}{hTop})^{2.5}}{\cosh(ExtFac \frac{1 - hBottom}{hTop})}$$

with

loc_{win}_{fl}	Foliage layer specific wind speed	(m s-1)
loc_{win}	Above-canopy wind speed	(m s-1)
hCum	Cumulative height	(m)
hBottom	Bottom height of tree crowns	(m)

The extinction factor depends linearly on plant area index:

$$extFac = \frac{4.0 \cdot DRAGC \cdot pai}{ROUGH^2 KARMAN^2}$$

$$pai = lai + mWood \cdot FEXT_W \cdot \exp(-0.1 \cdot lai)$$

with

extFac	Extinction factor	(-)
DRAGC = 0.1	Drag coefficient	(-)
ROUGH = 2.0	Roughness parameter of the ground (1-2)	(-)
KARMAN = 0.41	Karman constant (Hogstrom 1985)	(-)

Note

: The drag coefficient is actually a function of wind speed and leaf area clumping (see Cescatti and Marcolla 2004 Cescatti and Marcolla (2004)), which is not considered here.

Albedo Albedo is the fraction of reflected light relative to the total incoming shortwave radiation.

$$albedo = \frac{\sum_0^f l(sw_refl_{fl}) + sw_refl_a}{rad_{sw}}$$

$$sw_refl_{fl} = (rdiff_{fl} + rdir_{fl}) \cdot \frac{refl}{1.0 - refl}$$

$$refl = (pai \cdot 0.5) \cdot \left(1.0 - \frac{sqrt(1.0 - ALB)}{1.0 + sqrt(1.0 - ALB)}\right);$$

with

- fl: canopy layer counter
- sw_refl_a: reflected shortwave radiation from soil surface
- sw_refl: reflection coefficient Spitters (1986)

- `rdiff`: incoming diffuse radiation into this layer
- `rdir`: incoming direct radiation into this layer
- `pai`: plant area index (see Wind Speed)
- `ALB`: species-specific albedo factor

The reflection from the soil surface is assumed to be a fixed proportion (`FLITALB`) of the shortwave radiation that is released below the last canopy layer. This is added to the reflected radiation of all canopy layers, which in turn are influenced by plant area (that is a function of foliage and wood biomass) distribution and a species-specific albedo parameter (`ALB`). If more than one species has leaves in the same layer, plant area and `ALB` are scaled with leaf area fraction of the respective species.

Temperature CanopyECM calculates a temperature buffering effect in the canopy as leaf area-weighted connection between temperature above the soil and temperature above the canopy (field temperature)

Temperature above the soil T_s depends on atmospheric temperature above canopy T_{atm} , leaf area index and an empirical species - specific temperature damping parameter (`CDAMP`):

$$\begin{aligned} bvc &= \frac{LAI}{LAI + CDAMP} \\ T_s(t+1) &= bvc \cdot T_s(t) + (1 - bvc)T_{atm} \end{aligned}$$

Temperature within the canopy T_c is linearly correlated with canopy height z specific leaf area index:

$$\begin{aligned} \phi(z) &= \frac{\sum_0^z LAI}{\sum LAI} \\ T_c(z) &= T_s + \phi(T_{atm} - T_s) \end{aligned}$$

1.0.2.3 Microclimate libraries

Incoming longwave radiation Incoming longwave radiation is given by:

$$LWR_{in} = \varepsilon \sigma T^4,$$

wherein ε , σ , T refer to the emissivity, the Stefan-Boltzmann constant and air temperature, respectively.

The emissivity ε has two components, i.e., emissivity under clear (ε_{cl}) and clouded sky (ε_{cs}):

$$\varepsilon = (1 - f_{cl})\varepsilon_{cs} + f_{cl}\varepsilon_{cl}$$

The partitioning coefficient f_{cl} refers to the cloud fraction. For ε_{cl} , a constant value of 0.976 is used Greuell et al. (1997).

Clear sky atmospheric emissivity

Emissivity of incoming longwave radiation under clear sky conditions is calculated based on vapour pressure vp Brunt (1932) :

$$\varepsilon_{cs} = B_c + B_d\sqrt{vp}$$

The parameters B_c and B_d are set to 0.53 and 0.212, respectively Van Kraalingen and Stol (1997).

Cloudiness

Cloudiness is derived from global radiation using the Angstrom formula:

$$f_{cl} = \frac{\frac{SWR}{SWR^*} - A}{B}$$

using the Angstrom parameters $A = 0.29$ and $B = 0.52$ Van Kraalingen and Stol (1997).

Meteorological variables

Radiation

- Stefan–Boltzmann equation for the power radiated from a black body in terms of its absolute temperature T :

$$P = \sigma \cdot T^4$$

- Global radiation depending on latitude ...
- Mean temperature \bar{T} after Thornton [thornton:1997a:]

$$\bar{T} = 0.394 \cdot T_{min} + 0.606 \cdot T_{max}$$

Sun declination

Eccentricity factor for calculation of extraterrestrial radiation (Fortin et al. (2008))

Daily extraterrestrial radiation as developed by [sellers:1961a] (cit. in Fortin et al. (2008), and Cai et al. (2007)) note: formula of sun declination wrong in Fortin et al. (2008)

Ratio between diffuse and total solar irradiance after Friend (2001)

Lizaso et al. (2005)

Daylength

Daylength period

The daylength is calculated based on latitude and the day of the year according to Lee (2010), as:

$$dayl = 12.0 * \frac{PI + 2.0 * \arcsin(\sin ld_{cosld})}{PI}$$

with:

$$\sin ld_{cosld} = \frac{-\sin(\frac{-PI}{45.0}) + (\sin(lat_r) * \sin(sdec))}{\cos(lat_r) * \cos(sdec)}$$

With sdec beeing sun declination and lat_r latitude in radians:

$$sdec = 0.4093 * \sin(\frac{2.0 * PI * jday}{365.0 - 1.405}) \quad lat_r = lat * \frac{PI}{180.0}$$

Saturated vapor pressure according to Hamon (1963)

When foliage temperature is above 0oC, saturated vapor pressure is calculated as:

$$svp = 0.61078 * \exp(17.26939 * \frac{T}{T + 237.3})$$

When foliage temperature is below 0oC, it is:

$$svp = 0.61078 * \exp(21.87456 * \frac{T}{T + 265.5})$$

Annual mean temperature

Cloudiness

Cloudiness is derived from global radiation using the Angstrom formula:

$$f_{cl} = \frac{\frac{SWR}{SWR^*} - A}{B}$$

using the Angstrom parameters $A = 0.29$ and $B = 0.52$ Van Kraalingen and Stol (1997).

1.0.3 Watercycle

- global_state_watercycle
- EcHy - Ecosystem Hydrology
- WatercycleDNDC
- waterlibs

1.0.3.1 global_state_watercycle

Initialisation

1.0.3.2 EcHy - Ecosystem Hydrology

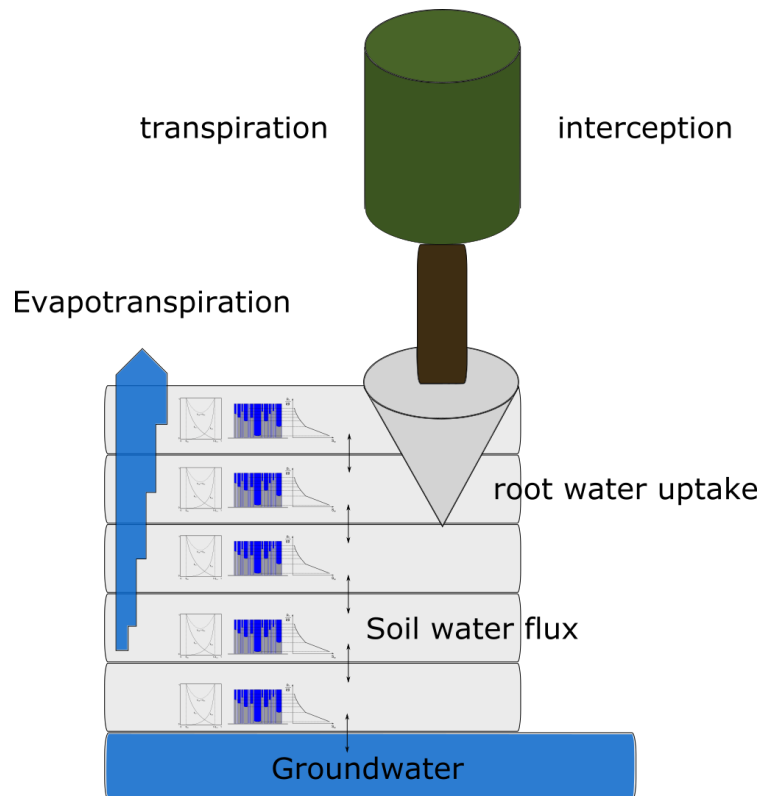


Figure 1.2: EcHy overview

User guide

Model structure EcHy requires further models for:

- plant growth (e.g., transpiration demand)

Parametrization The following lists include site parameters that might be calibrated in order to represent the hydrological cycle.

Evapotranspiration:

- *WCDNDC_INCREASE_POT_EVAPOTRANS*

Interception Interception describes the amount of precipitation, which is hold by the canopy, i.e., not reaching soil surface (see Interception capacity for more details)

Model options Available options: Default options are marked with bold letters.

- Potential evapotranspiration model (default: "potentialeapotranspiration" = **thornthwaite** / penman, priestleytaylor)

Potential evaporation (Echy) Actual evapotranspiration is the balance between atmospheric demand of water (potential evapotranspiration) and water supply by the surface. Implemented concepts for the calculation of potential evapotranspiration (default: Thornthwaite):

- Thornthwaite
- Priestley and Taylor
- Penman

Evapotranspiration distinguishes evaporation from leaf and soil water as well as transpiration of the prevalent vegetation. While leaf evaporation is not limited, soil evaporation and transpiration depend on:

- Soil water availability
- Soil texture and depth
- Fine root distribution

Soil layer specific transpiration $TR(z)$ and soil evaporation $EV(z)$ are given by:

$$\begin{aligned} TR(z) &= f_l(\theta) \cdot f_l(m_{fr}) \cdot f_{r,w}(z) \cdot PTR \\ EV(z) &= f_l(\theta) \cdot f_e(z) \cdot PSE \end{aligned}$$

The factors $f_l(\theta)$ and $f_l(m_{fr})$ refer to limitations due to water availability and fine roots abundance, while $f_{r,w}(z)$ and $f_e(z)$ are distribution factors of total transpiration and evaporation water needs across the soil profile. PTR and PSE refer to potential transpiration and soil evaporation, respectively.

Distribution factor for soil layer specific transpiration

Soillayer-specific transpiration depends on fine root abundance $m_{fr}(z)$ and water availability $\Delta\theta(z)$. For both, a soil layer specific relative share $f_x(z)$ is calculated and, in a

second step, harmonically weighted:

$$\begin{aligned} f_r(z) &= \frac{m_{f_r}(z)}{\sum m_{f_r}} \\ f_w(z) &= \frac{\Delta\theta(z)}{\sum \Delta\theta} \\ f_{r,w}(z) &= \frac{(f_r, f_w)_{harm.}(z)}{\sum (f_r, f_w)_{harm.}} \end{aligned}$$

Note, $\sum f_r = \sum f_r = \sum f_{r,w} = 1$. Hence respective factors do not limit transpiration but only distribute total transpiration needs across soil layers.

Distribution factor for soil layer specific evaporation

Soillayer-specific evaporation depends on depth:

$$\begin{aligned} f_d(z) &= 1 - \frac{z}{z_{limit}} \\ f_e(z) &= \frac{f_d(z)}{\sum f_d} \end{aligned}$$

Note, $\sum f_d = \sum f_e = 1$. Hence respective factors do not limit evaporation but only distribute total soil evaporation across soil layers.

Water limitation for transpiration

The reduction of transpiration depending on soil water availability $\Delta\theta$ is given by:

$$f_t(\theta) = \frac{\Delta\theta}{\Delta\theta^*}$$

The reference amount of available water $\Delta\theta^*$ that does not limit transpiration is given by the difference between field capacity and wilting point:

$$\Delta\theta^* = \theta_{max} - \theta_{min}$$

The amount of available water for transpiration $\Delta\theta$ is given by:

$$\Delta\theta = \theta - \theta_{min}$$

Water limitation for soil evaporation

The reduction of soil evaporation depending on soil water availability $\Delta\theta$ is given by:

$$f_t(\theta) = \frac{\Delta\theta}{\Delta\theta^*}$$

The reference amount of available water $\Delta\theta^*$ that does not limit soil evaporation is given by the difference between field capacity and residual water content:

$$\Delta\theta^* = \theta_{max} - \theta_{r,w}$$

The amount of available water for soil evaporation $\Delta\theta$ is given by:

$$\Delta\theta = \theta - \theta_{r,w}$$

Fine roots limitation

The reduction of transpiration depending on fine roots abundance is calculated by a Michaelis-Menten relationship:

$$f_l(m_{fr}) = \frac{m_{fr}^l}{m_{fr}^l + K_{mm,fr}}$$

The Michaelis-Menten constant is given in the site parameter $\text{ECHY_ROOTS} = \text{ECHY_KMM_ROOTS}$.

Percolation Vertical downward movement

Vertical downward movement of water q_z is calculated via the saturated hydraulic conductivity K_f and the relative permeability k_r , which depends on water saturation:

$$q_z = K_f \cdot k_r(\theta)$$

The relative permeability is derived from the van Genuchten soil parametrization following the work of Mualem (1976) :

$$k_r(\theta_e) = \theta_e \left[1 - \left(1 - \theta_e^{\frac{1}{m}} \right)^m \right]^2$$

Effective soil water saturation

The effective soil water saturation (θ_e) linearly scales between the residual water saturation ($\theta_e = 0$) and the residual air-filled porespace ($\theta_e = 1$). The residual water saturation is set by default to $\theta_{r,w} = 0.01$, while the residual air-filled porespace can be given as model input (default value is set to $\theta_{r,a} = 0$).

Groundwater influence

Percolation within the static groundwater table as given in the model input can be reduced by the site parameter $\text{GROUNDWATER_PERCOLATION}$.

Preferential flow Preferential flow due to, e.g., soil cracks is included by a simple concept, which is based on two parameters representing:

- Fraction of infiltrating surface water that is subject to preferential flow α_{pf}
- Specific soil depth z_{pf} until which preferential flow occurs

The amount of water that is subject to preferential flow is redistributed within z_{pf} . Soil layers are iteratively filled upwards until field capacity beginning with the soil layer at z_{pf} .

Snow and ice Snowfall and soil ice formation are calculated as presented in the library functions `Snow` and `ice` .

Pore space reduction

Soil ice formation leads to reduction of pore space ϕ . Likewise, field capacity θ_{max} and wilting point θ_{min} are reduced:

$$\begin{aligned} f(\theta_{ice}) &= 1 - \frac{\theta_{ice}}{\phi} \\ \theta_{max}^* &= \theta_{max} \cdot f(\theta_{ice}) \\ \theta_{min}^* &= \theta_{min} \cdot f(\theta_{ice}) \end{aligned}$$

1.0.3.3 WatercycleDNDC

User guide This WatercycleDNDC model is taken from the PnET-N-DNDC Model (Li 2000). It calculates daily dynamics of snowcover, soil ice content, potential evaporation and hourly dynamics of rainfall, interception, transpiration, percolation, and runoff.

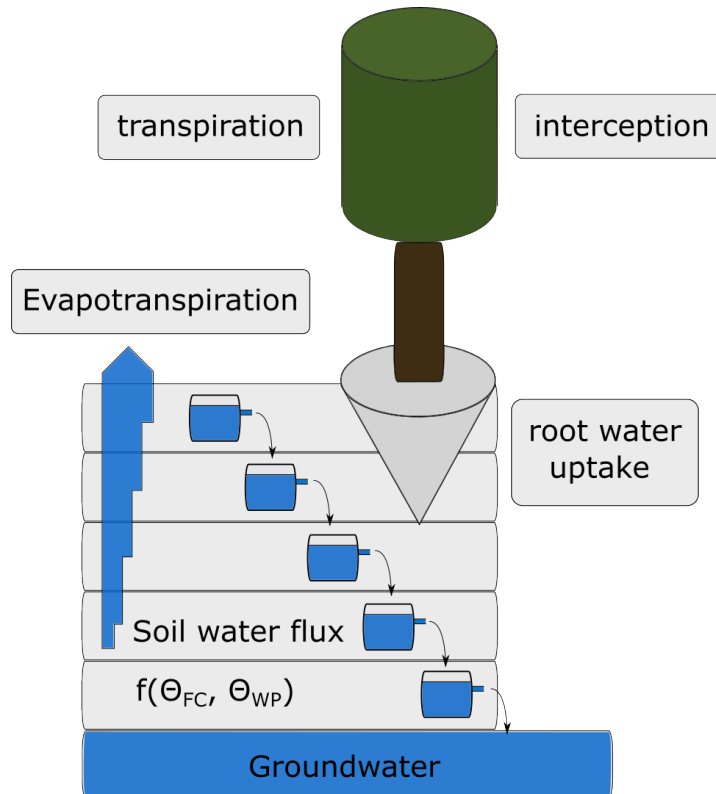


Figure 1.3: Watercycle overview

Model structure WatercycleDNDC requires further models for:

- plant growth (e.g., transpiration demand, fine roots distribution)

Parametrization The following lists include parameters that might be calibrated in order to adapt the model to site conditions:

Interception:

- MWWM (speciesparameter: specific interception capacity of wood mass (m kg-1↔DW))
- MWFM (speciesparameter: specific interception capacity of foliage (m m-2LAI))

Evapotranspiration:

- *ROOT_DEPENDENT_TRANS*
- *WCDNDC_INCREASE_POT_EVAPOTRANS*

Preferential flow

- *BY_PASSF*

Lateral runoff

- *FRUNOFF*

Percolation

- *FPERCOL*
- *IMPEDANCE_PAR*

Model options Available options: Default options are marked with bold letters.

- Potential evapotranspiration model (default: "potentialeapotranspiration" = **thorn-thwaite** / penman, priestleytaylor)
- Subdaily evapotranspiration distribution (default: "evapotranspiration" = **uniform** / non-uniform)
- Automatic irrigation (default: "automaticirrigation" = **-1.0**) Set to a number x within the interval $[0.0, 1.0]$ in order to automatically trigger irrigation as soon as the soil water content wc drops below a defined target water content depending on wilting point wp and field capacity fc :

$$wc < wp + x(fc - wp)$$

Management

Irrigation Irrigation events are simply added to rainfall.

Flooding Selectable flooding regimes via event input:

- Continuous surface water and fully saturated soil profile
 - Constant height of surface water table (set only: **watertable** > 0.0).
 - Minimum height of surface water table, e.g., precipitation can lead to higher surface water (set: **watertable** > 0.0 and **bundheight** > **watertable**).
 - Minimum height of surface water table, e.g., automatic irrigation as soon as defined minimum surface water is reached (set: **watertable** > 0.0 and **irrigationheight** > **watertable**).
- Alternating wetting and drying: Automatic irrigation as soon as soil water table drops below defined value. The specified value must be negative since it corresponds to a soil water depth below ground level. (set: **watertable** < 0.0 and **irrigationheight** > 0.0).
- Moist soil conditions: Soil layers above a specified depth are continuously set to field capacity, while soil layers below are set fully water saturated (set only **watertable** < 0.0)
- Fixed bund height (**bundheight** > 0.0). Water table is calculated dynamically depending on water input (precipitation & irrigation)
- Percolation rate (percolationrate > 0.0). Maximum value for soil water percolation. Can be defined in order to reflect soil puddling, which decreases soil water percolation under flooded conditions.

Rainfall distribution Rainfall per timestep set by a parameterized rainfall intensity (RI, mm timestep⁻¹). Thus, the number of timesteps (usually hours) with rainfall is given by:

$$nts_{rain} = \frac{P}{RI}$$

with

- P: precipitation (mm day⁻¹)

If the precipitation per day is larger than the parameterized rainfall intensity times the number of timesteps, rainfall intensity will be increased accordingly:

$$ri_{act} = \frac{P}{n_{timesteps}}$$

with

- `n_timesteps`: number of timesteps per day

Snow and ice Snowfall and soil ice formation are calculated as presented in the library functions `Snow` and `ice`.

Potential evapotranspiration Actual evapotranspiration is the balance between atmospheric demand of water (potential evapotranspiration) and water supply by the surface. Implemented concepts for the calculation of daily potential evapotranspiration (default: Thornthwaite):

- Thornthwaite
- Priestley and Taylor
- Penman

Interception Both, rainfall and irrigation are subject to interception. The amount of water that can be intercepted depends on:

- vegetation coverage
- vegetation specific interception capacity

The interception capacity is defined as the moisture quantity a plant species can harbour on the stems and at the foliage system (see `Interception capacity`).

All water that is not intercepted feeds into surface water from where it either infiltrates into the soil or is subject to lateral runoff.

Intercepted water contributes to total evapotranspiration. Leaf water evaporation equals the minimum of leaf water and potential evapotranspiration.

Remaining leaf water is redistributed depending on leaf area

Transpiration Update soilwater content due to transpiration.

Model options /n a) model configuration transpiration = true: water content is updated /n

b) model configuration transpiration = false: water content has been updated by external model

Minimum rule

- The water potentially used for transpiration (*pottrans*) is taken as the minimum value of the potential transpiration (provided by the physiology module, see Potential transpiration) and the potential evaporation (see Potential evaporation), reduced by evaporation of intercepted water. Both potential values are derived as daily averages. Therefore, transpiration occurs in the model also at night.
- Rooting depth and root mass or root length distribution are taken into account. The latter can be set with the site parameter ROOT_LENGTH_H2O_UP. As the default, the mass is used.
- The potentially available water in a layer (wc-wcmin) is reduced by soil properties (clay, organic carbon), resulting in an reduced available water amount.

1) By iterating rooted layers, determine:

- the total available soil water for uptake by transpiration (from field capacity to residual water)
- a value reflecting the sum of inverted soil water potentials (indicating the relative effort needed for water extraction)
- the fine root density sum (indicating relative extraction capacity).

2) Determine the dynamically changing uptake capacity, which is:

- decreasing with decreasing soil water content (considering a threshold value of relative available soil water content)
- increasing with increasing plant water deficit (nighttime driver)
- increasing with increasing transpiration demand (daytime driver).

3) Calculate actual uptake:

$$up_l = \min\left(\frac{c}{\sum_l c} * pottrans, H2Oavailableforuptake_l\right)$$

The soil water reservoirs are decreased accordingly. The routine iterates from top to bottom.

Transpiration after Couvreur This function is called if `ROOT_WATER_UPTAKE_COUVREUR = true (false)` and model configuration `transpiration = true`.

It updates the soil water content regarding the root water uptake for transpiration. The root water uptake is modeled by the Couvreur model (first derived in 3d Couvreur et al. (2012), 1d in Couvreur et al. (2014), in the notation in Ref. Cai et al. (2018) for every plant species individually. The potential transpiration is split up for different species by the mass fractions. As species parameters `KRSINIT`, `KCOMPINIT`, `FRTMASSINIT`, and `HLEAFCRIT` = **-16000cm** (constant by stomatal regulation) enter.

An effective soil water pressure head ($h < 0$ for unsaturated soil, [L][cm]) is determined by

$$h_{eff} = \sum_{sl=0}^{deepestrootedlayer} h(sl) \cdot frcfrts(sl)$$

The water potentials are determined via the van-Genuchten parametrisation.

The hydraulic conductivities of the root system K_{rs} [m/m/h] and for compensation K_{comp} [m/m/h] scale linearly with the root biomass in respect to the initial root biomass `FRMASSINIT`. The parameters for initialisation relate to the same plant stage/time.

$$K_{rs} = KRSINIT \cdot m_{frts} / FRTMASSINIT \quad K_{comp} = KCOMPINIT \cdot m_{frts} / FRTMASSINIT.$$

They can be understood as the volumetric fraction of water, which is extracted in an hour.

The root water uptake, as the intensive volumetric water fraction [m/m/timestep], from every layer is calculated by

$$S(sl) = (K_{rs} \cdot (h_{eff} - h_{leaf}) + K_{comp} \cdot (h(sl) - h_{eff})) \cdot \frac{massfrts(sl)/layerwidth}{massallfrts}.$$

In contrast to Cai 2017, we therefore use the fine root mass density fractions instead of the normalised root length density.

The potentially used water for transpiration (T_{pot}) is provided by another module (physiology). The pressure head of the leaves is derived from the potential transpiration, as long as this value remains above the critical leaf water pressure head `HLEAFCRIT`.

$$\tilde{h}_{leaf} = h_{eff} - \frac{T_{pot}}{K_{rs}}$$

- a) If $\tilde{h}_{leaf} > HLEAFCRIT$, it is $h_{leaf} = \tilde{h}_{leaf}$, then $T_{act} = T_{pot}$,
- b) otherwise $h_{leaf} = HLEAFCRIT$, then $T_{act} < T_{pot}$.

The values `wcmin` and `wcmax` are not used with this root water uptake model, but the water potentials related to the Van-Genuchten parameters. In contrast, in PlaMox, for the drought stress factor, which enters photosynthesis, `wcmin` and `wcmax` are used. Therefore,

if the hydraulic conductivity of the root system is unrealistically small, or if the Van-Genuchten parameters are not chosen in accordance to w_{min} and w_{max} , the actual transpiration can be smaller than the potential transpiration without the photosynthesis being affected from this. The Van-Genuchten parameters and w_{min} , w_{max} should be initialised consistently in the site file.

Evaporation

Evaporation from surface water If the potential evapotranspiration (from $CalcPotEvapoTranspiration()$ and reduced by evaporation from intercepted water, transpiration and evaporation from snow) is not yet zero, and if there is water remaining at the surface, water from this remaining surface water evaporates.

If the potential evapotranspiration is larger than the surface water, all the surface water evaporates.

If the amount of surface water is larger than the potential evapotranspiration, the potential evapotranspiration is reached as the actual evapotranspiration and some surface water still remains.

Snow evaporation Snow decrease from evaporation (original in unit: $evaporation_of_snow$) Since potential evaporation is 0 at freezing temperatures, snow evaporation occurs only for snow that can not melt fast enough. If there is more evaporation than can be expected with the sum of gross potential evaporation, hourly foliage evaporation and hourly transpiration, the remaining evaporation is assumed to occur from the snow surface.

Soil water evaporation Water from the soil evaporates

- down to $EVALIM$
- as long as the water content is above wilting point

$$\theta(sl) = WCDNDC_EVALIM_FRAC_WCMIN \cdot \theta_{wp}(sl)$$

- potential evapotranspiration is larger zero

Amount of water evaporating from a soil layer sl :

$$\frac{dE}{dT} = \text{bound} \left(0, \frac{potevapotrans}{EVALIM} \cdot limitwi \cdot \max \left(0, 1 - \frac{\min(EVALIM, depth(sl))}{EVALIM} \right), \theta(sl) \cdot limitwi \right)$$

- $potevapotrans$: water for potential evapotranspiration

- limiting factor for soil water infiltration $limitwi$:

$$limitwi = \begin{cases} 0, & \theta(sl) < wcminevap(sl) \\ \min \left(\left(\frac{wc(sl) - wcminevap(sl)}{wcmax(sl)} \right)^{clayfact}, 1 \right), & \text{else} \end{cases}$$

- factor including further soil properties

$$clayfact = 1 + SLOPE_CLAYF \cdot \min(1 - forg(sl), clay(sl))$$

- $forg(sl)$: fraction of organic matter

Comments:

- The water available for evapotranspiration is distributed homogeneously over all soil layers from which water potentially evaporates (down to EVALIM). The amount of water actually evaporating from every layer is further reduced linearly with the layer depth.
- Soil water evaporation for every layer takes place after the downwards percolation from that layer.

Soil water flow

Infiltration For the top soil layer, water inflow equals total surface water. For deeper soil layers, water inflow equals water outflow of the overlying soil layer.

Groundwater interaction For soil layers lying within the groundwater table, water flow out of the layer equals water inflow. In this way, soil water is discharged with groundwater with the percolation flow rate of the soil layer above the groundwater table.

Water flow at bottom If the last soil layer is above the groundwater, water flow out of the domain is given by:

1. Fully saturated conditions
Saturated hydraulic conductivity
2. Water content below saturation and above field capacity ($\phi > \theta > \theta_{fc}$)
Water flow is calculated in the same way as for all other soil layers (see below)
3. Water content between field capacity and wilting point ($\theta_{fc} > \theta > \theta_{wp}$)
Water flow out of the layer is calculated depending on the flow into the layer:
 $q_{out} = FPERCOL \cdot q_{in}$
4. Water content below wilting point ($\theta_{wp} > \theta$)
No flow

Water flow within domain Calculation of water flow out of soil layer is distinguished for different water contents:

1. Fully saturated conditions
Saturated hydraulic conductivity
2. Water content below saturation and above field capacity ($\phi > \theta > \theta_{fc}$)
See Water flow above field capacity
3. Water content between field capacity and wilting point ($\theta_{fc} > \theta > \theta_{wp}$)
See Water flow below field capacity
4. Water content below wilting point ($\theta_{wp} > \theta$)
No flow

Water flow above field capacity Water flow from layer sl to the layer $sl + 1$ below:

$$q = \left(1 - \frac{\theta_{fc}(sl)}{\theta(sl)}\right)^2 \cdot \theta(sl) \cdot \left(1 - e^{\frac{1}{\log(sks)}}\right) \cdot factimpedence$$

Water flow below field capacity Water flow from layer sl to the layer $sl + 1$ below:

$$q = \left(\frac{\theta(sl)}{\theta_{fc}(sl)} - \frac{\theta(sl+1)}{\theta_{fc}(sl+1)}\right) \cdot \theta(sl) \cdot \left(1 - e^{\frac{1}{\log(sks)}}\right) \cdot factimpedence$$

Capillary rise Similar to WaterFlowBelowFieldCapacity but restricts water flow by water availability from soil layer below

Preferential flow ...

Impedance Percolating water is delayed by an impedance factor, which considers the formation of ice lenses in (partially) frozen soil [Lundin (1990), Hansson et al. (2004).] The impedance factor depends on the parameter IMPEDANCE_PAR = 0.

- If no ice is present the impedance factor is 1 and no reduction occurs.
- If IMPEDANCE_PAR = 0 the impedance factor is 1 as well and no reduction occurs.

Surface runoff The surface flux gives the water, which runs off horizontally. This only happens if more water than stopped by the bunding (bund height is set in flooding events) is present.

- If the bund height > 0 : All water above the bund height runs off immediately.
- If the bund height $== 0$:

The fraction of water running off is determined by the site parameter FRUNOFF.

- If a time step is 24h (daily simulation), FRUNOFF corresponds to the fraction of water running off in these 24h. Hence, $FRUNOFF = 1$ corresponds to a complete run off, i.e. 100% of the surface water
- If a time step is 1h (hourly simulation), only the fraction $FRUNOFF/24$ runs off in this time step, the rest of the water remains as surface water for the next time step. For an hourly time step a complete run off corresponds to $FRUNOFF = 24$. A run off of 50% would be $FRUNOFF=12$.

1.0.3.4 waterlibs

Interception capacity Interception capacity I_c is given by:

$$I_c = m_{wood,above} \cdot MWWM + LAI \cdot MWFM$$

Author

- David Kraus

Date

13 Nov, 2017

Potential transpiration

Potential transpiration for non-woody plants This function calculates the potential transpiration T_{pot} (water in kg). Therefore, it is assumed that the loss of water is directly related to the gain of carbon (by photosynthesis):

$$T_{pot} = \frac{carbon_uptake \cdot scale}{wue}$$

$$wue = WUECMAX \cdot \frac{mc}{mco2}$$

$$scale = 1.3 - 0.0009 \cdot co2$$

with:

- carbon_uptake: CO2 uptake by photosynthesis [kg m-2 ground]
- mco2, mc: molar masses of CO2 and carbon, respectively [g mol-1]
- co2: CO2 concentration of the air [ppb]
- WUECMAX: parameter describing the species-specific water use efficiency [mgCO2 gH2O-1]

The function assumes an increase in carbon uptake efficiency (a decrease of water loss per unit carbon uptake) with increasing CO2 concentration in the air.

Potential transpiration for woody plants based on water use efficiency Similar as for non-woody plants, the potential transpiration T_{pot} for woody plants is assumed to correlate with the gain of carbon by photosynthesis. The water use efficiency, however, is allowed to vary with vapor pressure deficit Aber and Federer (1992) as well as relative available soil water. This accounts for the frequent observation that the efficiency of carbon uptake increases with increasing evaporation demand and decreasing water supply.

$$T_{pot} = \frac{\text{carbon_uptake}}{wue}$$

$$wue = \frac{wuec \cdot mc / mco2}{vpd}$$

$$wuec = (WUECMAX - WUECMIN) \cdot \text{sum}(rwa_sl \cdot \frac{h_sl}{rd})$$

$$rwa_sl = \frac{wc_sl - wc_wp_sl}{wc_fc_sl - wc_wp_sl}$$

with:

- sl: soil layer indicator for all layers within rooting depth
- vpd: vapor pressure deficit [kPa]
- carbon_uptake: CO2 uptake by photosynthesis [g m-2 ground]
- mco2, mc: molar masses of CO2 and carbon, respectively [g mol-1]
- rwa: relative available water
- h: height of a soil layer [m]
- rd: rooting depth [m]
- wc: water content in a soil layer [mm m-3]
- wc_fc: field capacity [mm m-3]

- `wc_wp`: wilting point [mm m-3]
- `WUECMAX`, `WUECMAX`: parameter describing the species-specific maximum and minimum water use efficiency respectively [gCO2 kgH2O-1]

Note

Transpiration demand is limited by potential evaporation determined from climatic factors.

Potential transpiration for woody plants based on stomatal conductance The potential transpiration stream (in m hr-1) is calculated from canopylayer-specific stomatal conductance and the vapor pressure deficits in each layer Jarvis and McNaughton (1986). These layered values are added up to scale to the whole-canopy. The canopylayer-specific transpiration tr_{fl} is thus calculated as:

$$tr_{fl} = \frac{vpd_{fl}}{P_{atm}} c_{fl} lai_{fl}$$

With stomatal conductance c_{fl} is either:

$$c_{fl} = GS_{MIN} + relativeconductance_{fl} (GS_{MIN} - GS_{MAX})$$

if stomatal conductance is not directly calculated, or:

$$c_{fl} = GS_{MIN} + frad_{fl}(gs_{fl} - GS_{MIN})$$

if stomatal conductance has been determined by the Berry Ball method.

with:

- `fl`: canopy layer indicator
- `vpd`: vapor pressure deficit
- `lai`: leaf area index
- `Patm`: atmospheric air pressure
- `GSMIN`, `GSMAX`: species-specific parameters for minimum (cuticular) and maximum stomatal conductance

This option is chosen in the setup file by selecting `transpirationmethod="potentialtranspiration"` (see Model options).

Layered water pressure head Returns the water pressure head [cm] of a specific soil layer: matrix h_m + gravitational/elevation h_g . The result is given in cm.

- h_m is determined by the van Genuchten equation of the water retention curve for the soil WITHOUT stones.
- $h_g = layerdepth$, [cm], (only relevant for moist soils close to field capacity)

Snow and ice calculations (SnowDNDC) Includes snow and ice formation and melting at the surface and soil layers as well as the resulting soil temperature changes.

Snowpack formation and melting All precipitation is assumed to be snow when air temperature is less or equal a given temperature limit (SNOWFALL_TEMPERATURE_LIMIT). It can be intercepted by the canopy, but otherwise accumulates at the soil surface.

When air temperatures (t_{air}) exceeds a limit temperature ($TLIMIT = 0$ oC), snow melts with a rate depending on air temperature and an empirical parameter $MCOEFF$:

$$\Delta\theta_{snow} = MCOEFF \cdot (t_{air} - TLIMIT)$$

Soil ice formation and melting Soil ice formation occurs when soil temperature T_{soil} drops below ice temperature T_{ice} . The amount of ice $\Delta\theta_{ice}$ that is formed depends on the enthalpy of ice formation H_m and the energy release Q_r , which is calculated by the difference between ice and soil temperature multiplied by the heat capacity of the wet soil:

$$\begin{aligned} Q_r &= (T_{ice} - T_{soil}) \cdot C_{p,wetsoil} \\ \Delta\theta_{ice} &= \frac{Q_r}{H_m} \end{aligned}$$

The change of soil temperature due to energy release is hence given by:

$$\Delta T = \frac{\Delta\theta_{ice} H_m}{C_{p,wetsoil}}$$

Soil ice melting occurs for $T_{soil} > 0$ oC. The amount of melted ice and associated energy uptake is given by:

$$\begin{aligned} Q_u &= T_{soil} \cdot C_{p,wetsoil} \\ \Delta\theta_{ice} &= -\frac{Q_u}{H_m} \end{aligned}$$

The change of soil temperature due to energy uptake is hence given by:

$$\Delta T = \frac{\Delta\theta_{ice} H_m}{C_{p,wetsoil}}$$

Heat capacity of the (wet) soil $C_{p,wetsoil}$ is calculated by heat capacity values of its components, i.e., soil organic matter, mineral soil, water and ice (air is neglected):

$$\begin{aligned} C_{p,wetsoil} &= C_{p,drysoil} + C_{p,water} + C_{p,ice} \\ C_{p,drysoil} &= (c_{p,som} \cdot c_{som} + c_{p,min} \cdot (1 - c_{som})) \cdot m_{soil} \\ C_{p,water} &= c_{p,water} \cdot m_{water} \\ C_{p,ice} &= c_{p,ice} \cdot m_{ice} \end{aligned}$$

Ice temperature Ice temperature T_{ice} depends on the ratio of ice and water mass and the parameter $TICE$:

$$T_{ice} = TICE \cdot \frac{m_{ice}}{m_{water}}$$

Potential evaporation

Penman

Authors

- Daniel van Kraalingen (original version Van Kraalingen and Stol (1997))
- David Kraus (implementation into LandscapeDNDC)

The underlying principle is that the energy between radiation, heat flux, and vaporizing water is balanced. It is set up for grass. For higher growing crops it should be adapted by a Penman crop factor in the original version. In the present implementation, the lai fulfils this role to some extend.

The **albedo** (reflection coefficient) a is determined by distinguishing

- dry soil (water table of less than 0.005mm): $rfs = 0.25 \cdot (1 - 0.5 \cdot watersaturation)$
- wet soil (water table of more than 0.005mm): $rfs = 0.05$

$$a = rfs \cdot \exp(-0.5 \cdot lai) + 0.25 \cdot (1 - \exp(-0.5 \cdot lai))$$

This equation represents, that the background (soil or water) is shielded by the crop/grass. In Van Kraalingen and Stol (1997) the albedo is a fixed parameter. The size of the plant is taken into account by the crop coefficient curve.

Net radiation R_n is given by:

$$R_n = (1 - a)R_{shortwave} + R_{longwave,in} - R_{longwave,out}$$

Evapotranspiration is separated in a radiation and an aerodynamic term:

$$PET = PET_r + PET_d = \frac{1}{\lambda} \left(\frac{\frac{dp_s}{dT} R_n}{\frac{dp_s}{dT} + \gamma} + \frac{\gamma \lambda E_a}{\frac{dp_s}{dT} + \gamma} \right)$$

- λ : latent heat of vaporising water

- γ : the psychrometric constant
- E_a : isothermal evaporation, $E_a = f_w \cdot (p_s(T_2) - p_2)$
- $p_s(T_2)$: saturated vapour pressure at the temperature at 2m height
- p_2 : vapour pressure at 2m height

Saturated vapour pressure

Saturated vapour pressure p_s and respective derivative with respect to temperature are given by:

$$\begin{aligned} p_s &= 0.61 \cdot e^{\left(\frac{17.32 \cdot T}{T + 238.102}\right)} \\ \frac{dp_s}{dT} &= 238.102 \cdot 17.32 \cdot \frac{p_s}{(T + 238.102)^2} \end{aligned}$$

Wind function

The wind function is chosen depending on the surface type.

Bare soil Van Kraalingen and Stol (1997) :

$$f_w = 2.63 \cdot (0.5 + 0.54v_w)$$

Short grass Van Kraalingen and Stol (1997) :

$$f_w = 2.63 \cdot (1.0 + 0.54v_w)$$

- v_w : wind speed

Priestley and Taylor The Priestley-Taylor evapotranspiration is a simplified Penman method. It is based on the assumption that the radiation driven part of evapotranspiration dominates. Therefore, it uses only the radiation driven part of the Penman equation and an empirical coefficient $\alpha_{PT} = 1.1$, which adapts the radiation term for the neglected aerodynamic term:

$$PET = \alpha_{PT} \frac{1}{\lambda} \frac{R_n s}{s + \gamma},$$

wherein λ and γ refer to the latent heat of vaporization and the psychrometric constant, respectively. This method should work well for humid and semi-arid climates. It fails, when net radiation gets negative (as in Dutch winters). It is set up for short grass. If one wants to use it for crops, the result should (originally) be multiplied by a Penman crop factor. Instead, in the present implementation, the lai is included in the albedo.

The slope of saturation vapor pressure for changing temperature at the temperature at 2m height is estimated by:

$$s = vps \cdot \frac{4098}{\sqrt{T + 237.3}}$$

Net radiation R_n is given by:

$$R_n = (1 - a)R_s + R_{l,in} - R_{l,out}$$

- The albedo a is determined in the same way as for Penman.

For more details, see Van Kraalingen and Stol (1997).

Thornthwaite Daily potential evapotranspiration PET [m] after Thornthwaite (1948) with additions from Willmott et al. (1985) is calculated depending on temperature by:

$$\begin{aligned} PET(T > 37.5) &= -415.85 + 32.24 \cdot 37.5 - 0.43 \cdot 37.5^2 \\ PET(37.5 \geq T > 26) &= -415.85 + 32.24 \cdot T - 0.43 \cdot T^2 \\ PET(26 \leq T) &= 16 \cdot \left(10 \cdot \frac{T}{h_i}\right)^{0.49239+0.0179h_i-0.0000771h_i^2+0.000000675h_i^3} \end{aligned}$$

These formulas give monthly values for an average of 12 hours daylight. They are corrected to the appropriate number of hours and divided to a daily value.

Depending on the heat index h_i there can be a jump at 26degreeC (maybe of 2mm per day).

The method is purely empirical.

The Thornthwaite heat index h_i is given by:

$$h_i = \sum_m (0.2 \cdot T_m)^{1.514}$$

The monthly temperature T_m is derived from the annual mean temperature T_a :

$$T_m = -0.5 \cdot T_a \cdot \cos\left(2\pi \frac{d_m}{d_y}\right)$$

wherein d_m and d_y refer to the midmonth day of year and total number of days per year, respectively.

1.0.4 Vegetation

- Vegetation global state
- ArableDNDC
- GrasslandDNDC
- PlaMox - Plant Growth Model
- PSIM - Physiological Simulation Model

- PnET tree plantation model
- TreeDyn - Tree dimensional Dynamics
- PhotoFarquhar - Farquhar Photosynthesis
- Vegetation Libraries
- MoBiLe Plant

1.0.4.1 Vegetation global state

Initialisation

1.0.4.2 ArableDNDC

User guide The crop growth model ArableDNDC originates from the DNDC Model (Li et al. (1994)). ArableDNDC simulates the carbon and nitrogen cycle of crops. Processes are described in a universal way and plants are primarily distinguished by species-specific parameters that can be accessed and calibrated externally. Dynamics of plant carbon (C) and nitrogen (N) are primarily calculated based on temperature driven crop development and associated N demand and N uptake/fixation.

Model structure ArableDNDC can be either run in subdaily or daily time resolution.

Parametrization The following lists includes species parameters that might be calibrated in order to represent a specific plant. See the description of respective sections for more details on parameter behaviour.

Nitrogen related parameters:

- nc_fruit_max (optimum nitrogen content of the fruit)
- nc_fruit_min (minimum nitrogen content of the fruit)
- nc_fineroots_max (optimum nitrogen content of fine roots)
- nc_fineroots_min (minimum nitrogen content of fine roots)
- nc_structural_tissue_max (optimum nitrogen content of structural tissue)
- nc_structural_tissue_min (minimum nitrogen content of structural tissue)
- nc_foliage_max (optimum nitrogen content of foliage)
- nc_foliage_min (minimum nitrogen content of foliage)

Allocation related parameters:

- `fraction_root` (root fraction of total biomass at maturity)
- `fraction_fruit` (fruit fraction of total biomass at maturity)
- `fraction_foliage` (foliage fraction of total biomass at maturity)

Plant development related parameters:

- `gdd_base_temperature`
- `gdd_max_temperature`
- `gdd_maturity`
- `gdd_grain_filling`
- `gdd_flowering`

Drought

- `h2oref_a` (determines drought resistance)

Nitrogen uptake

- `tlimit` (minimum temperature required for nitrogen uptake)
- `k_mm_nitrogen_uptake` (root affinity to soil nitrogen)

Nitrogen fixation

- `ini_n_fix` (fraction of total nitrogen that might be fixed)

Respiration

- `maintenance_temp_ref` (reference temperature for maintenance respiration)
- `mc_root` (maintenance respiration coefficient for roots)

Root exsudation

- `doc_resp_ratio` (ratio of doc exsudation in relation to root respiration)

Senescence

- senescence_drought (coefficient of senescence related to drought)
- senescence_frost (coefficient of senescence related to frost)
- senescence_age (coefficient of senescence related to age)

Fineroots turnover

- tofirtbas

water demand

- wuecmax (water use efficiency)

Structure

- exp_root_distribution (coefficient for exponential root distribution)
- height_max (maximum plant height)

Transpiration Calculates potential transpiration on

a) water use efficiency and carbon uptake: potential_crop_transpiration()

Roots Roots are described by the rooting depth, which grows linearly with $GZR \leftrightarrow TZ$ (default 1cm/day) up to a maximum value ZRTMC (default 1m) (see Fine root distribution). The distribution of fine roots follows a sigmoid function (see Sigmoid root distribution).

Crop development Crop development is determined by growing degree days GDD :

$$DVS = \frac{GDD}{GDD_{max}}$$

Vernalization

Growing degree days are only upgraded for:

$$\begin{aligned} T & \stackrel{!}{>} \max(0, \Psi_{TLIMIT}) \\ GDD & \stackrel{!}{<} \Psi_{GDD_MATURITY} \end{aligned}$$

Nitrogen demand and crop growth Carbon assimilation on biomass growth are calculated depending on nitrogen demand and uptake.

Nitrogen Uptake Crops are able to take up NO_3^- and NH_4^+ .

1.0.4.3 GrasslandDNDC

User guide The grassland growth model GrasslandDNDC originates from the DNDC Model (Li et al. (1994)). GrasslandDNDC simulates the carbon and nitrogen cycle of grass species only (no crops). Processes are described in a universal way and plants are primarily distinguished by species-specific parameters that can be accessed and calibrated externally.

Model structure GrasslandDNDC can be either run in subdaily or daily time resolution.

Parametrization The following lists includes species parameters that might be calibrated in order to represent a specific plant. See the description of respective sections for more details on parameter behaviour.

Nitrogen related parameters:

- nc_fruit_max (nitrogen content of the fruit)
- nc_fineroots_max (nitrogen content of fine roots)
- nc_structural_tissue_max (nitrogen content of structural tissue)

Allocation related parameters:

- root (assimilated carbon fraction allocated to roots)
- grain (assimilated carbon fraction allocated to the fruit)
- faleaf (determines fraction of carbon that is allocated to leafs)

Plant development related parameters:

- gdd_base_temperature
- gdd_maturity

Drought

- h2oref_a (determines drought resistance)

Nitrogen uptake

- tlimit (minimum temperature required for nitrogen uptake)
- k_mm_nitrogen_uptake (root affinity to soil nitrogen)

Nitrogen fixation

- ini_n_fix (fraction of total nitrogen that might be fixed)

Respiration

- maintenance_temp_ref (reference temperature for maintenance respiration)
- mc_root (maintenance respiration coefficient for roots)

Root exsudation

- doc_resp_ratio (ratio of doc exsudation in relation to root respiration)

Senescence

- senescence_drought (coefficient of senescence related to drought)
- senescence_frost (coefficient of senescence related to frost)
- senescence_age (coefficient of senescence related to age)

Fineroots turnover

- tofrtbas

water demand

- wuecmax (water use efficiency)

Structure

- exp_root_distribution (coefficient for exponential root distribution)
- height_max (maximum plant height)

Cutting and grazing After cutting and grazing events plant development is linearly reduced with nitrogen loss.

$$DVS(t_{i+1}) = \frac{N(t_{i+1})}{N(t_i)} \cdot DVS(t_i)$$

Plant Development Plant development is calculated by growing degree days (GDD):

$$GDD = \sum (T_{avg} - T_{base})$$

Plant development is given by:

$$DVS = \frac{GDD}{GDD_MATURITY}$$

1.0.4.4 PlaMox - Plant Growth Model

User guide PlaMox simulates the carbon and nitrogen cycle of crops and grass species. Processes are described in a universal way and plants are primarily distinguished by species-specific parameters that can be accessed and calibrated externally. However, for a growing number of specific species (e.g., rice, maize, ...), there exist specific functionalities, which are continuously developed.

Model structure PlaMox includes a submodel for photosynthesis calculation based on von Caemmerer and Farquahr 1981. Since the photosynthesis submodel requires a subdaily time step, PlaMox can also only be used with a subdaily time resolution. The recommendation is 24 time steps per day. PlaMox requires further models for:

- watercycle (e.g., transpiration)
- soilchemistry (e.g., nitrogen uptake)
- microclimate (e.g., radiation distribution within the canopy)

Parametrization The following lists include species parameters that might be calibrated in order to represent a specific plant. See the description of respective sections for more details on parameter behaviour.

Photosynthesis:

- *C4_TYPE*

- *VCMAX25* (rubisco activity)
- *SLAMAX* (leaf area)
- *SLADECLINE* (decline of specific leaf area with plant development)

Nitrogen related parameters:

- *NC_FRUIT_MAX* (optimum nitrogen content of the fruit)
- *NC_FRUIT_MIN* (minimum nitrogen content of the fruit)
- *NC_FINEROOTS_MAX* (optimum nitrogen content of fine roots)
- *NC_FINEROOTS_MIN* (minimum nitrogen content of fine roots)
- *NC_FOLIAGE_MAX* (optimum nitrogen content of foliage)
- *NC_FOLIAGE_MIN* (minimum nitrogen content of foliage)
- *NC_STRUCTURAL_TISSUE_MAX* (optimum nitrogen content of structural tissue)
- *NC_STRUCTURAL_TISSUE_MIN* (minimum nitrogen content of structural tissue)

Allocation related parameters:

- *FRACTION_ROOT* (assimilated carbon fraction allocated to roots)
- *FRACTION_FRUIT* (assimilated carbon fraction allocated to the fruit)
- *FRACTION_FOLIAGE* (assimilated carbon fraction allocated to foliage)
- *MFOLOPT* (optimum foliage biomass)

Plant development related parameters:

- *GDD_BASE_TEMPERATURE*
- *GDD_MAX_TEMPERATURE*
- *GDD_STEM_ELONGATION*
- *GDD_FLOWERING*
- *GDD_GRAIN_FILLING*
- *GDD_MATURITY*

Vernalization related parameters:

- *CHILL_TEMP_MAX*
- *CHILL_UNITS*

Cutting

- *SHOOT_STIMULATION_REPROD* (changes root/shoot ratio before first cutting)

Stress

- *H2OREF_A* (determines drought resistance)

Nitrogen uptake

- *TLIMIT* (minimum temperature required for nitrogen uptake)
- *K_MM_NITROGEN_UPTAKE* (root affinity to soil nitrogen)

Nitrogen fixation

- *INI_N_FIX* (fraction of total nitrogen that might be fixed)
- *NFIX_RATE* (maximum daily rate of nitrogen fixation)

Respiration

- *MAINTENANCE_TEMP_REF* (reference temperature for maintenance respiration)
- *MC_LEAF* (maintenance respiration coefficient for leafs)
- *MC_ROOT* (maintenance respiration coefficient for roots)
- *MC_STEM* (maintenance respiration coefficient for stems)
- *MC_STORAGE* (maintenance respiration coefficient for fruit/storage organs)
- *FYIELD* (growth respiration efficiency)

Root exudation

- *DOC_RESP_RATIO* (ratio of doc exudation in relation to root respiration)

Senescence

- *SENESCENCE_DROUGHT* (coefficient of senescence related to drought)
- *SENESCENCE_FROST* (coefficient of senescence related to frost)
- *SENESCENCE_HEAT* (coefficient of senescence related to heat)
- *SENESCENCE_AGE* (coefficient of senescence related to age)
- *FRET_N*

Fineroots turnover

- *TOFRTBAS*

water demand

- *WUECMAX* (maximum water use efficiency under drought conditions)
- *WUECMIN* (minimum water use efficiency under non-drought conditions)

Structure

- *EXP_ROOT_DISTRIBUTION* (coefficient for exponential root distribution)
- *RS_CONDUCT* (conductivity of root aerenchyma)
- *HEIGHT_MAX* (maximum plant height)

Model options Available options: Default options are marked with bold letters.

- Potential nitrogen use (npot: **no** / yes)
- Transpiration method (transpirationmethod: **wateruseefficiency** / stomatalconductance)
- Drought stress switch (droughtstress: no / **yes**)
- Drought stress method (droughtstressmethod: uniform / **rootweighted**)
- Considered species (plantfamilies: **crops grass**)

Management Considered field mangement includes:

- Planting
- Harvest
- Grazing
- Cutting

Planting event For planting events, the following event inputs are considered:

- Plant type and name
- Initial biomass

All other quantities are determined by the model:

- Annual nitrogen fixation is assumed to be zero at planting
- Plant development index and growing degree days are set to 0
- Tissue nitrogen concentration is set to optimum

The N-contents of fine roots, foliage, and structural tissue are set to optimum (parameters NC_FINEROOTS_MAX, NC_FOLIAGE_MAX, and NC_STRUCTURAL_TISSUE_MAX). Mass is only distributed to fine roots and foliage by FRACTION_ROOT and 1 - FRACTION_ROOT.

Harvest event For harvest events, the following event inputs are considered:

- Export root wood
- Remains
- Stubble height

The term wood with regard to the export of roots is neglected and all root parts are considered. The fraction given as remains determines the fraction of straw that remains on the field. If there is not remains fraction given, the amount of straw can be determined via stubble height. If neither remains nor stubble height are given all aboveground biomass is removed from the field.

Grazing After grazing the development index of the plant is set to 0.

Cutting After cutting the development index of the plant is set to 0.

Phenology Phenology of plant growth depends on the plant development stage DVS , which is defined between 0 (germination) and 1 (maturity).

Growing degree days Plant development depends on accumulated growing degree days $AGDD$, which is the sum of growing degree days over the complete vegetation period:

$$AGDD = \sum GDD$$

Growing degree days depend on daily mean temperature and a species-specific base temperature:

$$GDD = (T_{avg} - GDD_BASE_TEMPERATURE) f_{chill}$$

The factor f_{chill} retards plant development due to insufficient vernalization (see: vernalization).

Plant development $\frac{dDVS}{dt}$ is given by:

$$\frac{dDVS}{dt} = \frac{GDD}{GDD_MATURITY}$$

In addition to DVS , there exists a mortality state index MOS that is calculated in the same way as DVS but interpreted differently and not reset after grazing and cutting events.

Emergence Emergence is regulate by accumulated growing degree days $AGDD$, drought stress and snow. Three conditions must be satisfied for emergence:

$$AGDD > GDD_EMERGENCE f_h 2o > H2OREF_FLUSHING_{snow} < 0.01[m]$$

In case $GDD_EMERGENCE$ is not defined, the plant development index must be greater 5%

Vernalization Vernalization is only implemented for crops. The following species-specific parameters determine vernalization:

- $CHILL_UNITS$
- $CHILL_TEMP_MAX$
- $GDD_FLOWERING$

The state of chilling if calculated following Haenninen (1990) (see: Vernalization).

Allocation Allocation of assimilated carbon and nitrogen is determined by the plant development stage *DVS*. PlaMox distinguishes the following compartments:

- Fruit / Reserves (θ_{fruit})
- Roots (θ_{root})
- Stem (θ_{stem})
- Leaves (θ_{leaf})

Crops

Fruit fraction The fruit fraction θ_{fruit} generally is given by:

$$\theta_{fruit} = \begin{cases} 0 & AGDD \leq GDD_GRAIN_FILLING \text{ AND } m_{fruit} < m_{fruit,pot} \\ 1 & \text{ELSE} \end{cases}$$

The potential fruit biomass $m_{fruit,pot}$ at a given time step is given by:

$$m_{fruit,pot} = \frac{AGDD - GDD_GRAIN_FILLING}{GDD_MATURITY - GDD_GRAIN_FILLING} \cdot M_FRUIT_OPT \cdot \phi_{heat}$$

If there was heatstress during the flowering phase, the potential fruit fraction is reduced by the heat factor ϕ_{heat} (see: Heat Stress Limitation)

Root fraction The default root fraction θ_{root} is given by:

$$\theta_{root} = (1 - \theta_{fruit}) \frac{FRACTION_ROOT}{1 - FRACTION_FRUIT}$$

For some species families specific calculations exist:

- Rice

$$\theta_{root}^* = (1 - DVS) \cdot FRACTION_ROOT_START + DVS \cdot FRACTION_ROOT$$

$$\theta_{root} = \begin{cases} (1 - \theta_{fruit})0.8 & \frac{m_{fruit}}{m_{total}} < \theta_{root}^* \\ (1 - \theta_{fruit})\theta_{root}^* & \text{ELSE} \end{cases}$$

According to Yoshida (1981), root fraction of rice declines from about 20% at seedling stage to 10% at maturity.

- Corn

$$\theta_{root} = FRACTION_ROOT_START \cdot (1 - DVS)^{1.7} + DVS \cdot FRACTION_ROOT$$

Using $FRACTION_ROOT_START = 0.4$ and $FRACTION_ROOT = 0.15$, this function can be fitted to the mean root-shoot ratio RS reported by Amos and Walters (2006) :

$$RS = 0.45 \cdot (0.15 + 0.5 \cdot e^{-3 \cdot DVS}) .$$

- Rapeseed

$$\theta_{root} = \begin{cases} FRACTION_ROOT_START \cdot \frac{GDD_GRAIN_FILLING - AGDD}{GDD_GRAIN_FILLING} \cdot (FRACTION_ROOT_START + FRACTION_ROOT) \\ FRACTION_ROOT \end{cases}$$

Using $FRACTION_ROOT_START = 0.25$ and $FRACTION_ROOT = 0.05$, this function can be approximately fitted to a root-shoot ratio RS of 0.3 at planting declining to 0.05 at onset of grain filling as reported by Robertson and Lilley (2016)

- Milt
- Sorg
 - Wheat

$$target_{root} = 1 - DVS \cdot 0.5 + DVS \cdot FRACTION_ROOT$$

$$value_{root} = \frac{fineroots}{total_biomass}$$

If the target biomass is larger than the current value,

$$\theta_{root} = target_{root}$$

Stem and leaf fraction

- If the number of growing degree days is larger than $GDD_STEM_ELONGATION = 0$ (for crops), no C is allocated to stems, but only to leaves.
- Otherwise, and in case of drought, no C is allocated to leaves. Instead it goes into stems.
- Otherwise, and without drought, it is

$$\theta_{stem} = (1 - \theta_{fruit} - \theta_{root}) \cdot (1 - FAL EAF) \theta_{leaf} = 1 - \theta_{fruit} - \theta_{root} - \theta_{stem}$$

where $FAL EAF$ is the fraction of straw (leaves + stems) forming leaves.

Grass

The reserve/fruit fraction (θ_{fruit}) increases linearly with the plant development in accordance to $FRACTION_FRUIT$:

$$\theta_{fruit} = DVS \cdot FRACTION_FRUIT$$

A cutting event influences the root/shoot ratio by a factor γ_{roots} (here determined by the fraction of roots θ_{roots}):

- Before the first cutting of the year:

$$\gamma_{roots} = \frac{1.0}{1.0 + SHOOT_STIMULATION_REPROD}, \text{ with } SHOOT_STIMULATION_REPROD = 0$$

- After the first cutting of the year:

$$\gamma_{roots} = 1.0$$

The root fraction is given by:

$$\theta_{roots} = (1.0 - \theta_{fruit}) \frac{\gamma_{roots} FRACTION_ROOT}{1 - FRACTION_FRUIT - (1 - \gamma_{roots}) FRACTION_ROOT}$$

As a default or after the first cutting of the year it is

$$\theta_{roots} = \frac{1.0 - \theta_{fruit}}{1 - FRACTION_FRUIT} \cdot FRACTION_ROOT.$$

If the current root mass is higher than predicted by the allocation factor, the root allocation factor is decreased exponentially.

The straw fraction is given by

$$FRACTION_STRAW = 1 - \theta_{roots} - \theta_{fruit}.$$

The current foliage to straw ratio is given by

$$f_{aleaf} = \frac{m_{fol}}{m_{fol} + m_{stem}}.$$

If the foliage biomass, m_{fol} , is 0, $f_{aleaf} = 0$.

Bud emergence Translocation of stored carbon from buds to foliage, e.g., during spring, after defoliation (grazing, cutting)

Redistribution If some reserves exist in the stem and after grain filling, some biomass from the stem goes into the grain (reproductive tissue).

Photosynthesis Actual photosynthesis is calculated by the external model Photo↔Farquhar (Berry Ball). This requires the canopy height specific information of:

- Rubisco activity
- Electron transport
- Photorespiration

The latter two quantities are calculated depending on the rubisco activity and with the species specific parameters QJVC (Maximum electron transport rate and RubP saturated rate of carboxylation) and QRD25, respectively.

The rubisco activity depends on the species specific parameter VCMAX25 (Maximum RubP saturated rate of carboxylation at 25oC for sun leaves). Further, the following properties are factored in:

- Severe drought stress reduces enzyme activity
- Plant age reduces enzyme activity
- Temperature: Heat and frost stress
- Nitrogen availability

Nitrogen uptake Nitrogen availability can be dependent on location specific N-distribution. Only the share ϕ_L of total N that is either located close to the plant or that is homogeneously distributed is available.

Daily nitrogen demand is calculated by:

demand = n_opt() – total plant nitrogen

After maturity the N uptake is reduced linearly to zero with increasing GDD.

Nitrogen uptake is calculated for every layer individually. Only layers containing roots are considered.

Temperature dependency of N uptake is given by:

$$\phi_T = \begin{cases} 0, & T < 0.8 \cdot TLIMIT \\ \frac{t - 0.8 \cdot TLIMIT}{TLIMIT - 0.8 \cdot TLIMIT}, & 0.8 \cdot TLIMIT < T < TLIMIT \\ 1, & T > TLIMIT \end{cases}$$

Nitrogen uptake of N_x (NH4, NO3, DON) is determined by

$$\frac{dN_x}{dt} = US_N_x \cdot plant_available_n \cdot m_{roots} \cdot \phi_L \cdot \phi_T \frac{N_x}{N_x + K_MM_NITROGEN_UPTAKE},$$

where $m_{\{roots\}}$ is the root mass in the soil layer. With environmental roots, the root length rather than the mass is used.

Nitrogen fixation Two different approaches are considered:

- Nitrogen fixation based on potential nitrogen fixation rate under consideration of water availability, temperature and the nodule surface. This approach is chosen as soon as: $NFIX_RATE > 0.0$.
- Nitrogen fixation based on total fixable nitrogen (TFN) amount and plant development. This approach is chosen as soon as: $NFIX_RATE = 0.0$ and $INI_N_FIX > 0.0$.

Approach $NFIX_RATE > 0.0$

- **Plant N demand:**

$$- N_{demand} = N_{optimum} - N_{plant}$$

See also

$$n_opt()$$

- **Water availability** Sinclair (1986)

$$- f_w = \text{NitrogenFixation}::\text{get_fact_water}()$$

- **Temperature**

$$- f_t = \text{NitrogenFixation}::\text{get_fact_temperature}()$$

- **Nitrogen availability**

- Hurley Pasture Model (Thornley, 1998)

$$- f_n = \frac{1}{1 + \frac{\text{Fine root nitrogen concentration}}{0.01}}$$

- **Nodule surface:** (Weisz et al., 1985)

- Nodule surface area represented by vegetative plant biomass

- **Actual nitrogen fixation rate:**

- If the plant N demand is > 0 :

* f = Potential N fixation rate * Nodule surface area * Water availability * Temperature * Nitrogen availability

* the carbon costs of the nitrogen fixation are restricted by the fine root biomass and are determined:

· $\text{MIN}(\text{Actual fixation rate} * \text{NFI}_{\text{CEFF}}, 0.99 * \text{Fine root biomass carbon content})$

Approach $\text{INI}_{\text{N}_{\text{FIX}}} > 0.0$

- **Plant N demand:**

$$- \text{N}_{\text{demand}} = \text{N}_{\text{optimum}} - \text{N}_{\text{plant}}$$

See also

$\text{n}_{\text{opt}}()$

- **Total nitrogen demand:**

- f_n = Foliage biomass under optimal, closed canopy conditions (parameter MFOLOPT) * optimum nitrogen concentration of foliage (parameter $\text{NC}_{\leftrightarrow \text{FOLIAGE_MAX}}$)

- **Potential N fixation rate:**

$$- f_{pot} = \text{MIN}(\text{plant development stage} * \text{parameter INI_N_FIX (0-10)} * \text{total foliage nitrogen demand} - \text{the yearly nitrogen fixation, } N_{\text{demand}})$$

- **Fine root carbon costs:**

$$- f_{pot} * \text{carbon use efficiency for nitrogen fixation (parameter NFIX_CEFF)}$$

- **Biological nitrogen fixation** (BNF) happens if the potential N fixation rate > 0 AND fine root carbon costs (total transport and uptake respiration) $<$ total fine root carbon

Respiration **Maintenance respiration** is calculated after Spitters et al. (1989) :

- Maintenance respiration coefficient of leaves, roots, stems and storage organs (parameter MC_LEAF, MC_ROOT, MC_STEM and MC_STORAGE (the latter three are by default chosen differently to Spitters et al. (1989)) are used.
- If the plant is in chilling stadium (`get_chill_factor()`) there is no maintenance respiration.
- Maintenance respiration is based on the cost of metabolic activity (lower temperature, higher age of plant (latter not for grass)):

- **Temperature scale factor:**

$$* f_{ts} = \text{get_frost_factor()} * (2.0^{\{((T - \text{Reference temperature for maintenance respiration})/10)\}} * 1/24)$$

- **Temperature chill factor:**

$$* f_{tc} = f_{ts} * \text{Carbon Content} * \text{get_chill_factor()}$$

– **Reduction with age:**

Maintenance **respiration** is reduced to 50% of daily photosynthesis as long as plant has only little foliage biomass
(guarantees accrue of plant growth)

$$* f_a = \text{MIN}((1.0 - \text{dvsFlush} * 0.5), \text{get_age_factor}()) \text{ for crops}$$

$$* f_a = 1 \text{ for grass species}$$

– **Respiration** is calculated for all compartments separately and then added up to the complete maintenance respiration:

$$* r_{fol} = MC_LEAF \cdot \text{Foliage Biomass} * f_a * f_{tc}$$

$$* r_{root} = MC_ROOT \cdot \text{Fine Root Biomass} * f_a * f_{tc}$$

$$* r_{stem} = MC_STEM \cdot \text{Sapwood Biomass} * f_a * f_{tc}$$

$$* r_{storage} = MC_STORAGE \cdot \text{Bud Biomass} * f_{tc}$$

Growth respiration:

- The fraction of growth respiration (respired C) relative to gross assimilation (assimilated C) *FYIELD* is used to calculate the respired C from the uptaken carbon. The assimilated part goes into biomass, the respired C is used energetically for building this biomass.

$$C_{resp} = \frac{FYIELD}{1.0 - FYIELD} * carbonuptake$$

- The separate growth respiration rates for foliage, sapwood, storage organs (buds), and fine roots are calculated by multiplying C_{resp} with the (static?) fractions of foliage, sapwood, buds, or fine roots.
- A maximum of 90% of the biomass of every compartment is allowed for growth respiration.
Respiration of storage organs is only added if the plant species is a tuber plant (parameter TUBER), which means it has belowground storage organs, otherwise this factor is 0.

Root exudation

- Exudation is modelled as a loss of fine root biomass. The exudation losses are calculated using the parameter *DOC_RESP_RATIO*, which gives the ratio between root exudates and losses from root respiration. The total exudation losses are calculated by

$$C_{loss} = DOC_RESP_RATIO * \text{Belowground Respiration} .$$

- A maximum of 10% of living root biomass is allowed to be used for exudation:
 $C_{maxloss} = 0.1 * \text{Fine Root Biomass} * \text{Carbon Content}$

Senescence Senescence calculates fluxes from living to dead plant tissue separately for above- and belowground plant parts.

Aboveground senescence List of senescence processes affecting aboveground tissue:

- Drought
- Frost
- Heat
- Age

Drought stress

$$\Phi_d = \text{SENESCENCE_DROUGHT} \cdot \phi_d$$

The drought stress factor ϕ_d is given by: Linear relationship

Water stress

$$\Phi_h = \text{SENESCENCE_HEAT} \cdot (1 - \phi_h)$$

The heat stress factor ϕ_h is given by: Heat factor

Frost stress Frost stress for $T < 0$ is given by:

$$\Phi_f = \begin{cases} 0, T \geq 0 \\ \text{SENESCENCE_FROST} \cdot \frac{T}{-20}, -20 < T < 0 \\ \text{SENESCENCE_FROST}, T \leq -20 \end{cases}$$

Heat stress

$$\Phi_h = \text{SENESCENCE_HEAT} \cdot (1 - \phi_h)$$

The heat stress factor ϕ_h is given by: Heat factor

Senescence due to age Grass:

$$\Phi_{a,leaf} = SENESCENCE_AGE \cdot DVS \Phi_{a,stem} = SENESCENCE_AGE \cdot DVS$$

Crops:

$$\Phi_{a,leaf} = SENESCENCE_AGE \cdot \frac{GDD - GDD_GRAIN_FILLING}{GDD_MATURITY - GDD_GRAIN_FILLING} \Phi_{a,stem} = 0.0$$

Belowground senescence List of senescence processes affecting belowground tissue:

- Drought (layer dependent)
- Water (layer dependent)
- Frost (layer dependent)
- Age (layer independent)

For grass only temperature, i.e. frost (layer independent) is considered.

Drought stress

$$\Phi_d = SENESCENCE_DROUGHT \cdot \phi_d$$

Water stress

$$\Phi_w = SENESCENCE_WATER \cdot hypoxia_sl$$

Frost stress Frost stress for $T < 0$ is given by:

$$\Phi_f = \begin{cases} 0, T \geq 0 \\ SENESCENCE_FROST \cdot \frac{T}{-20}, -20 < T < 0 \\ SENESCENCE_FROST, T \leq -20 \end{cases}$$

Age or temperature stress For grass, temperature (frost) stress is the only factor, the parameter is TOFRTBAS.

For non-grass, age is considered (layer independent) similarly to above ground biomass, the parameter is TOFRTBAS.

Transpiration Calculates potential transpiration on

a) water use efficiency and carbon uptake:

- Potentialcroptranspiration

b) stomatal conductance and vapour pressure deficit:

- Potentialtranspiration

If an hourly timestep is chosen, this is done hourly. However, only the accumulated potential transpiration is stored.

Root Structure

Distribution Roots are represented in a one-dimensional way by the fine root mass distribution and the total fine root mass.

Currently available distribution functions for vertical root distribution:

- root depth dependend (see Standard empirical root distribution)
- exponential (see Exponential root distribution)
- sigmoid (see Sigmoid root distribution)

The environmental function is used for *ROOTS_ENVIRONMENTAL = true*. If *ROOTS_ENVIRONMENTAL = false*, the exponential function is used for *EXP_ROOT_DISTRIBUTION > 0*. If *ROOTS_ENVIRONMENTAL = false* and *EXP_ROOT_DISTRIBUTION <= 0*, the sigmoid function is used.

Environmentally/dynamic determined root growth See Sink-strength driven root distribution.

Default static root growth See Empirical root growth distribution

Root conductivity Gaseous conductivity of roots is expressed by an root aerenchyme transport r_{tc} coefficient:

$$r_{tc} = m_r \cdot RS_CONDUCT$$

Ground coverage Ground coverage of grass is always assumed to be 100%

Ground coverage of crops is estimated by lai:

$$gc = \frac{lai^{0.5}}{3}$$

Full cover is reached with a leaf area index of three (FAO).

Specific leaf area weight (sla) Calculates specific leaf area weight sla kg m⁻² in each canopy layer:

- sla is assumed to be homogeneously distributed throughout the whole canopy.
- sla decreases with plant development dvs depending on the species parameter SL↔ADECLINE (mostly **0** or **0.5**)

$$sla = SLAMAX \cdot (1 - dvs \cdot SLADECLINE \cdot dvsMort)$$

For selected species (mungbean, rice, grass), specific formulations exist.

Temperature factor is calculated depending on species parameter TLIMIT = Temperature limit for plant growth

For simplification reasons the soil temperature from the top soiler layer is used instead of the global temperature

- If the temperature $T < (0.9 * TLIMIT)$:

$$- f_t = 0.0$$

- If the temperature $T < (1.1 * TLIMIT)$ for a smother transition:

$$- f_t = T - \frac{(0.9 * TLIMIT)}{(0.2 * TLIMIT)}$$

- All other cases:

$$- f_t = 1.0$$

Common

Heat Stress Limitation If the plant experiences heat stress during the critical time around flowering, the pod set is reduced. The approach follows the ones introduced by Challinor et al. 2005 and Nendel 2011.

The relevant temperature for this heat stress factor is the temperature during the photoactive period (T_d), since it affects the time during which flowers are open.

$$T_d = T_{max} - \frac{T_{max} - T_{min}}{4}$$

(following Mirschel & Wenke (2007)).

Challinor et al. 2005 introduced a variable Temperature threshold T_{crit} dependent on timing and duration of the heat stress during the flowering period.

The daily influence ($heat_d$) of the heat limitation is calculated dependent on the daily fraction of flowers open:

$$heat_{daily} = 1 - \left(\frac{(T_d - T_{crit})}{(T_{zero} - T_{crit})} \right) * frac_flower;$$

The daily fraction of flowers newly opened:

$$frac_flower = openFlowers_{today} - openFlowers_{yesterday}$$

The open Flowers on a specific day after flowering (daf) (Moriondo et al. 2011) :

$$openFlowers = \frac{1}{\left(1 + \frac{1}{0.015-1} * \exp -1.4 * daf\right)};$$

The overall influence on the grain reduction is:

$$influence_heat_reduction_grainfilling = min(heat_{daily})$$

Heat factor Heat factor ϕ_h is given by:

$$\phi_h = 1 - \frac{1}{1 + e^{-2(T_{leaf} - PSNTMAX)}}$$

Nitrogen deficiency Nitrogen deficiency factor ϕ_n is given by:

$$\phi_n = \frac{C_{N,fol}}{C_{N,fol,opt}} N_DEF_FACTOR$$

Aging The age factor is calculated dependend on the growing degree days (GDD) (see vernalization()), the minimum temperature sum for foliage activity onset (parameter GDDFOLSTART) and temperature degree days for full plant development .

For grass:

- If $GDDFOLSTART > GDD$:

$$f_a = 1.0 - \frac{(GDDFOLSTART - GDD)}{GDDFOLSTART}$$

- else: $f_a = 1.0$.

For all other species:

- If $GDD < (0.9 * GDD_MATURITY)$: $f_a = 1.0$

- else:

$$f_a = \max \left(0.0, 1.0 - \frac{GDD - (0.9 * GDD_MATURITY)}{GDD_MATURITY - (0.9 * GDD_MATURITY)} \right)$$

Optimum nitrogen concentration Grass: foliage nitrogen concentration is constant (from species parameter NC_FOLIAGE_MAX)

Crops: foliage nitrogen concentration is highest at planting (NC_FOLIAGE_MAX) and decreases until harvest to NC_FOLIAGE_MIN.

1.0.4.5 PSIM - Physiological Simulation Model

The PSIM runs in sub-daily (hourly) time steps and gets assimilated carbon based on a Farquhar approach Farquhar et al. (1980), calculated in the photofarquhar.cpp, which is considered along with the ideas of Ball et al. (1987) regarding consideration of stomatal conductance (ld_berryball.cpp).

Processes are generally calculated specifically for species (as cohorts containing trees of equal dimensions), canopy- (2-40) and soil layers (individually set in the site properties). In addition, long-living foliage is considered in different age classes.

In the module itself, respiration is considered to originate from either biomass growth, nitrate conversion, or maintenance of different compartments (foliage, fine roots, structural reserves, living wood) and depends on temperature and nitrogen concentrations Cannell

and Thornley (2000). Allocation from net photosynthesis (or nitrogen uptake) into the respective compartments is realized according to its sink strength that is determined from targeted allometric relations and dynamic gain and loss processes Grote (1998). Therefore, the model assumes a certain longevity of each compartment, resulting in an empirically determined senescence.

Specifically, the main physiological processes of carbon and nitrogen in the plant are:

- hydraulic conductance (PSIM_HydraulicConductance)
- growth of new foliage from buds (PSIM_BudBurst)
- senescence (PSIM_Senescence)
- carbon allocation and growth (PSIM_CarAllocation)
- nitrogen allocation (PSIM_NitAllocation)
- respiration (PSIM_Respiration)
- nitrogen uptake (PSIM_NitrogenUptake) Which all are described further down.

In addition, a change in enzymatic capacity is derived indicating a seasonality and stress-dependence of photosynthetic enzyme activity (PSIM_PhotosynthesisRates).

Besides from the photosynthesis input (see PhotoFarquhar), the module depends on variables describing:

- microclimate, i.e. daily average canopy temperature for budburst, soil temperature for root growth limitations, and temperature in all canopy- and soil layers for maintenance respiration
- air and soil chemistry, i.e. nitrogen concentrations in the air (no₂, nh₃) and the soil (no₃, nh₄) in all canopy- and soil layers for nitrogen uptake
- vegetation structure, i.e. distribution of foliage and fine roots throughout canopy and soil layers. In addition, tree dimensions are needed for sapwood allocation.

Modes The calculations are reduced to the seasonality, flushing and senescence modules if the model runs in the MoBiLE_IsOneLeaf mode where plant growth is not of interest.

Author

- Ruediger Grote

Model options Available options (default options are marked with bold letters):

- Branch fraction ("branchfraction" = **diameter** / volume)
Branch fraction is either estimated from parameterized tree diameter relationship (option: diameter) or from crown volume (option: volume).
- Crown length ("crownlength" = **diameter** / height)
Crown length is either estimated from a parameterized relation to tree height (option: height, see: veglibs_crown-length_parameter) or based on crown diameter (option: diameter).
- Competition ("competition" = **true** / false)
The Competition effect for stand density on height/diameter ratios is either neglected (option: false) or considered (option: true).
- Forest structure ("foreststructure" = **true** / false)
Structural growth either neglected (option: false) or considered (option: true). If structural growth is not included, seasonal woody biomass growth is reset in order to avoid structural growth. Removed woody biomass is added to the litter pools (see: PSIM_ResetBiomassFromLastYear)
- Limit root growth considering texture ("limitedrootgrowth" = false / **true**)
Depth of root growth affected by bulk density and stone content. (option: false) or considered (option: true).
- Transpiration (transpirationmethod: **wateruseefficiency** / potentialtranspiration)

Transpiration is either calculated using fixed relations to photosynthesis (WUEC↔ MAX, WUECMIN), or the transpiration that is defined by stomatal conductance, depending on vapor pressure deficit and plant hydraulic conductance (with GSMIN as minimum conductance).

- Stomatal conductance (stomatalconductance: **leuning_1995** / ballberry_1987 / medlyn_2011(a,b) / eller_2020)
Various stomatal conductance routines are available with and without consideration of soil water supply. While Leuning et al. LEUNING (1995) with linear reduction of conductance with relative available soil water is the standard option Knauer et al. (2015), Eller et al. Eller et al. (2020) is the only option that considers plant water potential instead soil water availability.

Hydraulic conductance The hydraulic approach calculates canopy water potential based on soil water potential, which then affects stomal conductance following the 'Stomata on Xylem' (SOX) model (see: Farquhar model): First, xylem water potential is derived from the soil conditions, weighting soil layer importance by fine root abundance

and considering a threshold soil water potential at which plant tissues are decoupled from the soil:

$$psi_sr = Sum[(min(CSR_REF; psi_sl \cdot fFrt_{sl})]$$

with

- *psi*: Soil water potential (MPa) (see *assign_soillayer_van_genuchten_parameter*)
- *fFrt*: Biomass fraction of fine roots in a particular soil layer
- *sl*: Indicator for a specific soil layer

Canopy water potential is then calculated from the gradient between the water potential in the xylem and from evaporative demand, also including the gravitational force.

$$psi_can = (psi_sr + psidecline_cum) - (\frac{transp}{CWP_REF \cdot kxyl}) - dps_i$$

with

- *psidecline_cum*: previous day cumulative water deficit within the tree
- *kxyl*: previous day root-to-canopy (plant hydraulic) conductance (in mol MPa-1 s-1 m-2leaf)
- *transp*: current day transpiration (mol m-2leaf s-1)
- *CWP_REF*: reference (=maximum) value for the (leaf area-normalized) specific xylem conductance (mol MPa-1 m-2leaf s-1)
- *dpsi*: water potential decline due to plant height (MPa)

The water deficit is build from the water that is transpired but was not available from the rooting zone. It is supposed to reflect the water resources within a tree, i.e. the stem water content. Surplus on water supply will refill this storage while additional deficits will empty it further.

The total plant, or xylem, conductance is calculated based on empirical relations with species-specific parameters (*PSI_REF*, *PSI_EXP*).

$$kxyl = 1.0 - (1.0 - exp(-((\frac{psi_can}{PSI_REF})^{PSI_EXP})))$$

Phenology Leaf flushing is calculated using the growing degree days approach, which is using the temperature sum since this years 1st January, considering chilling requirements and drought stress limitations.

Therefore, temperature sum (cumulative growing degree days, gdd), is first calculated from daily temperature sum (Lehning et al. (2001)):

$$gdd_cum = temp \cdot \frac{dayl}{12.0}$$

with

- temp: daily average leaf surface temperature (oC)
- dayl: daylength (h)

When cumulative gdd reaches a threshold value (gdd_thresh) that depends on the degree chilling requirements are met, flushing is initiated. This value is calculated as:

$$gdd_thresh = 100.0 + GDDSTART \cdot \exp(-0.0075 \cdot chilldays)$$

with

- GDDSTART: temperature sum value for flushing without considering chilling, ON TOP of the minimum GDD which is assumed to be 100.

Chilling days (chilldays) are calculated from average temperature and amplitude Linkosalo et al. (2008) :

$$chilldays = 2.0 \cdot \arccos(1.0 - (\max(0.0, -\frac{temp_avg - 0.5 \cdot temp_ampl}{0.5 \cdot temp_ampl})) \cdot \frac{diy}{2.0 \cdot PI})$$

with

- temp_avg: average annual temperature (oC)
- temp_ampl: annual temperature amplitude (oC)
- diy: number of days in year (-)
- PI: constant (3.1416)

After temperature requirements are met, flushing goes on provided water supply is above a species-specific threshold value (H2OREF_FLUSHING) and there is no water deficit in the stem.

Senescence Dry matter senescence loss is calculated assuming fixed tissue longevity separately for foliage, fine roots, and living (sap-)wood. Fine root and sapwood senescence is decreased by a species-specific fraction each day. Senescence of buds is directly related to foliage growth, which is driven by a similar function than foliage senescence (see Carbon allocation and growth).

Foliage senescence (sFol) is empirically determined (for evergreen species in every age class, na) based on a mortality factor ranging between 1 and 0:

$$sFol = mFol_na \cdot \left(1.0 - \frac{1.0 - dvmort}{1.0 - dvmort_old}\right)$$

$$dvmort = \exp\left(-1.0 \cdot \frac{foliage_age - DLEAFSHED)^2}{(0.5 \cdot NDMORTA)^2 \cdot \log(2.0)}\right)$$

with:

- mFol: foliage biomass (kgDW m⁻²)
- foliage_age: age of foliage (age class) (days)
- DLEAFSHED: parameter describing the day where all foliage (of one age class) is shed (days)
- NDMORTA : parameter indicating the duration of senescence (days)

The nitrogen loss is defined by the nitrogen concentration in the tissue considering a species-specific retranslocation rate that is the same for all tissues. The maximum retranslocation rate is reduced if the overall nitrogen demand is smaller than the maximum amount of nitrogen that could be retranslocated.

Under some circumstances, stress induced senescence (i.e. xylem and foliage loss due to extensive drought stress) is also considered. This part is under development.

Carbon allocation and growth Carbon provided by photosynthesis (minus growth respiration) is distributed into any compartment that didn't comply with parameterized allometric relations which define the optimum biomass. Allocation strength is linearly related to the difference between actual and optimum biomass Grote (1998) .

$$dc_C = cPool \cdot afc_C - res_COld$$

$$afc_C = \frac{dem_C}{cPool}$$

$$dem_C = \frac{\max(0.0, m_COpt - m_C) \cdot CCDDM}{1.0 - FYIELD} + res_COld$$

with

- C: indicator for plant compartments foliage, fine roots, sapwood, buds (= structural reserves), and the free available carbon (nonstructural reserves) that are represented in percent of all other living tissues (fac)
- cPool: available carbon for allocation originating from photosynthesis minus growth respiration
- afc: allocation factor (0-1)
- res: (maintenance) respiration from the compartments in the last timesteps (C m-2)
- dem: carbon demand (C m-2)
- m: biomass (DW m-2)
- m_Opt: optimum biomass of a compartment (DW m-2)
- CCDM: constant transforming biomass to carbon values (carbon content)
- FYIELD: species-specific parameter for growth efficiency (growth respiration fraction)

The foliage compartment is primarily increased by the depletion of reserves (bud compartment), and therefore has no 'demand' to its own. The transfer and thus the increase of foliage biomass is triggering the demand of buds, sapwood, and fine roots via allometric relations:

$$m_{Frt}Opt = QRF \cdot mFol;$$

$$m_{Sap}Opt = qsfm \cdot mFol;$$

$$m_{Bud}Opt = MFOLOPT \cdot farea \cdot fheight \cdot \frac{qsfm}{qsfm_{act}};$$

$$m_{Fac}Opt = sum(m_C) \cdot (FACMAX - fac);$$

with

- frt, sap, bud, fac: descriptors for plant compartments finroots, sapwood, buds (= constitutive reserves)
- qsfm, qsfm_act: desired and actual relation between sapwood and foliage biomass
- farea, fheight: fraction of crown covered area, and fraction to which maximum crown length has been established
- QRF: species-specific parameter describing the desired relation between fine roots and foliage biomass
- MFOLOPT: species-specific parameter for foliage biomass per area (kgDW m-2ground)

- FACMAX: species-specific parameter for maximum percentage of free available carbon

qsfm is derived from a desired relation between sapwood area and foliage area (Huber value, QSFA) and the dimension of the tree (assuming species-specific taper functions and fixed fractions for branchiness and coarse roots).

Sink-limitations apply for the compartments 'buds', which is only supported if sapwood area is sufficient to supply current leaves, and 'sapwood', which is not growing under drought stress (positive plant water deficit).

If the supply is larger than all demands, the surplus is distributed between buds, foliage, and fine roots in case of herbaceous plants, wood and buds in case of determined growth (FREEGROWTH = false) or into foliage growth if species are growing leaves continuously (FREEGROWTH = true).

Free available carbon can be depleted only by respiration demands higher than supply rates.

Carbon exudation is assumed to be species specific fraction of total fine root growth (see: PSIM_SoilCarbonRelease).

Nitrogen allocation The nitrogen provided from uptake and retranslocation is distributed according to biomass growth and optimum tissue concentrations Grote (1998).

Respiration Respiration consists of growth (rGro) and maintenance respiration, with the latter split up into respiration that is related to nutrient uptake and transport (rTra), and into remaining (residual) respiration (rRes). I Growth respiration is a fraction of growth is assumed to apply equally for every tissue

$$rGro = \text{sum}(dc_C \cdot (1.0 - FYIELD))$$

with

- C: indicator for plant compartments foliage, fine roots, sapwood, buds (= structural reserves)
- FYIELD: species-specific parameter expressing fraction of growth parameters

II Transport respiration summarizes carbon costs due to uptake of nitrogen and other nutrients (rUpt), phloem transport of carbon into the roots (rPhl), and the reduction of oxygenized nitrogen compounds (rNit). Uptake of nitrogen compounds is explicitly modeled, while additional costs from uptake and incorporation of other nutrients are estimated from biomass growth, assuming that all requirements are met.

$$rTra = rUpt + rPhl + rNit$$

$$rUpt = PAMM \cdot (uptNH4 + uptNH3) + PNIT \cdot (uptNO3 + uptNOx) + PMIN \cdot growth \cdot \frac{FMIN}{CCDM}$$

$$rPhl = PPHLOE \cdot (dcFrt + dcSap + exsuLoss)$$

$$rNit = PREDFRT \cdot uptNO3 \cdot FRFRT + PREDSAP \cdot uptNO3 \cdot (1.0 - FRFRT) + PREDSAP \cdot uptNOx$$

with

- $uptNH4$, $uptNH3$: taken up reduced nitrogen from the air ($NH4$) and the soil ($NH3$)
- $uptNOx$, $uptNO3$: taken up oxygenized nitrogen from the air (NOx) and the soil ($NO3$)
- $dcFrt$, $dcSap$: carbon increase of fineroots and sapwood (C)
- $exsuLoss$: carbon loss by exudation out of fine roots into the soil (C)
- $PAMM$, $PNIT$, $PMIN$: parameters for uptake cost of ammonia, nitrate, and other mineral components (0.17, 0.34, 0.06)
- $FMIN$: parameter for fraction of mineral components other than nitrogen to total plant biomass (0.05)
- $CCDM$: constant indicating the carbon content of plant dry matter (0.45)
- $PPHLOE$: parameter for phloem loading costs to support growth in sapwood, fine roots as well a exudates (0.06)
- $PREDFRT$, $PREDSAP$: parameters for reduction costs of taken up oxygenized nitrogen forms in fine roots and sapwood, respectively (1.72, 0.855)
- $FRFRT$: parameter indicating the fraction of nitrate that is reduced in the roots (0.5)

III Residual (maintenance) respiration according to temperature and nitrogen content Cannell and Thornley (2000)

$$rRes = sum(km \cdot fsub \cdot n_C)$$

$$km = KM20 \cdot (temp_C - TRMIN)^2 \cdot (TRMAX - temp_C) \cdot \frac{1.0}{(TROPT - TRMIN)^2 \cdot (TRMAX - TROPT)}$$

$$fsub = \frac{\frac{ffac}{FFACMAX}}{KMMM + \frac{ffac}{FFACMAX}}$$

with

- C : indicator for plant compartments foliage, fine roots, sapwood, buds (= structural reserves)

- n : nitrogen within a plant compartment
- f_{sub} : reduction factor due to depleted non-structural reserves
- k_m : temperature modification factor
- $temp$: tissue temperature
- $ffac$: actual fraction of non-structural carbon reserves (0-1)
- $FFACMAX$: maximum fraction of non-structural carbon reserves (0-1)
- $KMMM$: Michaelis-Menton constant for the importance of relative available non-structural carbon on respiration

Nitrogen uptake Uptake of ammonia and nitrate from the soil and canopy is calculated according to supply, soil water availability and fine root density. Total nitrogen uptake is limited to the current whole plant demand. Nitrogen uptake/emission from the canopy depends on NO_x air concentration.

Note

Uptake through the canopy may be small but could be significant relative to NO_x emissions from the soil. Parameterization should be species specific but necessary information is yet not available. Instead, rough estimates from a tropical landscape are used Sparks et al. (2001).

Nitrogen fixation is considered similar to agricultural plants, using a species-specific parameter (INI_N_FIX) that indicates that a fraction of nitrogen demand is covered by fixation at no cost (see $PSIM_NitrogenFixation$).

Daily enzyme activity

$$v_{25E} = V_{25E} \cdot f_{dorm} \cdot f_{nit} \cdot f_{wat}$$

with

- v_{25} : value for velocity at 25 °C (μmol m⁻² s⁻¹)
- E : indicator for different enzymes (carboxylation reactivity, electron transport activity, dark respiration)
- V_{25} : parameterized standard values for enzyme velocities at 25 °C (μmol m⁻² s⁻¹)
- f_{dorm} , f_{nit} , and f_{wat} : multiplicative reduction factors for phenology, nitrogen- and water supply, respectively

The reduction factor for phenology is differently calculated for deciduous species, where enzyme activity is assumed to develop in parallel to flushing and senescence, and for ever-green species, where the activity is determined from temperature development according to Maekelae et al. Mäkelä et al. (2004) :

$$f_{dorm} = C1 \cdot (tFol24 + \frac{24.0}{TAU} \cdot (temp - tFol24) - PSNTFROST)$$

with

- temp: (leaf surface) temperature (oC)
- tFol24: temperature average of the previousl 24 hours (oC)
- C1, TAU: empirical model constants (0.0367, 330.0, respectively) Mäkelä et al. (2004)
- PSNTFROST: species-specific temperature at which photosynthesis enzymes start to decline (oC)

The reduction factor for nitrogen supply is defined as the degree to which the optimum (equal to maximum) foliage nitrogen concentration has been established:

$$f_{nit} = \frac{ncFol - NCFOL_MIN}{NCFOL_OPT - NCFOL_MIN}$$

with

- ncFol: foliage nitrogen concentration (gN gDM-1)
- NC_FOL (MIN, OPT): species-specific minimum and optimum foliage nitrogen concentrations (gN gDM-1)

The reduction factor for water supply is based on the same function as has been used for determining the loss of hydraulic conductance according to Tuzet et al. (2003). The recovery of the water damaged enzyme activity is not very well determined. In the literature, periods between 3 (33% recovery rate) and >20 (about 5% recovery rate are indicated Manzi et al. (2021). The value is currently set to 5% for all species.

$$f_{wat} = \frac{1.0 + \exp(A_REF \cdot A_EXP)}{1.0 + \exp((A_REF - psi_mean) \cdot A_EXP)}$$

with

- psi_mean: mean canopy water potential (MPa)
- A_REF, A_EXP: species-specific empirical parameters that describe the sensitivity (EXP) and a reference water potential (REF) of the drought impact on enzyme activity

Note

vcAct25 is not changed in dependence on season alone as is e.g. indicated in Ito et al. (2006).

1.0.4.6 PnET tree plantation model

The PNET module represents mechanisms of the PNET2 Model Aber et al. (1995), which is a monthly-timestep plantation model (monospecific, evenly structured forests) based on daily photosynthesis calculations Aber and Federer (1992). General descriptions can be found at <http://www.pnet.sr.unh.edu>. The functions are taken from the Download of PNET_VERSION 4.1, Oct. 12, 2001.

Note

Water balance and soil respiration calculations in the original model have been deleted and the water and nitrogen availability is now provided by other modules of LandscapeDNDC.

Model options Available model options: Default options are marked with bold letters.

- Branch fraction ("branchfraction" = **diameter** / volume)
Branch fraction is either estimated from parameterized tree diameter relationship (option: diameter) or from crown volume (option: volume).
- Crown length ("crownlength" = **height** / volume)
Crown length is either estimated from parameterized height relationship (option: height) or from crown volume (option: volume).
- Competition ("competition" = **true** / false)
The Competition effect for stand density on height/diameter ratios is either neglected (option: false) or considered (option: true).
- Limit root growth considering texture ("limitedrootgrowth" = false / **true**)
Depth of root growth affected by bulk density and stone content. (option: false) or considered (option: true).

Calculates allocation to the different plant parts **CHANGED**: The parameter of root growth has been made dependent on physiological parameter describing fine root demand C-Allocation out of roots (respiration and senescence)

1.0.4.7 TreeDyn - Tree dimensional Dynamics

Mortality Tree mortality rate (*mort*) is assumed to have a fixed component not related to stand density (*mort_natural*), e.g. caused by diseases, and a stand density related component (*mort_dens*). The latter only applies if trees are growing across a threshold of tree canopy coverage. Then, the number of trees is reduced to this threshold.

$$mort = \max(mort_dens, mort_natural)$$

$$mort_natural = \frac{MORTNORM}{365}$$

$$if(relcover > 1) mort_dens = 1.0 - (MORTCROWD \cdot \frac{cdr^2}{cdr_pot^2})$$

$$relcover = \frac{(dbh \cdot cdr)^2 \cdot PI \cdot 0.25 \cdot tree_number}{10000 \cdot MORTCROWD}$$

with

- dbh: diameter at breast height (1.3m) (m)
- cdr: ratio between dbh and crown diameter
- *cdr_pot*: ratio between dbh and potential crown diameter under unconstrained conditions
- tree_number: number of trees per hectare
- relcover: relation between actual tree cover and potential coverage with no constraints
- PI: constant (3.146)
- MORTNORM, MORTCROWD: parameters for annual intrinsic mortality rate and maximum tree coverage, respectively

Dimensional growth All dimensional growth is calculated on the basis of the new wood volume which consists of sapwood and core(or heart)wood, reduced by fractions for underground wood parts (coarse roots) and branches.

$$vol = \frac{(m_sap + m_cor) \cdot (1.0 - UGWDF) \cdot (1.0 - f_branch)}{DSAP}$$

with:

- m_sap: living sapwood
- m_cor: core (or heart)wood

- `f_branch`: fraction of branch biomass of aboveground woody biomass
- `UGWDF`: species-specific paramter describing the belowground fraction of total woody biomass
- `DSAP`: species-specific wood density (kgDW dm-3)

The branch fraction is calculated based on a allometric relationship to stem diameter or based on crown volume (= option 'branchfraction, Model options). See Branch fraction. The new volume is then distributed into height- and diameter growth considering the a stand-density related optimum height:diameter ratio (Height-diameter ratio).

Sapwood:Foliage relation Assuming a relation between sapwood area and foliage area (Sapwood to foliage area ration), which is calculated empirically in dependence on tree height, the sapwood biomass necessary to supply the maximum foliage in the crown can be determined assuming a cone shape decline within the canopy and throughout the rooting zone. This optimum sapwood biomass (`mSap_opt`) is then divided by current foliage (and bud) masses in order to gain a sapwood/foliage biomass ratio.

$$qsm = \frac{mSap_opt}{mFol + mBud}$$

$$mSap_opt = 1000 \cdot DSAP \cdot mSap_demand \cdot (height_base + \frac{rooting_depth}{3.0} + \frac{height - height_base}{3.0})$$

$$mSap_demand = lai_max \cdot qsfa$$

with

- `mFol`, `mBud`: biomass of foliage and structural reserves (buds) (kg m-2)
- `height_base`: crown base height (m)
- `rooting_depth`: rooting depth (m)
- `lai_pot`: potential leaf area calculated from foliage and bud mass weighted by specific leaf area, derived from canopy length and species-specific parameters (`SLA_MAX`, `SLAMIN`)
- `qsfa`: relation between sapwood area and foliage area using `QSF_P1`, and `QSF_P2` (sap-fol-ratio)
- `DSAP`: species-specific sapwood density (kg dm3)

The height at crown base is calculated EITHER from a parameterized relationship to tree height (= option 'height, described under 'PSIM') using the species-specific parameters `HREF` (tree height at which crown base height starts to increase) and `CB` (relation between crown base height and top height at a mature state) or based on crown diameter (crown-length) using the species specific parameters (`CL_P1` and `CL_P2`).

Biomass and leaf area distribution Foliage biomass throughout the foliated canopy and fine root biomass throughout the rooted soil are empirically distributed using the same function that depends on distribution length (either canopy depth or rooting depth) with different parameters Grote (2003), `veglibs_biomass_distribution`.

Leaf area throughout the foliated canopy follows foliage biomass distribution but is weighted by specific leaf area per canopy layer. The latter varies linearly between a predefined minimum (at the top of the canopy) and maximum value (SLAMIN, SLAMAX).

Forest disturbances

- Defoliate
- Regrowth
- Throwing
- Thinning
- Harvest

1.0.4.8 PhotoFarquhar - Farquhar Photosynthesis

Farquhar model precalculations

Light dependency The electron transport rate depends on radiation intensity Evans (1989).

$$jPot = \frac{(i_S + jMax - ((i_S + jMax)^2 - 4.0 \cdot THETA \cdot i_S \cdot jMax))^{0.5}}{2.0 \cdot THETA}$$

with

- jPot: potential rate of electron transport (umol m⁻² s⁻¹)
- S: indicator for sunlit and shaded canopy fractions
- THETA: species-specific slope parameter

The radiation perceived by the photosystem is calculated separately for sunlit and shaded fractions in each canopy layer

$$i_S = par_S \cdot (1.0 - 0.15) \cdot 0.5$$

with

- par: absorbed photosynthetic active radiation

The losses of absorbed radiation are fix ($(1.0 - 0.15) * 0.5 = 0.425$), assuming a constant correction for spectral quality of 0.15 Evans (1987). (reduction by a factor of 0.5 is considering an equal distribution between two photosystems).

could be improved by

- variable light use efficiency (mol electrons mol⁻¹ photons) with canopy depth (0.4-20-0.24, Harley and Baldocchi (1995))
- dependency of light use efficiency with temperature (0.34-0.72, Harley et al. (1985)).

Temperature dependency Carboxylation and oxygenation activities as well as the electron transport rate depend on temperature using an Arrhenius function based on Long (1991) that has been corrected for high temperatures according to Medlyn et al. (2002).

$$v_E = (v_{25E} \cdot \exp(AE_E \cdot term_{arrh}) \cdot add_{peak})$$

$$term_{arrh} = \frac{tempK - TK25}{TK25 \cdot tempK \cdot RGAS}$$

$$add_{peak} = \frac{1.0 + \exp(\frac{TK25 \cdot SDJ - HDJ}{TK25 \cdot RGAS})}{1.0 + \exp(\frac{tempK \cdot SDJ - HDJ}{tempK \cdot RGAS})}$$

with

- v: enzymatic velocity (umol m⁻² s⁻¹)
- E: indicator for different enzymes (kc, ko, vcMax, voMax, rd)
- v25: standard value for velocity at 25 oC (umol m⁻² s⁻¹)
- tempK: tissue temperature [K]
- TK25: standard temperature [303.15 K]
- AE: activation energies for the respective enzymatic process (J mol⁻¹)
- SDJ: entropy factor (-)
- HDJ: deactivation energy (J mol⁻¹)
- RGAS: general gas constant (=8.3143) [J mol⁻¹ K⁻¹]

For these dependencies oxygenation activity vo is assumed to be in a fixed relation (Q_{VOVC}) to parameterized carboxylation activity at 25 oC (VCMAX25). Similarly, the electron transport as well as the photorespiration rate at 25 oC is assumed to be in a fixed relation to carboxylation velocity (Q_{JVC} , Q_{RD25}).

could be improved by

- introduction of specific activation and deactivation energies for each process Harley et al. (1992) (disregarded except for vcMax and jMax, Harley and Baldocchi (1995))
- acclimation to carbon dioxide Cannell and Thornley (1998)

Internal co2 concentration The internal co2 concentration is calculated iteratively considering assimilation and stomatal conductance (which depends on assimilation) until $c_i = c_{iPot}$. With

$$c_{iPot} = c_a - \frac{ass_i}{g_s/FGC}$$

with

- c_a : air co2 concentration
- g_s : stomatal conductance for water
- FGC: constant describing the relation between water and co2 molecules

Note that there is no iteration if $ass_i < 0$ because dark respiration is not influenced by c_i and the rest impact is supposed to be negligible. Furthermore, stomatal conductance of water is constraint by minimum and maximum values (GSMIN and GSMAX, respectively).

The co2 compensation point which is also used for defining g_s is derived from carboxylation (vc) as well as oxygenation (vo) velocities Von Caemmerer and Farquhar (1981) using an empirical estimate of O2 concentrations in the plant tissue Long (1991), kinetic values that are derived from temperature-corrected species-specific parameteres (KO25, KC25) and enzyme activities (AEKC, AEKO).

$$c_{star} = 0.5 \cdot v_o \cdot k_c \cdot \frac{o_i}{v_c \cdot k_o}$$

with

- o_i : internal o2 concentration
- k_c, k_o : temperature corrected Michaelis-Menten parameters for carboxylation and oxygenation
- v_c, v_o : temperature corrected carboxylation and oxygenation velocities

Farquhar model This gas exchange module calculates stomatal conductance and photosynthesis based on Farquhar et al. (1980). The implementation is according to Von Caemmerer et al. (2009).

$$A = \left(1.0 - \frac{c^*}{c_i}\right) \cdot \min(w_c, w_j, w_p) - r_d$$

with

- A : assimilation rate
- c^* : carbon dioxide compensation point
- c_i : internal carbon dioxide concentration
- w_c : carboxylation limited assimilation rate
- w_j : electron transport limited assimilation rate
- w_p : phosphorylation limited assimilation rate
- rd : dark respiration

The calculation of w_c , w_j and w_p depend on c_i , w_c additionally on o_i , w_j and w_p additionally on the compensation point:

$$w_c = vc \cdot \frac{c_i}{c_i + kc \cdot (1.0 + \frac{o_i}{ko})}$$

$$w_j = \frac{j}{4.0 + 8.0 \cdot \frac{c^*}{c_i}}$$

$$w_p = \frac{3.0 \cdot tpu}{1.0 - \frac{c^*}{c_i}}$$

with c^* according to Von Caemmerer and Farquhar (1981) :

$$c^* = 0.5 \cdot vo \cdot kc \cdot \frac{o_i}{vc \cdot ko}$$

with

- vc : carboxylation activity (umol m⁻² s⁻¹)
- vo : oxygenation activity (umol m⁻² s⁻¹)
- j : electron transport rate (umol m⁻² s⁻¹)
- tpu : rate of phosphate release (umol m⁻² s⁻¹)
- ko : Michaelis Menten constant for O₂ (mmol mol⁻¹, empirically determined according to Long 1991 Long (1991))
- kc : Michaelis Menten constant for CO₂ (mmol mol⁻¹)
- oi : intercellular concentration of oxygen (mmol mol⁻¹)

All enzyme activities (*vc, vo, j, tpu, rd*) rates are calculated using canopy layer-specific temperature and radiation. Regarding temperature dependencies an Arrhenius function is used Long (1991) that has been corrected for high temperatures according to Medlyn et al. (2002). For these dependencies, process-specific activation energies (AEVC, AEVO, A \leftrightarrow EJM, AETP, AERD), and activity rates at 25oC are parameterized (VCMAX25, TPU25) or put into a fixed relation to carboxylation activity (QJVC, QVOVC, QRD25). Similarly, also for Michaelis-Menten constants the rates at 25oC have been parameterized (KO25, KC25) and temperature corrected in the same way as carboxylation and oxygenation (using AEKC, AEKO). For C4 plants simplified assumptions are applied for carboxylation dependencies Harley et al. (1992) and phosphorylation limits Collatz et al. (1992).

Radiation intensity is needed to define electron transport rate only Evans (1989), using a species-specific parameter to define the slope of the relationship (THETA). Furthermore, it is assumed that the potential (parameterized) carboxylation activity, electron transport rate and photorespiration at 25oC is reduced with increasing canopy depth (linked to specific leaf area) and can be further reduced if nitrogen supply is not sufficient to reach a predefined target value. In addition, the enzymatic activities depend on phenological developments, and are eventually reduced by heat, frost or drought stress (Daily enzyme activity).

Modes Internal carbon dioxide concentration is calculated with the Berry-Ball Ball et al. (1987) optimization approach (standard) or the Jarvis Jarvis (1976) multiplicative approach (optional).

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Stomatal conductance models

Ball, Woodrow, and Berry 1987 The model Ball et al. (1987) is the original version to use iteratively with the Farquhar model Farquhar et al. (1980). The stomatal conductance of every foliage layer is determined by

$$gs = G_{SMIN} + SLOPE_GSA \cdot assi \cdot \frac{rh}{ca}$$

with

- *assi*: the assimilated carbon (per canopy layer)
- *rh*: the relative humidity (per canopy layer)
- *ca*: the mole fraction of CO₂ (per canopy layer)

- *GSMIN*, *SLOPE_GSA*: species-specific parameters (for minimum leaf conductance and sensitivity to assimilation)

Leuning 1995 The model LEUNING (1995) has been modified by adding an additional soil water impact Knauer et al. (2015). Stomatal conductance of every foliage layer is determined by

$$gs = GSMIN + SLOPE_GSA \cdot fwat \cdot assi \cdot \frac{rh}{ca - c_star}$$

$$fwat = \min \left(1.0, \frac{wc - wc_min}{wc_max - wc_min} \cdot \frac{H2OREF_GS}{H2OREF_GS} \right)$$

with:

- *assi*: assimilated carbon (per canopy layer)
- *rh*: relative humidity (per canopy layer)
- *ca*: mole fraction of CO2 air concentration (per canopy layer)
- *c_star*: CO2 compensation point
- *fwat*: drought stress factor, see also *wc*: soil water content (mm m-3)
- *wc_max*, *wc_min*: maximum and minimum water content within the rooting zone (field capacity and wilting point)
- *H2OREF_GS*: species-specific threshold relative water content at which stomata start to close
- *GSMIN*, *SLOPE_GSA*: species-specific parameters (for minimum leaf conductance and sensitivity to assimilation)

Eller et al. 2020 The model Eller et al. (2020) considers canopy water potential as influential for stomatal conductance. Stomatal conductance of every foliage layer is determined by

$$gs = GSMIN + 0.5 \cdot qac \cdot (\sqrt{1.0 + (4.0 \cdot \frac{epsilon}{qac})} - 1.0)$$

$$qac = \frac{assi_ref - assi}{ca - ci}$$

with

- *assi*: photosynthesis rate

- *assi_ref*: photosynthesis rate under standard conditions (25oC)
- *ca*: the mole fraction of CO₂
- *ci*: plant internal mole fraction of CO₂
- *GSMIN*: species-specific parameter (for minimum leaf conductance)

The conductance impact 'epsilon' is a complex interaction of plant conductance modified by canopy water potential and evaporative demand:

$$\epsilon = \frac{2.0}{qkr \cdot r_{plant} \cdot 1.6 \cdot vpd_mmol}$$

$$qkr = \left(\frac{kcr - kcr_ref}{psi_mean - (0.5 \cdot (psi_mean + PSI_REF))} \right) / kcr$$

$$kcr = 1.0 - (1.0 - \exp(-(\frac{psi_mean}{PSI_REF})^{PSI_EXP}))$$

$$kcr_ref = 1.0 - (1.0 - \exp(-(\frac{0.5 \cdot (psi_mean - PSI_EXP)}{PSI_REF})^{PSI_EXP}))$$

with

- *rplant*: plant resistance (MPa m² s mmol⁻¹)
- *kcr*: relative conductance between roots and canopy
- *vpd_mmol*: vapor pressure deficit (mmol)
- *psi_mean*: mean between canopy water potential and predawn water potential (MPa)
- *PSI_EXP*, *PSI_REF*: species-specific parameter

1.0.4.9 Vegetation Libraries

Stem dimensions The shape of tree stems is defined by the relation between tree height, diameter and stem volume. While the volume is only constraint by stem biomass and wood density, a change in volume can thus be related to a change in tree height and diameter based on:

- a height-diameter relationship that is dynamically related to stand density
- an empirically defined taper (shape) function

Because the taper function is based on tree height and diameter at breast height - but the latter is unavailable for trees shorter than 1.3 m - it is assumed that the form of short trees (*height* < 0.5 · *HLIMIT*) is that of a cone. Thus, dimensional growth can be determined from volume growth with only a given height-diameter ratio. The stem volume of large trees (*height* > *HLIMIT*) is determined by a taper function.

Height-diameter ratio Both calculations of stem dimensional developments (for short as well as tall trees) require an indication of the optimal height-diameter relationship, which is given as:

$$hd_opt = (HDMIN + (HDMAX - HDMIN) \cdot \exp(-HDEXP \cdot dbh)) \cdot competition_factor$$

with

- dbh: diameter at breast height (1.3m) (m)
- competition_factor: stand density factor (see separate section)
- HDMIN, HDMAX, HDEXP: species-specific parameters for height-diameter function

If the optimum height:diameter ratio (hd ratio) can be achieved based on the current tree dimensions, it is realized. Otherwise diameter growth will be established iteratively with a hd ratio as close as possible to the optimum one until the new wood volume (vol, m³) matches the calculated volume growth (see taper).

Competition factor considering stand density The competition factor is calculated empirically as:

$$competition_factor = \left(\frac{areacover_openrange}{DFLIMIT} \right)^{DFEXP}$$

To estimate the stand density impact on crown size, crown coverage without competition is calculated first:

$$areacover_openrange = (dbh \cdot cdr_open)^2 \cdot PI \cdot 0.25 \cdot N_trees$$

$$cdr_open = CDR_{P1} + CDR_{P2} \cdot \log(dbh) + CDR_{P3} \cdot \log(height)$$

with

- dbh: diameter at breast height (1.3m) (m)
- height: tree (cohort upper) height (m)
- N_{trees}: tree number per ha
- CDR_P1, CDR_P2, CDR_P3: species-specific parameters for crown width-diameter function
- DFLIM, DFEXP: species-specific parameters for competition function

Cone-shape based dimensional growth For short trees, a cone-shaped trunk is assumed where the relationship between volume, height, and (base) diameter can be calculated as:

$$vol_{cone} = \frac{PI \cdot (d_base \cdot 0.5)^2 \cdot height}{3.0}$$

All dimensional changes based on wood volume increase can thus be derived considering the previously defined height-diameter relationship $f_{hd}(d)$:

$$height = \frac{vol_{cone} \cdot 3.0}{PI \cdot (d_base \cdot 0.5)^2}$$

$$d_base = \frac{height}{hd_opt}$$

with

- PI: constant (3.146)
- d_base: base diameter (m)

Taper-function based dimensional growth The taper function that has been selected for the calculation of stem volume [m^3] depends on tree height $h[m]$ and tree diameter $d[m]$:

$$vol_{tap} = 0.001 \cdot (100 \cdot dbh)^{TAP_P1} \cdot height^{TAP_P2} \cdot exp(TAP_P3)$$

with

- TAP_P1, -P2, P3: species-specific parameters It has been particularly advocated in Dik (1984) with parameters for various species (see citation in Zianis et al. (2005)).

The taper parameters TAP_P1, TAP_P2, TAP_P3 are species-specific. Default parameters for coniferous trees are:

- TAP_P1 : 1.75
- TAP_P2 : 1.1
- TAP_P3 : -2.75

Default parameters for deciduous trees are:

- TAP_P1 : 1.95
- TAP_P2 : 0.75
- TAP_P3 : -2.4

According to the taper equation, tree height is can be defined in dependence on tree volume V [m³] and tree diameter at breast height [m]:

$$height = \left(\frac{vol_{tap}}{0.001 \cdot (100 \cdot dbh)^{TAP_P1}} \cdot exp(TAP_P3) \right)^{\frac{1}{TAP_P2}}$$

Also, tree diameter at breast height can be calculated with this equation based on tree volume V [m³] and tree height [m] using the same taper parameters:

$$dbh = 0.01 \cdot \left(\frac{vol_{tap}}{0.001 \cdot height^{TAP_P2}} \cdot exp(TAP_P3) \right)^{\frac{1}{TAP_P1}}$$

For larger trees ($h > HLIMIT$), diameter at ground height is determined depending on diameter at breast height dbh and tree height $height$:

$$d_{base} = dbh + \frac{HLIMIT}{height} \cdot dbh$$

Transition phase dimensional growth For $0.5 \cdot HLIMIT < height \leq HLIMIT$ a linear transition between the two shapes is assumed:

$$vol = \phi \cdot vol_{tap} + (1.0 - \phi) \cdot vol_{cone}$$

with ϕ representing a linear scaling factor. Accordingly, the diameter used for allometric scaling (e.g. regarding height/diameter ratio) is shifting during this period between ground height (d_{base}) and breast height (dbh), and is regarded as effective tree diameter (Condés and Sterba (2005)). As described for the volume, the effective tree diameter is defined by a linear transition using the scaling factor ϕ :

$$d_{eff} = (1 - \phi) \cdot d_{base} + \phi \cdot dbh$$

Iteration between volume and dimensional growth Since the optimum height-diameter ratio might not be achievable given the dimensions of the previous state, a change in trunk volume is translated into height and diameter changes iteratively:

$$\begin{aligned} d_{test} &= DBHLIMIT \\ \text{while } (vol_{test} < vol) : \\ \quad height_{test} &= d_{test} \cdot hd_opt(d_{test}) \\ \quad vol_{test} &= V(d_{test}, height_{test}) \\ \quad d_{test} &= d_{test} + increment \end{aligned}$$

With the increment used for diameter modification is plus or minus 10, 1, and 0.5 cm steps.

Iteration between volume and dimensional growth Stem volume for small trees is approached with a cone function iteratively approachng a new volume with a fixed HD ratio With the increment used for diameter modification is plus or minus 1 mm steps.

Iteration between volume and dimensional growth Since the optimum height-diameter ratio might not be achievable given the dimensions of the previous state, a change in trunk volume is translated into height and diameter changes iteratively:

$$\begin{aligned}
 d_{test} &= DBHLIMIT \\
 \text{while } (vol_{test} < vol) : \\
 \quad height_{test} &= d_{test} \cdot hd_opt(d_{test}) \\
 \quad vol_{test} &= V(d_{test}, height_{test}) \\
 \quad d_{test} &= d_{test} + increment
 \end{aligned}$$

With the increment used for diameter modification is plus or minus 10, 1, and 0.1 cm steps.

Crown dimensions The crown is generally described by crown length, diameter and a shape function that defines the extension of the crown in each canopy layer. The concept is descript in Grote and Pretzsch (2002). The resulting volume is also used to calculate the total demand of branches. Since it is assumed that foliage biomass scales linearly with crown volume, the shape function used to describe the relative canopy volume of each layer and the foliage biomass distribution within the canopy is the same. It is documended under `veglibs_biomass_distribution`.

Branch fraction The branch fraction is used to calculate the stem biomass and volume that is needed for tree dimensional growth (Dimensional growth). It is EITHER defined using the crown size by assuming a specific branch density per unit volume (Branch fraction from canopy volume) or based on species-specific limit values (Branch fraction from stem diameter). See option settings in Model options.

Branch fraction from canopy volume The crown volume is calculated assuming that every layer can be described as a disc with a horizontal extension defined by the biomass distribution function `veglibs_canopy`. The total volume can then be integrated across all canopy layers.

$$\begin{aligned}
 f_branch &= \frac{m_branch}{(m_stem + m_branch)} \\
 m_branch &= DBRANCH \cdot can_vol \\
 can_vol &= \int \left(\left(\frac{fFol_{fl}}{fFol_max} \cdot crown_diam \right)^2 \cdot PI \cdot 0.25 \cdot hfl_{fl} \right)
 \end{aligned}$$

with:

- fl: counter for canopy layers (1 - flmax)
- fFol: crown extension relative to maximum crown diameter (0 - 1)
- crown_diam: maximum crown diameter (see Crown diameter)
- hfl: height of the canopy layer (m)
- m_branch, m_stem: branch and stem biomass, respectively (kg m² ground)
- PI: constant (3.1416)
- DBRANCH: species-specific parameter describing the density of branches within the canopy volume (kg m³)

Branch fraction from stem diameter If this option is selected (Model options), the branch fraction is empirically related to stem diameter at breast height (dbh). Since the development of this term is different in young seedlings (where no dbh is available) and mature trees, branch fraction is calculated as the maximum of two functions:

$$f_branch = \max(fbranch_young, fbranch_mature)$$

For young trees, a maximum value is initiated that decreases steeply with increasing size, expressed as diameter at ground height.

$$fbranch_young = FBRAF_Y \cdot (1.0 - \exp(FSLOPE_Y \cdot dbas))^{FEXP_Y}$$

After a minimum branch fraction has reached, it is slowly increasing again approaching a final value for mature trees.

$$fbranch_mature = FBRAF_M + (1.0 - FBRAF_M) \cdot \exp(FSLOPE_M \cdot \frac{dbh}{DIAMMAX})$$

with

- dbas, dbh: stem diameter at ground height and breast height (1.3m), respectively (m)
- FBRAF_Y, FSLOPE_Y, FEXP_Y: species-specific allometric parameters for branch development in young trees
- FBRAF_M, FSLOPE_M: species-specific allometric parameters for branch development in more mature trees
- DIAMMAX: tree diameter at which a mature state is defined (m)

Crown diameter Crown diameter calculation is based on the open-range calculations that depend on breast-height diameter and tree height as presented by Condes and Sterba (2005).

$$crown_diam = CDR_P1 + (CDR_P2 \cdot \log(dbh)) + (CDR_P3 \cdot \log(height))$$

with

- dbh: breast-height (1.3m) diameter (m) (limited to values above 1cm)
- height: tree height (m)
- CDR_P1, -P2, -P3: species specific allometry parameters

In case that the canopy coverage of crowns calculated for open-grown trees is larger than a predefined species-specific threshold value (MORDCROWD), the crown diameter is reduced by a reduction factor that restricts the coverage to the threshold.

Crown length For all vegetation types other than woody species, crown length is equal to height. For trees, it is calculated depending on the setup-option selected (options depicted in 'PSIM' descriptions).

The first option is to calculate crown length based on an allometric relationship to tree height and diameter at breast height (= option height):

$$crown_length = \min(HLIMIT, height_eff \cdot CB)$$

$$height_eff = height - HREF \cdot \left(1.0 - \frac{dbh}{DIAMMAX}\right)$$

with: h_{cs} : height at canopy start

h_{max} : height at canopy top

$DIAMMAX$: tree diameter at which a mature state is defined

CB : relation between crown base height and top height at a mature state ($dbh \geq DIAMMAX$)

$HREF$: tree height at which crown base height starts to increase

The second option is to calculate crown length from crown diameter (option 'diameter') according to Thorpe et al. (2010) .

$$crown_length = CL_P1 \cdot (crown_diam)^{CL_P2}$$

with:

- crown_diam: crown diameter (m)
- CL_P1, CL_P2: species-specific allometric parameters

Crown length is limited by tree height. The crown base height (or crown start) is defined as tree height - crown length.

Canopy structure The distribution of foliage biomass $m(z)$ within the canopy depends on canopy length with a tendency to put more weight to the bottom of the distribution with larger length (Grote (2003), Grote (2007)):

$$m(z) = M \cdot \frac{r_{ih}f(z)}{\int r_{ih}f(z)} r_{ih} = \frac{CL - z}{CL} f(z) = p^{100 \frac{z}{CL^2}}$$

CL : canopy length (difference between start and end of canopy, m)

z : distribution depth for which the percentage foliage should be defined (between 0-1, refers to canopy start and top height)

p : shape parameter

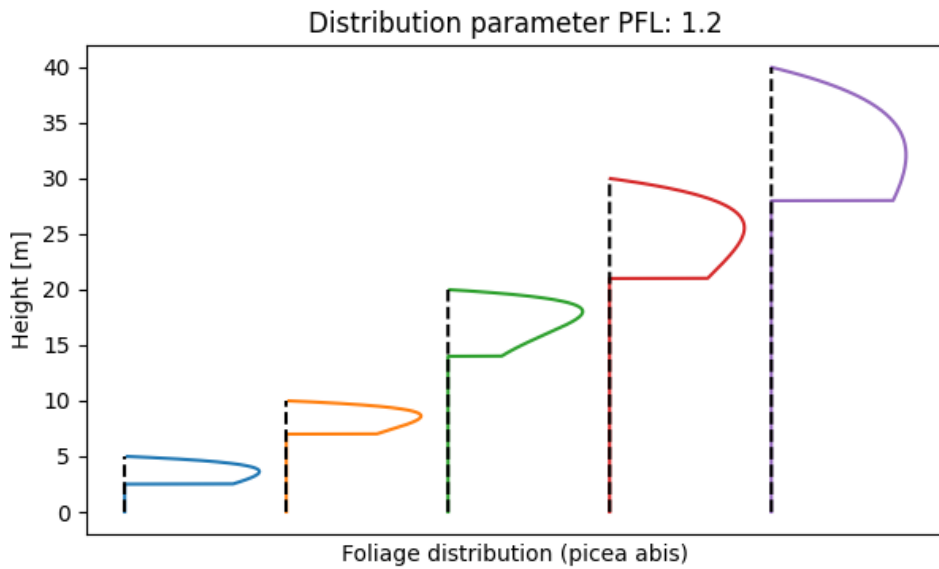


Figure 1.4: Canopy biomass distribution

Root system

Fine root distribution Root distribution and root properties are generally fixed throughout the simulation period. Only, if the initial condition of planting doesn't allow the soil profile to be fully rooted (e.g. plants are too small), rooting depth increases linearly with $GZRTZ$ until the maximum root depth (defined by the soil profile) is reached ($ZRTMC$).

Standard empirical root distribution The distribution of fine root biomass $m(z)$ within the rooting space depends on the rooting depth and is calculated with the same empirical equation as the foliage biomass (veglibs_canopy). The main difference is that the parameter 'p' is generally below 1 now to get a concave distribution (Grote and Pretzsch (2002)).

$$m(z) = M \cdot \frac{r_{ih}f(z)}{\int r_{ih}f(z)} r_{ih} = \frac{RD - z}{RD} f(z) = p^{100 \frac{z}{RD^2}}$$

RD : root depth (m)

z : distribution depth for which the percentage roots should be defined (between 0-1, from upper soil boundary to rooting depth)

p : shape parameter

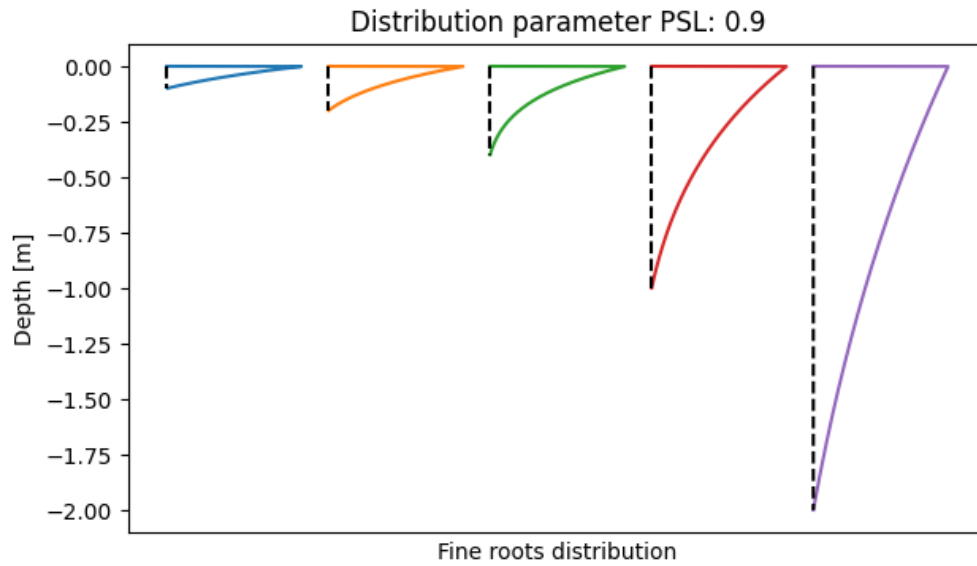


Figure 1.5: Fine roots biomass distribution

Note

This function is currently the standard option for PSIM/TREEDYN (implicitly) and PLAMOX

Sigmoid root distribution The root distribution decreases sigmoidel with the soil depth:

$$m(z) = M \cdot \frac{f(z)}{\int f(z)} f(z) = \left(\frac{e^{\left(-\frac{(z-0.1 \cdot RD)^2}{0.01 \cdot RD}\right)}}{RD} + 0.1 \cdot L \right)$$

with M : root growth (kg m⁻²)

RD : root depth (m)

z : distribution depth for which the percentage roots should be defined (between 0-1, from upper soil boundary to rooting depth)

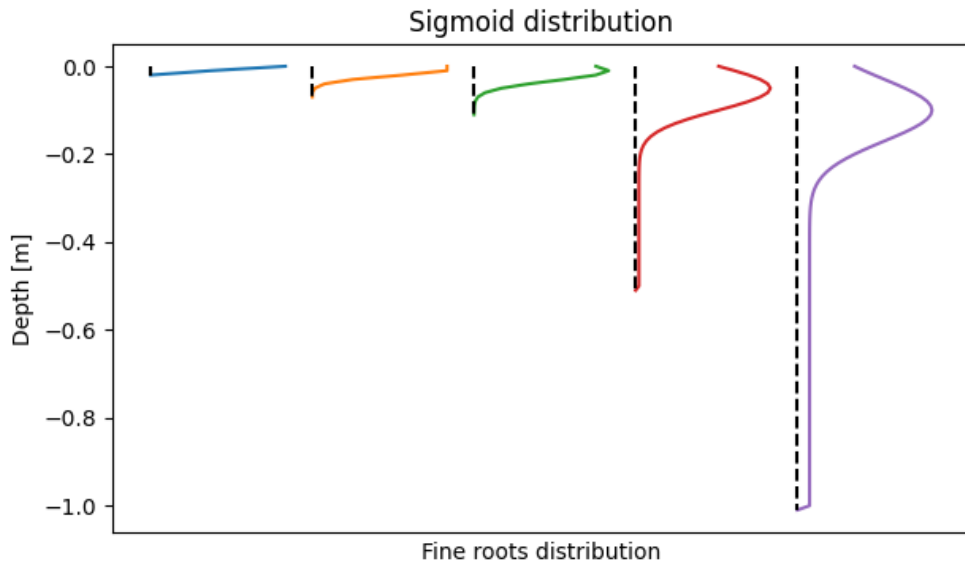


Figure 1.6: Fine roots biomass distribution

Note

This function is currently the standard option for ARABLE-DNDC and an option to select in PLAMOX and GRASSLAND

Exponential root distribution The root distribution decreases exponentially with the soil depth:

$$m(z) = M \cdot \frac{f(z)}{\int f(z)} f(z) = \exp(-EXP_ROOT_DISTRIBUTION \cdot z)$$

with: M : root growth (kg m⁻²)

z : distribution depth for which the percentage roots should be defined (between 0-1, from upper soil boundary to rooting depth)

$EXP_ROOT_DISTRIBUTION$: species-specific distribution parameter

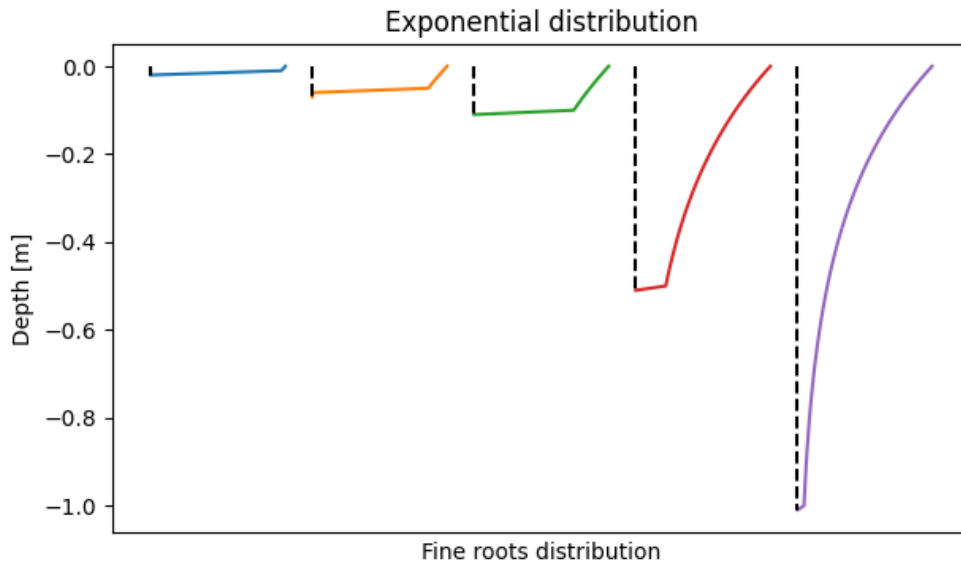


Figure 1.7: Fine roots biomass distribution

Note

This function is currently the standard option in ORYZA and GRASSLAND and can be selected in PLAMOX.

Root growth The function is entered with total carbon allocated to the roots (with costs for growth respiration already considered before), and it is then decided where to put the new biomass according to specific rules. There is no active redistribution of old root biomass but root biomass which is not supported by growth will continuously decrease due to senescence.

Empirical root growth distribution If no other options are defined, new root biomass is distributed to the different soil layers according to the selected root distribution scheme (standard, sigmoidal, or exponential). Therefore, the overall distribution stays constant.

Nutrient-based root distribution Carbon distribution to roots is based on previous nitrogen uptake of a particular layer. Thus, roots grow stronger in soil layers with high nitrogen availability.

Note

This function is currently not used at all in LDNDC

Sink-strength driven root distribution Root biomass distribution may be limited by various influences that prevent the realization of a particular distribution scheme. Based on an optimum root biomass distribution assuming either exponential or sigmoidal functions, these restrictions are calculated separately for all relevant layers, following Allan Jones et al. (1991).

Note

This function is available as an option in PLAMOX.

Sink driven allocation starts and ends with germination period. Outside this period, carbon distribution is done empirically. The different restrictions within the relevant period are considered as follows:

Update rooting depth

I Restrictions due to coarse fragments

$$S_{Fc}(sl) = 1 - stone_content[volume\ fraction](sl)$$

with

- sl: counter of soil layers

II Restrictions due to bulk density The bulk density enters via S_{BD} , which is given by

$$S_{BD} = 1, \quad BD < BD_O, S_{BD} = \frac{BD_X - BD}{BD_X - BD_O}, \quad BD_O \leq BD \leq BD_X, S_{BD} = 0, \quad BD > BD_X,$$

where the threshold BD_O is the bulk density at which root growth is first affected, and BD_X is the bulk density above which no root growth occurs. Following Allan Jones et al. (1991), these parameters can be estimated from the sand content [weight fraction] *sand*

$$BD_O = 1.1 + 0.005 \cdot sand, BD_X = 1.6 + 0.004 \cdot sand.$$

III Restrictions due to poor aeration Plants do not have any stress if the water filled porosity is below a critical value, whereas above this critical value the stress factor scales linearly between 1 and 0 in a fully saturated soil.

$$S_{AI} = S_{FT} + (1 - WFP) \cdot \frac{1 - S_{FT}}{1 - CWP}, \quad WFP \geq CWP, S_{AI} = 1, \quad WFP < CWP.$$

With the fraction of water filled pore space calculated as:

$$WFP = \frac{\text{water filled porosity}}{\text{total porosity}}$$

The critical value of water filled pore space depends on the clay content:

$$CWP = 0.4 + 0.004 \cdot \text{clay}.$$

IV Restriction due to temperature stress If the soil temperature is below a critical value (T_{BS}), root growth doesn't occur. Similar, too hot conditions also restricted carbon allocation into roots. Here, it is assumed that the limitations occur symmetrically around an species-specific optimum temperature T_{OP} , using a sinus function around an optimum temperature to describe the dependency.

$$S_{TP} = 0, \quad T < T_{BS}, S_{TP} = \sin\left(\frac{\pi}{2} \frac{T - T_{BS}}{T_{OP} - T_{BS}}\right), \quad T_{BS} \leq T \leq 2T_{OP} - T_{BS}, S_{TP} = 0, \quad T > 2T_{OP} - T_{BS}.$$

V Restriction due to flooding In addition, a species-(or genotype-)specific sensitivity to flooding S_{FT} is introduced.

$$S_{FT} = 0, \quad \text{corn, maize, soybean, etc.}, S_{FT} = 1, \quad \text{rice, etc.}$$

The combination of individual restrictions is then done following Allan Jones et al. (1991) :

$$\Delta rd_{red} = \Delta rd_{pot} \cdot \min\left(S_{TP}, \min(S_{ST}, S_{AI}, SCF)^{0.5}\right),$$

The restrictions in the bottom layer are assumed to represent a reasonable simplification as long as the time steps are small so that root elongation is also small in comparison to the soil layer widths.

Root length While root biomass is defined by one of the rooting distribution schemes, root length is calculated based on root biomass but considering a specific root length for every single soil layer. Specific root lengths scales linearly between $SRLMIN$ and $SRLMAX$ as:

$$\text{specific_rootlength}_{sl} = SRLMAX - \text{dvsFlush} \cdot (SRLMAX - SRLMIN) \cdot \text{scale}_{sl};$$

$$\text{scale} = 1.0 - \frac{\text{depth}_{sl}}{\text{depth_root}}$$

with

- *sl*: counter of soil layers
- *dvsFlush*: foliage development stage (0-1, 1 if fully grown leaves/needles are established)
- *depth*: depth of the respective soil layer
- *depth_root*: rooting depth

Sapwood

Optimum sapwood biomass Assumptions:

- Sap wood area is constant from the ground to crown base
- Stem in the crown is only sapwood,
- Stem in the crown + branches are cone shaped
- Coarse root volume is cone shaped

Sapwood to foliage area ration Ratio between sapwood and foliage area (Huber Value) The sapwood to foliage area relationship (m² sapwood area m⁻² leaf area) is calculated following Kostner et al. (2002), which is assumed to scale linearly with tree height.

$$qsfa = QSF_P1 + height \cdot QSF_P2$$

with

- *height*: tree height (m)
- *QSF_P1*: species-specific allometric parameter
- *QSF_P2*: species-specific allometric parameter

Vernalization Vernalization after Haenninen (1990).

Influence of vernalization starts as soon as accumulated growing degree days *AGDD* are greater than half of the required growing degree days for the state of flowering *GDD_FLOWERING*:

$$AGDD > 0.5 \cdot GDD_FLOWERING$$

Chill factor f_{chill} is given by:

$$f_{chill} = 1 - \frac{AGDD - 0.5 \cdot GDD_FLOWERING}{0.5 \cdot GDD_FLOWERING} + \frac{ACU}{CHILL_UNITS}$$

wherein ACU and $CHILL_UNITS$ refer to accumulated chill units and required chill units for complete vernalization, respectively. The factor f_{chill} is bound between 0 and 1.

Accumulated chilling units ACU are given by:

$$\begin{aligned} ACU &= \sum CU \\ CU &= \frac{CHILL_TEMP_MAX - T_{avg}}{CHILL_TEMP_MAX} \end{aligned}$$

$CHILL_TEMP_MAX$ and T_{avg} refer to a species-specific parameter and daily mean temperature, respectively.

Drought stress

Exponential relationship Exponential drought stress factor ϕ_d :

$$\phi_d = \frac{1 - e^{-f_{H_2O} gsslope}}{1 - e^{-gsslope}}$$

Related literature: Soil drought impact on stomatal conductance Van Wijk et al. (2000)

$$\phi_d = 1.016 - 0.016 \cdot e^{4.1 \cdot (1.0 - f_{h2o})}$$

A general relationship for 5 tree species was developed by Granier et al. (2000)

$$\phi_d = (1.154 + 3.0195 \cdot f_{h2o} - ((1.154 + 3.0195 \cdot f_{h2o})^2 - 2.8 \cdot 1.154 \cdot 3.0195 \cdot f_{h2o})^{0.5}) / 1.4);$$

Linear relationship Linearly calculated soil drought impact on stomatal conductance (ϕ_d) according to Wang and Leuning (1998) (more flexible due to species-specific sensitivity):

$$\phi_d = \min \left(\frac{f_{H_2O}}{f_{H_2O,ref}}, 1 \right)$$

Non-stomatal water limitation Non-stomatal impact of drought stress Tuzet et al. (2003).

1.0.4.10 MoBiLe Plant

1.0.5 Soilchemistry

- global_state_soil
- MeTrx - Metabolism and Transport of x
- SoilchemistryDNDC - Denitrification and Decomposition
- soillibs

1.0.5.1 global_state_soil

Initialisation Initialization of the global soil state is separated into two parts:

1. Initialization of soil state directly from site input information
2. Initialization of remaining soil state (state variables not directly provided by site input)

Initialisation from site input

Accessing individual items from site input

Stone fraction For each stratum the following procedure applies for:

1. Take value if provided in the site input
2. If not provided in the site input, use value according to the humus or layer-specific soil type (determined by the clay, sand and silt content in the specific layer, note layer specific soil types are only determined if clay+sand+silt summs up to 1.0. If not, e.g. for peat soils, the soil type that covers the complete soil profile is used as specified in the site input.)

Soil texture Soil texture includes:

- clay
- sand
- silt

For each stratum the following procedure applies for clay, sand and silt:

1. Take value if provided in the site input
2. If not provided in the site input, use value according to the humus/soil type
3. If the sum of all three fractions is greater than 1.0, all fractions are scaled down to exactly 1.0.

Bulk density For each stratum the following procedure applies for:

1. Take value if provided in the site input
2. If not provided in the site input, use value according to the humus or layer-specific soil type (determined by the clay, sand and silt content in the specific layer, note layer specific soil types are only determined if clay+sand+silt sums up to 1.0. If not, e.g. for peat soils, the soil type that covers the complete soil profile is used as specified in the site input.)

Carbon and nitrogen content For each stratum the following procedure applies for:

1. Take value of soil organic carbon content if provided in the site input
2. If soil organic carbon content is not provided in the site input, use humus type specific value for the litter layer. For the soil below the litter layer, if soil organic nitrogen content is provided determine ecosystem-specific C/N ratio to calculate the soil organic carbon content. If soil organic nitrogen content is also not provided, determine a exponential decay function using the soil organic carbon content in 5 and 30 cm soil depth as provided in the site input.
3. Take value of soil organic nitrogen content if provided in the site input
4. If soil organic carbon nitrogen is not provided in the site input, use humus type specific C/N ratio for the litter layer and determine ecosystem-specific C/N ratio for the soil below the litter layer to determine soil organic nitrogen content.

Porosity For each stratum the following procedure applies for:

1. Take value of porosity if provided in the site input
2. If not explicitly provided, calculate porosity based on soil texture, soil organic carbon content and bulk density.

Field capacity and wilting point ...

Linking/interpretating individual items

Soil texture Soil texture is determined depending on clay, sand and silt content. Only if the sum of these fractions does add up to 1.0, the soil type is determined layer-specific and used for further gap-filling. Otherwise, the soil type that covers the complete soil profile is used.

Stone fraction Bulk soil characterization may in- or exclude rocks/stones/gravel depending on different measurement approaches and points of view. While smaller gravel is most likely included in soil samples of, e.g., bulk density, greater stones or rocks are commonly excluded. Within the context of LandscapeDNDC, all soil input refers to the bulk soil excluding rocks/stones/gravel. Accordingly, the stone fraction represents the volumetric sum of rocks/stones/gravel.

pH value Depending on the model selection, pH may be dynamically calculated (e.g. after urea application). The pH value provided in the site input is interpreted as a mean value that is measured frequently over a longer time period.

Bulk density Internally used bulk density ρ includes bulk density of the soil without stones ρ^* and bulk density of stones ρ_{min} :

$$\rho = \rho^*(1 - x_{stone}) + \rho_{min}x_{stone}$$

Iron Total iron content is distributed equally to ferric and ferrous iron pools.

Organic carbon and nitrogen Internally used organic carbon and nitrogen contents include stones:

$$c_{org} = c_{org}^*(1 - x_{stone})\frac{\rho}{\rho^*}$$

Porosity ...

Field capacity and wilting point ...

van Genuchten parameters

Maximum and minimum water filled pore space ...

Van Genuchten parameters ...

1.0.5.2 MeTrx - Metabolism and Transport of x

User guide MeTrx simulates carbon and nitrogen cycle of soils. Focus lies on the production and consumption of the greenhouse gases CO_2 , CH_4 and N_2O . Therewith related outputs include leaching of NO_3 and emissions of NH_3 . Depending on the ecosystem of interest, several model options should be considered (see also: `metrxoptions`):

- Forests:
 - Depending on litter fall, the amount of carbon in the litter layers (defined in the site file) may considerably change. This can result in a change of the height of the litter layer. Wether the height of the litter is allowed to change can be regulated by the model option: "nochangelitterheight"
- Agricultural rice production systems:
 - Flooded agricultural rice systems are subject to the growth of algae. Wether algae growth sould be considered can be regulated by the model option: "algae"
- Initial conditions of systems not in equilibrium, e.g., drained wetlands:
 - During the spin up phase, soil organic matter pools are intended to establish equilibrium conditions as best as possible by shifting carbon and nitrogen between soil organic matter pools. However, if the system is known not to be in equilibrium initially, e.g., drained wetlands, this can be considered by defining an annual carbon loss or build-up rate using the model option: "spinupdeltac"

Microbial processes are especially relevant in the upper soil layers. Choose a spatial discretization of at maximum 0.5 cm for the upper 1cm soil depth. For a soil depth greater 1cm and smaller 10 cm, a spatial discretization of 1-2 cm per soil layer is recommended.

Model structure MeTrx requires further models for:

- watercycle (e.g., soil water content)
- plant growth (e.g., litter production / nitrogen uptake)

Model parameters MeTrx includes the following siteparameters:

- GROUNDWATER_NUTRIENT_RENEWAL
- METRX_AMAX
- METRX_AMAX_ALGAE
- METRX_BETA_LITTER_TYPE
- METRX_BIOSYNTH_EFF
- METRX_CN_ALGAE
- METRX_CN_FRAC_HUM3
- METRX_CN_MIC_MAX
- METRX_CN_MIC_MIN
- METRX_D_EFF_REDUCTION
- METRX_FE_REDUCTION
- METRX_FRAC_FE_CH4_PROD
- METRX_F_RANVF_1
- METRX_F_RANVF_2
- METRX_F_SANVF_1
- METRX_F_SANVF_2
- METRX_F_CONNECTIVITY_1
- METRX_F_CONNECTIVITY_2
- METRX_F_CH4_OXIDATION_T_EXP_1
- METRX_F_CH4_OXIDATION_T_EXP_2
- METRX_F_CH4_PRODUCTION_PH_1
- METRX_F_CH4_PRODUCTION_PH_2
- METRX_F_CH4_PRODUCTION_PH_3
- METRX_F_CH4_PRODUCTION_T_EXP_1
- METRX_F_CH4_PRODUCTION_T_EXP_2

- METRX_F_CHEMODENIT_PH_1
- METRX_F_CHEMODENIT_PH_2
- METRX_F_CHEMODENIT_T_1
- METRX_F_CHEMODENIT_T_2
- METRX_F_MIC_M_WEIBULL_1
- METRX_F_MIC_M_WEIBULL_2
- METRX_F_DECOMP_M_WEIBULL_1
- METRX_F_DECOMP_M_WEIBULL_2
- METRX_F_DECOMP_T_EXP_1
- METRX_F_DECOMP_T_EXP_2
- METRX_F_DECOMP_PH_1
- METRX_F_DECOMP_PH_2
- METRX_F_DECOMP_CLAY_1
- METRX_F_DECOMP_CLAY_2
- METRX_F_MIC_T_EXP_1
- METRX_F_MIC_T_EXP_2
- METRX_F_DENIT_N2_1
- METRX_F_DENIT_N2_2
- METRX_F_DENIT_NO
- METRX_F_DENIT_M_WEIBULL_1
- METRX_F_DENIT_M_WEIBULL_2
- METRX_F_DENIT_PH_1
- METRX_F_DENIT_PH_2
- METRX_F_DENIT_N2O_PH_1
- METRX_F_DENIT_N2O_PH_2
- METRX_F_N_ALGAE

-
- METRX_F_N_CH4_OXIDATION
 - METRX_F_NIT_FRAC_MIC
 - METRX_F_NIT_NO_N2O_M_WEIBULL_1
 - METRX_F_NIT_NO_N2O_M_WEIBULL_2
 - METRX_F_NIT_NO_M_EXP_1
 - METRX_F_NIT_NO_M_EXP_2
 - METRX_F_NIT_NO_N2O_T_EXP_1
 - METRX_F_NIT_NO_N2O_T_EXP_2
 - METRX_MIC_EFF_AEROBIC_RESPIRATION
 - METRX_MIC_EFF_ANAEROBIC_RESPIRATION
 - METRX_MIC_EFF_METHANE_OXIDATION
 - METRX_MUEMAX_C_ALGAE
 - METRX_MUEMAX_C_CH4_OX_HA
 - METRX_MUEMAX_C_CH4_OX_LA
 - METRX_MUEMAX_C_CH4_PROD
 - METRX_MUEMAX_C_DENIT
 - METRX_MUEMAX_C_FERM
 - METRX_MUEMAX_C_MIC
 - METRX_MUEMAX_C_FE_RED
 - METRX_MUEMAX_H2_CH4_PROD
 - METRX_MUEMAX_N_ASSI
 - METRX_NITRIFY_MAX
 - METRX_KA_C_MIC
 - METRX_KF_NIT_NO_N2O
 - METRX_K_O2_CH4_PROD
 - METRX_K_O2_FE_RED

- METRX_K_FE_FE_RED
- METRX_KMM_AC_CH4_PROD
- METRX_KMM_AC_FE_RED
- METRX_KMM_H2_FE_RED
- METRX_KMM_C_DENIT
- METRX_KMM_CH4_CH4_OX
- METRX_KMM_C_MIC
- METRX_KMM_O2_NIT
- METRX_KMM_H2_FERM
- METRX_KMM_H2_CH4_PROD
- METRX_KMM_N_ALGAE
- METRX_KMM_N_CH4_OX
- METRX_KMM_N_DENIT
- METRX_KMM_N_MIC
- METRX_KMM_NH4_NIT
- METRX_KMM_NO2_NIT
- METRX_KMM_O2_CH4_OX
- METRX_KMM_O2_FE_OX
- METRX_KMM_PH_INCREASE_FROM_UREA
- METRX_KR_ANVF_DIFF_GAS
- METRX_KR_ANVF_DIFF_LIQ
- METRX_KR_FRAG_ALGAE
- METRX_KR_FRAG_RAW_LITTER
- METRX_KR_FRAG_STUBBLE
- METRX_KR_FRAG_WOOD
- METRX_KR_DC_AORG

- METRX_KR_DC_CEL
- METRX_KR_DC_HUM1
- METRX_KR_DC_HUM2
- METRX_KR_DC_HUM3
- METRX_KR_DC_LIG
- METRX_KR_DC_SOL
- METRX_KR_DENIT_CHEMO
- METRX_KR_OX_FE
- METRX_KR_HU_AORG_HUM1
- METRX_KR_HU_AORG_HUM2
- METRX_KR_HU_CEL
- METRX_KR_HU_SOL
- METRX_KR_HU_HUM1
- METRX_KR_HU_HUM2
- METRX_KR_HU_LIG
- METRX_KR_UREAHYDROLYSIS
- METRX_KR_REDUCTION_CN
- METRX_KR_REDUCTION_ANVF
- METRX_KR_REDUCTION_CONIFEROUS
- METRX_LIG_HUMIFICATION
- METRX_RET_HUMUS
- METRX_RET_LITTER
- METRX_RET_MICROBES
- METRX_TILL_STIMULATION_1
- METRX_TILL_STIMULATION_2
- METRX_V_EBULLITION

- RETDOC
- RETNH4
- RETNO3
- TEXP

Calibration of N trace gases The calibration of nitrogen trace gas emissions primarily addresses microbial metabolism, anaerobic conditions, and transport. The processes of decomposition and humification of SOM should be excluded or managed carefully in order to avoid compromising the overall stability of SOM by inadvertently inducing unrealistically high losses or gains.

Nitrification

- METRX_F_NIT_FRAC_MIC
- METRX_KMM_NH4_NIT
- METRX_KMM_NO2_NIT
- METRX_KMM_O2_NIT
- METRX_KF_NIT_NO_N2O
- METRX_F_NIT_NO_N2O_M_WEIBULL_1
- METRX_F_NIT_NO_M_EXP_1
- METRX_F_NIT_NO_M_EXP_2
- METRX_F_NIT_NO_N2O_T_EXP_1
- METRX_F_NIT_NO_N2O_T_EXP_2

Denitrification

- METRX_MUEMAX_C_DENIT
- METRX_KMM_C_DENIT
- METRX_KMM_N_DENIT
- METRX_MIC_EFF_ANAEROBIC_RESPIRATION
- METRX_F_DENIT_PH_1 (relevant for low pH only)
- METRX_F_DENIT_PH_2 (relevant for low pH only)

- METRX_F_DENIT_N2O_PH_1 (relevant for low pH only)
- METRX_F_DENIT_N2O_PH_2 (relevant for low pH only)
- METRX_F_DENIT_M_WEIBULL_1
- METRX_F_DENIT_N2_1
- METRX_F_DENIT_N2_2
- METRX_F_DENIT_NO

Microbial N assimilation

- METRX_MUEMAX_N_ASSI

Microbial turnover (decay constants)

- METRX_AMAX
- METRX_KA_C_MIC

Transport between aerobic/anaerobic microsites

- METRX_KR_ANVF_DIFF_LIQ
- METRX_KR_ANVF_DIFF_GAS

Anaerobicity

- METRX_F_RANVF_1
- METRX_F_RANVF_2
- METRX_F_SANVF_1
- METRX_F_SANVF_2

Determining ratio between CO₂ and DOC production from microbial turnover

- METRX_BIOSYNTH_EFF
- METRX_CN_MIC_MIN
- METRX_CN_MIC_MAX
- METRX_MIC_EFF_AEROBIC_RESPIRATION

Decomposition/humification

- METRX_KR_DC_AORG
- METRX_KR_REDUCTION_ANVF

Model options Available model options: Default options are marked with bold letters.

- Algae (default: "algae" = **no** / yes) Set to **yes** for agricultural rice production ecosystems for which growth of algae should be considered.
- Drywet (default: "drywet" = **no** / yes) Under construction.
- Surface bulk, e.g., water table (default: "surfacebulk" = **yes** / no) Automatically includes additional surface layers in case surface water table builds up.
- Freeze thaw (default: "freezethaw" = **no** / yes) Under construction.
- Canopy transport (default: "canopytransport" = **no** / yes) Considers diffusive transport of NH_3 through the canopy.
- River connection (default: "riverconnection" = **no** / yes) Considers adjacent river connection: Dissolved constituents of surface water are in equilibrium with the atmosphere.
- Change litter height (default: "nochangelitterheight" = **no** / yes) Spatial discretization of litter height changes depending on litter input from vegetation.
- Effective diffusion coefficient (default: "effectivediffusion" = **parameter** / millington←_and_quirk_1961) Diffusion coefficients in the air phase are reduced due to soil tortuosity
- Spin up years (default: "spinupyears" = **2** / any integer number) During spin up years humus pools are scaled in order to balance decomposition with humification.
- Spin up carbon loss (negative number) / build-up (positive number) rate (kg:ha⁻¹:yr⁻¹) (default: "spinupdeltac" = **0** / any floating point number) During spin up years humus pools are assumed to have an annual lost/build-up rate.

MeTrx includes several model-specific output options:

- metrxdaily
- metrxyearly
- metrxlayerdaily
- metrxlayeryearly
- metrxsubdaily
- metrxfluxes

In order to include a MeTrx specific output, add the according attribute to the sinks section in the project file. Example:

```
<sinks sinkprefix="output/metrx_" >
  <metrxdaily sink="metrx-daily.txt" format="txt" />
</sinks>
```

Model initialisation

C/N ratio The allocation of soil organic matter to various humus pools is primarily influenced by the C/N ratio within each pool, while adhering to the overall constraint of maintaining the soil's overarching C/N ratio.

The target C/N ratio of all mineral associated organic matter pools depend on the overall soil C/N ratio. Humus pool 1 represents non-protected organic matter. Humus pool 2 and 3 represent "old" and "very old" protected soil organic matter, respectively:

$$\begin{aligned} C/N_{hum,1} &= C/N_{soil} \\ C/N_{hum,2} &= 1.5 \cdot C/N_{soil} \\ C/N_{hum,3} &= METRX_CN_FRAC_HUM3 \cdot C/N_{soil} \end{aligned}$$

Pool distribution Active organic material is assigned to microbial necromass (15%) and mineral associated but non-protected organic matter (humus pool 1: 85%).

Fragmentation Incoming litter from, e.g., plants, algae, animals is fragmented to 'soil organic' litter (no more distinguishable from soil organic matter)

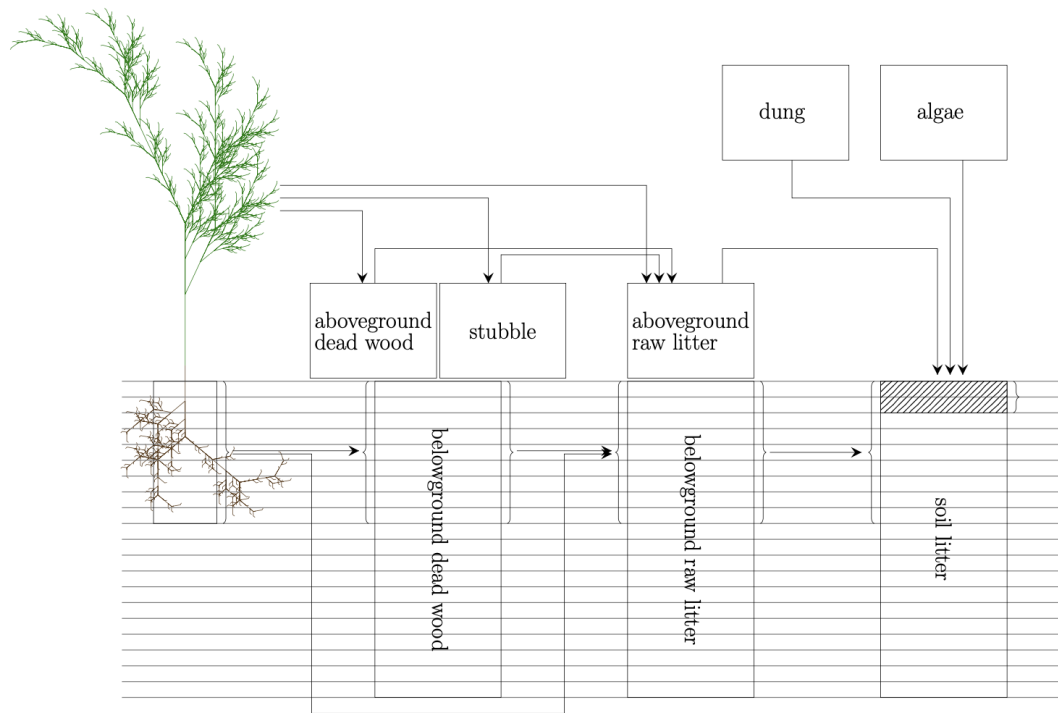


Figure 1.8: Litter flow

Soil organic matter turnover Turnover of soil organic matter (SOM) includes

- Decomposition to inorganic carbon dioxide (CO_2)
- Decomposition to dissolved organic carbon (DOC)
- Redistribution (humification) of SOM within different pools (e.g., from younger to older humus pools)

Dissolved organic carbon is distinguished between the aerob and the anaerob soil and facilitates microbial metabolism (e.g., nitrification, denitrification, fermentation, ...). During fermentation and syntrophic metabolism, anaerob DOC can be further metabolized to acetate and molecular hydrogen, which serves methanogenic microbes as substrate. Decomposed nitrogen is always transferred to the dissolved organic nitrogen pool (DON) from where it is subsequently redistributed depending on pool specific target CN ratios.

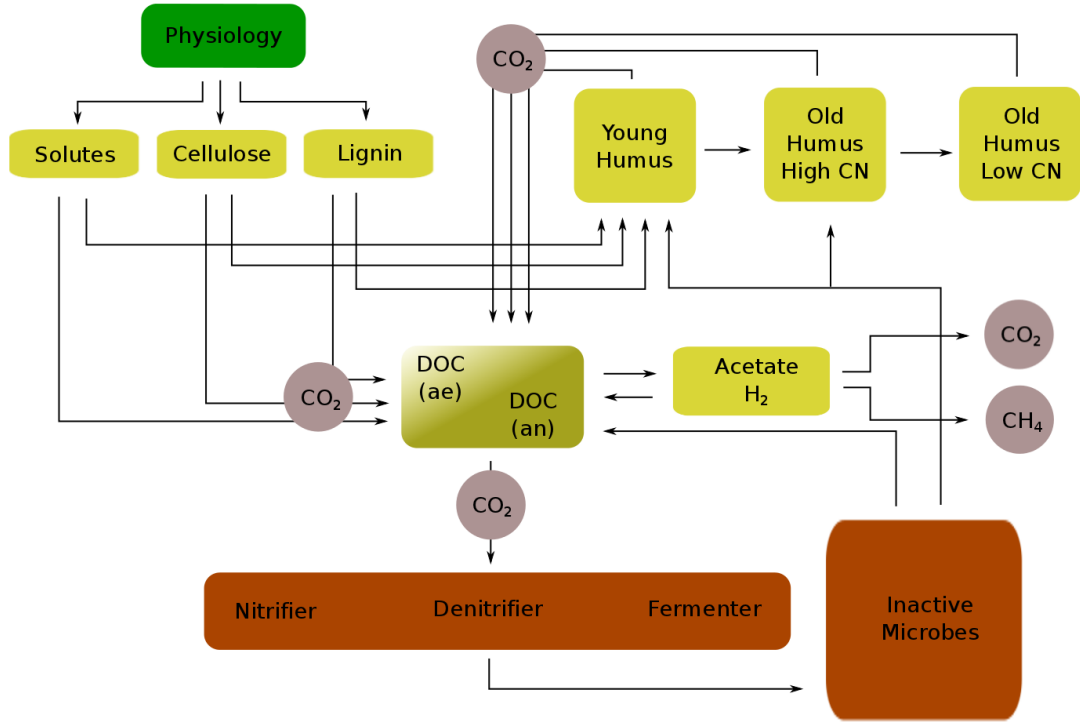


Figure 1.9: Scheme of Soil organic carbon turnover

Turnover of microbial necromass Turnover of microbial necromass involves:

- Decomposition (transfer to dissolved organic carbon pool)
- Humification (transfer to humus pools)

Decomposition of inactive microbial carbon m_{imc} and nitrogen m_{imn} depends on soil temperature, soil moisture and soil anaerobicity:

$$\begin{aligned}\Delta m_{imc \rightarrow doc_{ae}} &= K_DC_AORG \cdot m_{imc} \cdot \phi_{tm} \cdot \phi_{till} \cdot (1 - anv f) \\ \Delta m_{imc \rightarrow doc_{an}} &= K_DC_AORG \cdot m_{imc} \cdot \phi_{tm} \cdot \phi_{till} \cdot anv f \\ \Delta m_{imn} &= \frac{\Delta m_{imc \rightarrow doc_{ae}} + \Delta m_{imc \rightarrow doc_{an}}}{CN_{im}}\end{aligned}$$

Temperature moisture factor

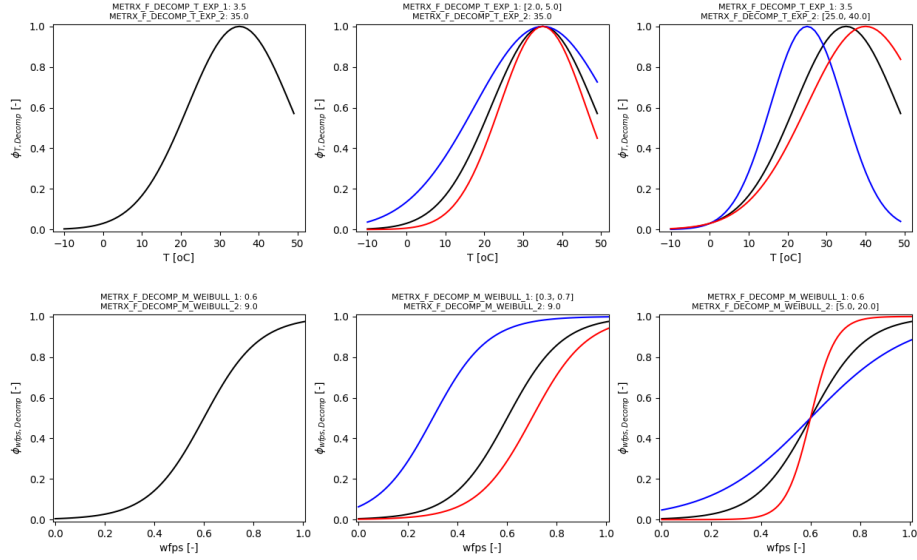


Figure 1.10: Response function of decomposition of inactive microbes depending on temperature and moisture

Humification of inactive microbial carbon is given by:

$$\Delta m_{imc \rightarrow hum(young)} = METRX_KR_HU_AORG_HUM_0 \cdot m_{imc}$$

$$\Delta m_{imc \rightarrow hum(old, highCN)} = METRX_KR_HU_AORG_HUM_1 \cdot m_{imc}$$

Turnover of soil organic matter and plant debris Turnover of SOM and plant debris includes:

- Decomposition (transfer to dissolved organic carbon pool)
- Humification (transfer to humus pools)

Turnover rates depend on:

- Climatic factors (temperature, moisture)
- Soil related factors (clay content, pH, aerobicity)
- Chemical composition (litter type, CN ratio)

- Management (tilling)

Depending on the litter or humus pool the general turnover rate is given by:

$$\frac{dm_x}{dt} = K_x \cdot m_x \cdot \Pi_i \phi_i$$

with $\Pi_i \phi_i$ being the multiplicative combination of pool specific environmental reduction factors ϕ_i (e.g., temperature, moisture,...) determining turnover.

The influence of temperature and moisture is given by:

$$\phi_{t,m} = \frac{2}{\frac{1}{\phi_t} + \frac{1}{\phi_m}}$$

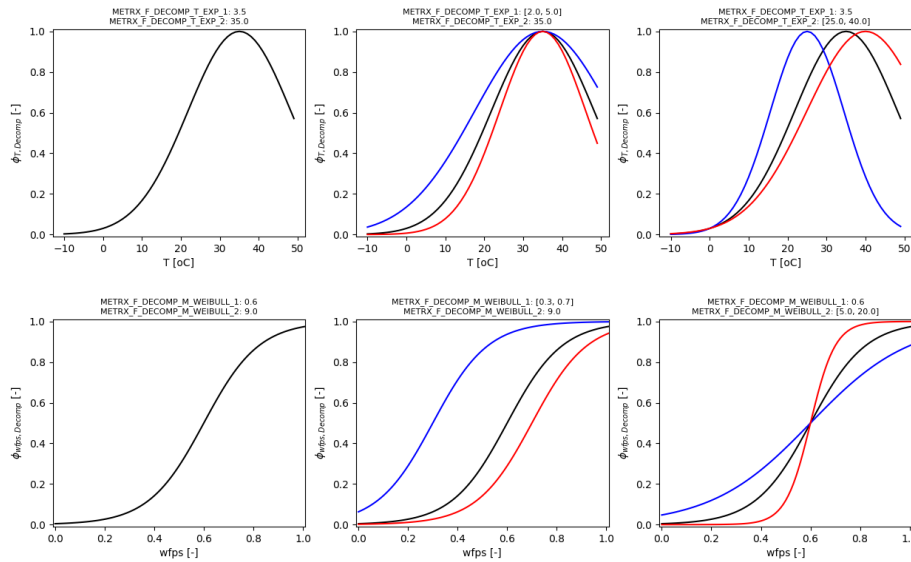


Figure 1.11: Response function of decomposition depending on temperature and moisture

The influence of the lignin content of the litter is given by:

$$\phi_{lig} = e^{-METRX_BETA_LITTER_TYPE \cdot \frac{c_{lig}}{c_{tot}}}$$

The influence of litter quality (C/N ratio) is given by:

$$\phi_{litter} = 1 - METRX_KR_REDUCTION_CN \cdot \frac{C_{lit}}{N_{lit}}$$

The influence of C/N ratio on anaerobic decomposition of humus pool 2 / organic soil

$$\phi_{cn,org.soil} = 1 - \frac{1}{1 + e^{-0.5(C/N-30)}}$$

The influence of clay content is given by

$$\phi_{clay} = METRX_F_DECOMP_CLAY_1 + (1 - METRX_F_DECOMP_CLAY_1) \cdot e^{-METRX_F_DECOMP_CLAY_2 \cdot clay}$$

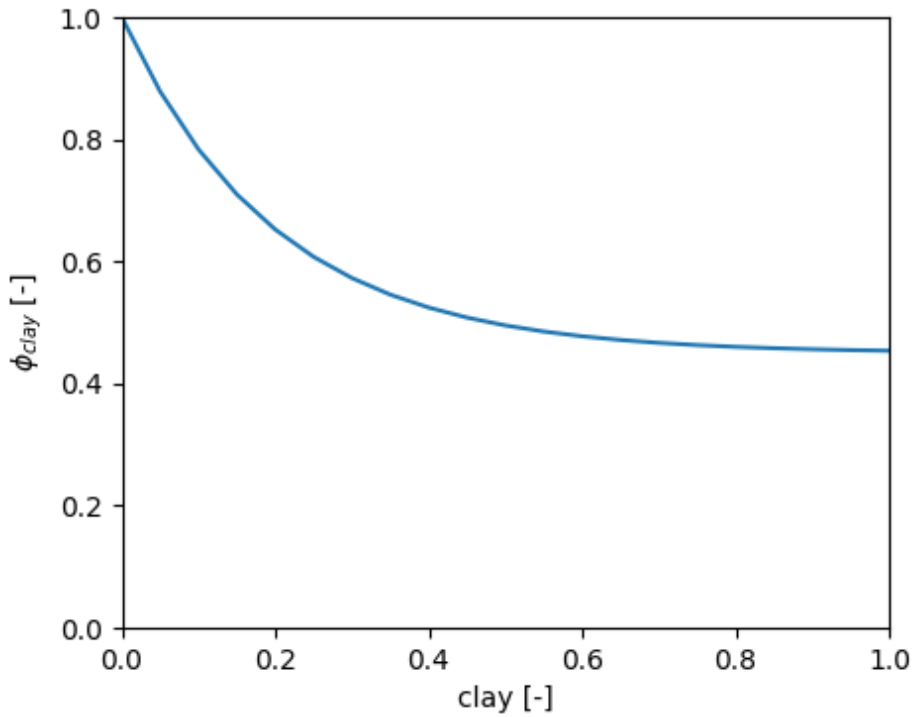


Figure 1.12: Response function of decomposition depending on clay

The influence of O₂ availability is given by the anaerobic volume fraction (*anvf*). The carbon flux from each litter and humus pool due to decomposition is distinguished by *anvf*:

$$\begin{aligned} \frac{dm_x}{dt} &= \frac{dm_{x,anvf}}{dt} + \frac{dm_{x,aevf}}{dt} \\ \frac{dm_{x,anvf}}{dt} &= K_x \cdot m_x \cdot \Pi_j \phi_j \cdot METRX_KR_REDUCTION_ANVF \cdot anvf \\ \frac{dm_{x,aevf}}{dt} &= K_x \cdot m_x \cdot \Pi_j \phi_j \cdot (1 - anvf) \end{aligned}$$

The influence of pH is given by:

$$\phi_{pH} = \frac{1}{1 + e^{-METRX_F_DECOMP_PH_1 \cdot (pH - METRX_F_DECOMP_PH_2)}}$$

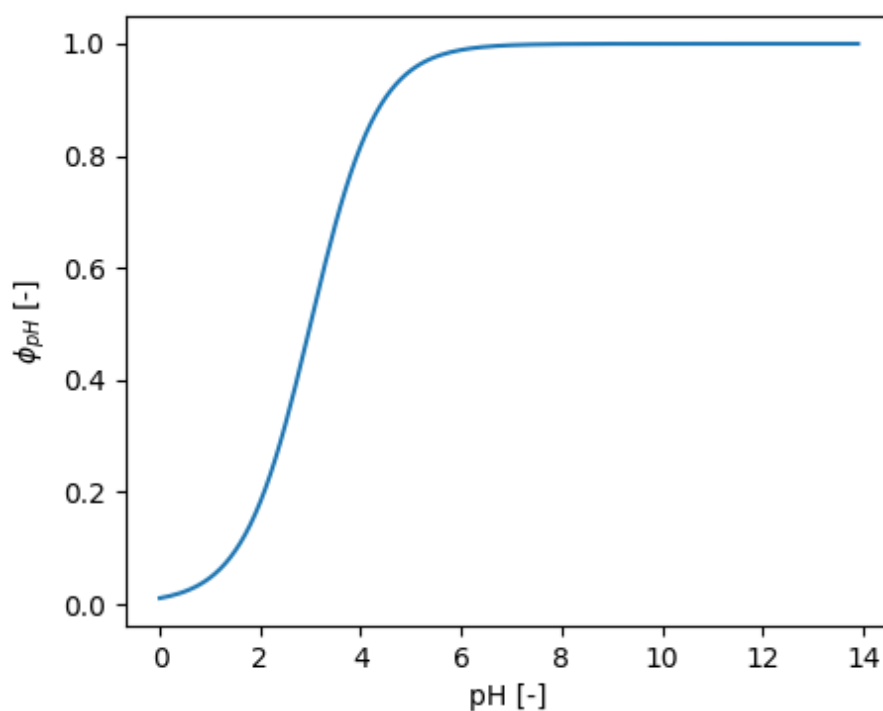


Figure 1.13: Response function of decomposition depending on pH

Overview of reduction factors for decomposition of litter and humus pools

Pool	Pa- rame- ter	tilling	Temp. Mois- ture	pH	litter type	litter C/N	clay	O2
Solutes	MET↔ RX_↔ KR_↔ DC_S↔ OL	yes	yes	yes	yes	yes	no	yes

Pool	Parameter	tilling	Temp. Moisture	pH	litter type	litter C/N	clay	O2
Cellulose	MET↔ RX_↔ KR_↔ DC_↔ CEL	yes	yes	yes	yes	yes	no	yes
Lignin	MET↔ RX_↔ KR_↔ DC_↔ CEL	yes	yes	yes	yes	yes	no	yes
Humus 1	MET↔ RX_↔ KR_↔ DC_↔ HUM1	yes	yes	yes	no	no	yes	yes
Humus 2	MET↔ RX_↔ KR_↔ DC_↔ HUM2	yes	yes	yes	no	no	yes	yes
Humus 3	MET↔ RX_↔ KR_↔ DC_↔ HUM3	yes	yes	yes	no	no	yes	yes

Decomposed carbon is added to DOC:

$$\begin{aligned}\frac{dDOC_{ae}}{dt} &= -\frac{dC_{x,aevf}}{dt} \\ \frac{dDOC_{an}}{dt} &= -\frac{dC_{x,anvf}}{dt}\end{aligned}$$

Decomposed nitrogen is partly mineralized and partly added to DON:

$$\begin{aligned}\frac{dNH_4}{dt} &= -0.5\frac{dN_x}{dt} \\ \frac{dDON}{dt} &= -0.5\frac{dN_x}{dt}\end{aligned}$$

Microbial dynamics Microbial growth is given by:

$$\frac{c_{mic}}{dt} = c_{mic} a_{mic} \mu_{mic} \phi_{DOC}$$

c_{mic} : Microbial biomass

a_{mic} : Microbial activity

μ_{mic} : Potential microbial growth rate

ϕ_{DOC} : Microbial growth dependency on DOC

The activity coefficient of microbes a_{mic} is given by a harmonic mean of a soil temperature (ϕ_T) and a soil water (ϕ_{wfps}) depending response coefficient.

$$a_{mic} = \frac{\phi_T + \phi_{wfps}}{\frac{1}{\phi_T} + \frac{1}{\phi_{wfps}}}$$

with ϕ_T given by:

$$\phi_T = e^{-METRX_F_MIC_T_EXP_1 \cdot \left(\frac{1-T}{METRX_F_MIC_T_EXP_2} \right)^2}$$

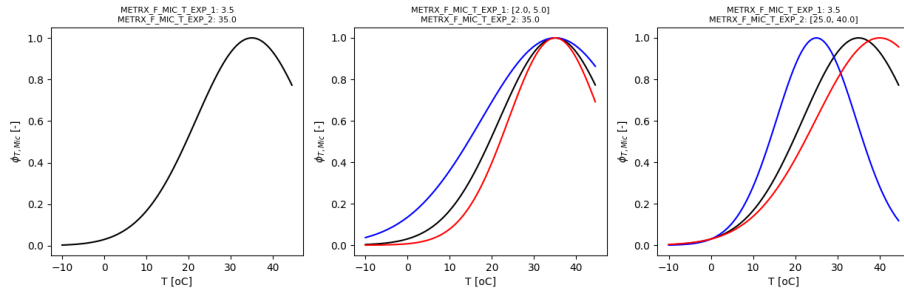


Figure 1.14: Microbial activity dependency on temperature

and with ϕ_{wfps} given by:

$$\phi_{wfps} = 1 - \frac{1}{1 + e^{(wfps - METRX_F_MIC_M_WEIBULL_1) \cdot METRX_F_MIC_M_WEIBULL_2}}$$

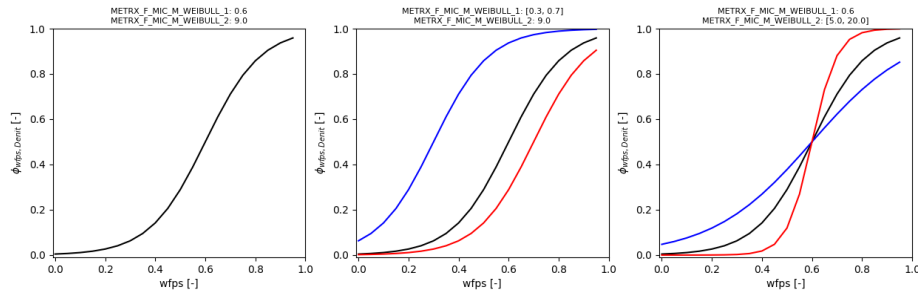


Figure 1.15: Microbial activity dependency on water

The potential microbial growth rate is given by the parameter: $MUE_MAX_C_MICRO_1$.

The dependency of microbial growth on DOC is given by:

$$\phi_{DOC} = \frac{DOC}{DOC + METRX_KMM_C_MIC}$$

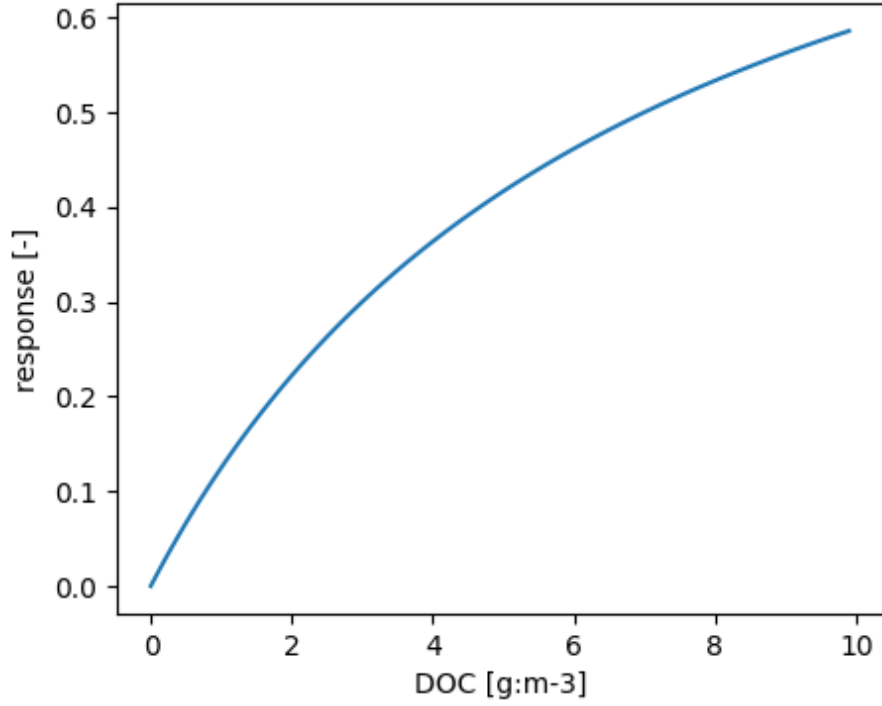


Figure 1.16: Microbial growth dependency on DOC

Microbial loss of biomass via maintenance respiration $\frac{c_{mic,r}}{dt}$ and death are calculated after Blagodatsky and Richter (1998) :

$$\begin{aligned}\frac{c_{mic,r}}{dt} &= c_{mic}a_{mic}a_{max}(1 - Y_r) \\ \frac{c_{mic,d}}{dt} &= c_{mic}a_{mic}a_{max} \frac{1}{1 + k_a \cdot DOC}\end{aligned}$$

c_{mic} : Microbial biomass

$c_{mic,r}$: Microbial biomass subject to respiration

$c_{mic,d}$: Microbial biomass subject to death

a_{mic} : Microbial activity

a_{max} : Maximum microbial death rate

Nitrification Nitrification is modeled as a two-stage process:



depending on microbial biomass.

NH4 nitrification The first step of Nitrification is given by:

$$\frac{dNH_4^+}{dt} = -c_{mic}a_{mic}\mu_{mic}\phi_{NH_4^+}\phi_{O_2}\phi_{ph}\phi_{ni}$$

c_{mic} : Microbial biomass

a_{mic} : Microbial activity

μ_{mic} : Microbial growth rate

$\phi_{NH_4^+}$: Microbial growth dependency on DOC

ϕ_{O_2} : Microbial growth dependency on O2

ϕ_{ph} : Microbial growth dependency on NH4

ϕ_{ni} : Effect of nitrification inhibitor

The activity coefficient of nitrifier a_{mic} is given by a harmonic mean of a soil temperature (ϕ_T) and a soil water (ϕ_{wfps}) depending response coefficient.

$$a_{mic} = \frac{\phi_T + \phi_{wfps}}{\frac{1}{\phi_T} + \frac{1}{\phi_{wfps}}}$$

with ϕ_T given by:

$$\phi_T = e^{-METRX_F_MIC_T_EXP_1 \cdot \left(\frac{1-T}{METRX_F_MIC_T_EXP_2} \right)^2}$$

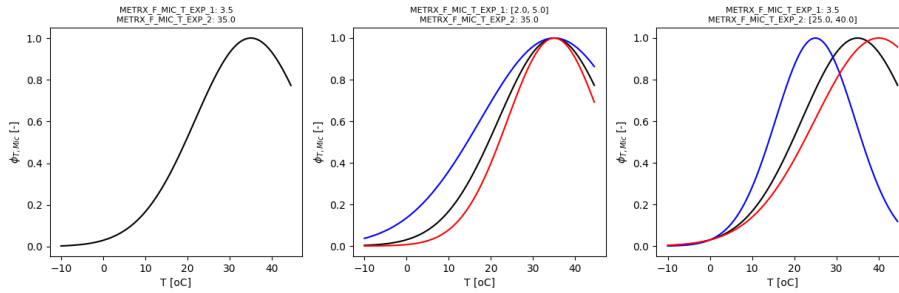


Figure 1.17: Response function depending on temperature

and with ϕ_{wfps} given by:

$$\phi_{wfps} = 1 - \frac{1}{1 + e^{(wfps - METRX_F_MIC_M_WEIBULL_1) \cdot METRX_F_MIC_M_WEIBULL_2}}$$

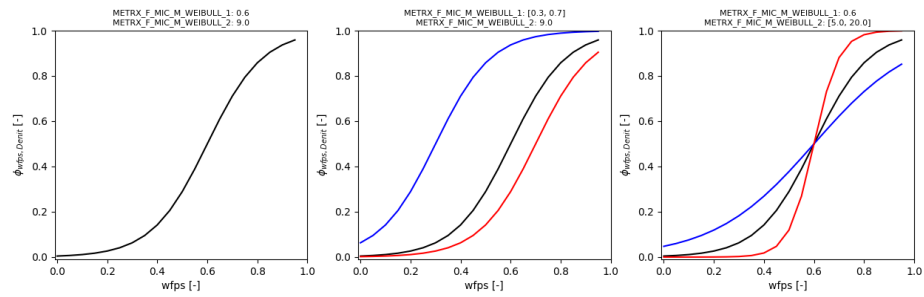


Figure 1.18: Response function depending on soilwater

The influence of NH_4^+ on nitrification of NH_4^+ is given by:

$$\phi_{NH_4^+} = \frac{NH_4^+}{NH_4^+ + METRX_KMM_NH4_NIT}$$

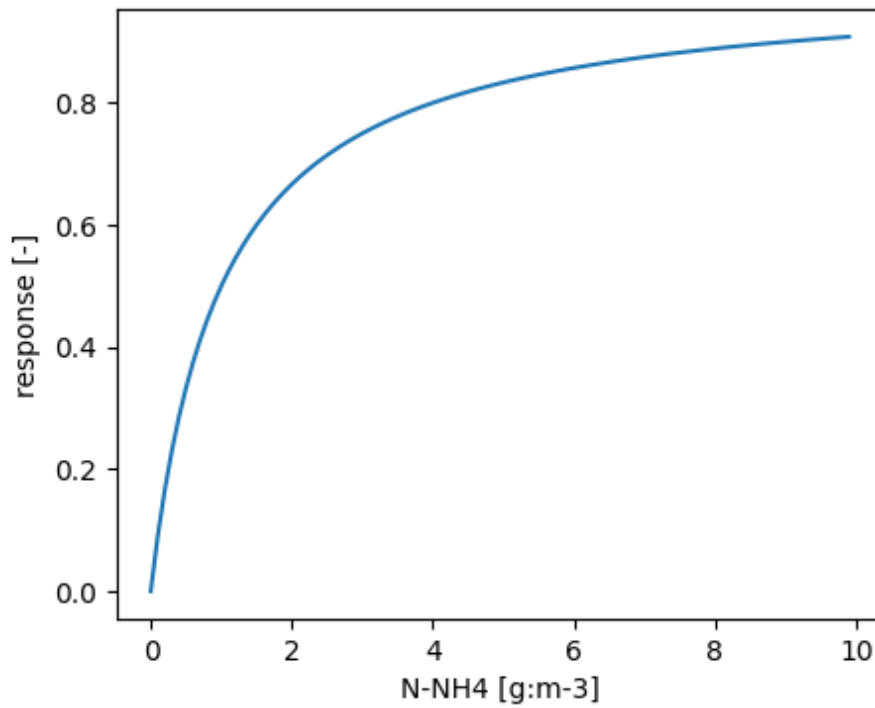


Figure 1.19: Nitrification of NH_4 depending on NH_4

The influence of O_2 on nitrification of NH_4^+ is given by:

$$\phi_{O_2} = \frac{O_2}{O_2 + METRX_KMM_O2_NIT}$$

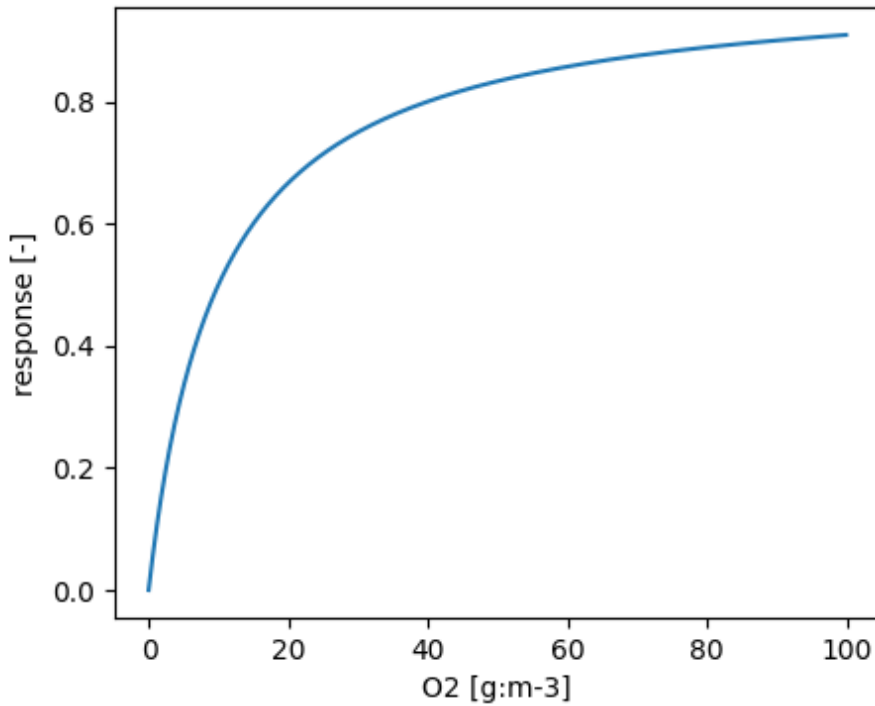


Figure 1.20: Nitrification of NH_4 depending on O_2

The influence of nitrification inhibitor is given by Enhanced efficiency nitrogen fertilizers.

Production of NO and N₂O during nitrification During the first step of nitrification a certain amount of N is lost in form of NO and N_2O . The relevant processes are a mix of:

- chemical decomposition of the metabolite hydroxylamine (NH_2OH) to NO
- nitrifier denitrification (denitrification within the nitrifying microbe)

Reported production of NO during nitrification:

- 0.1 - 10% of gross NH_4 oxidation (Ludwig et al., 2001)
- 0.6 - 2.5% of gross NH_4 oxidation (Garrido et al. 2002)

All N_2O produced in connection with nitrification was initially NO . Emissions of NO and N_2O during nitrification are influenced by soil temperature and moisture, 0.03% at 5oC and 40% WFPS to 0.12% at 25oC and 60% WFPS (Chen et al. 2010)

$$\frac{d(NO + N_2O)}{dt} = -METRX_KF_NIT_NO_N_2O \cdot \frac{dNH_4^+}{dt} \phi_{NO+N_2O,T,wfps}$$

The associated factor $\phi_{NO+N_2O,T,wfps}$ is given by a harmonic mean of a soil temperature ($\phi_{NO+N_2O,T}$) and a soil water ($\phi_{NO+N_2O,wfps}$) depending response coefficient:

$$\phi_{NO+N_2O,T,wfps} = \frac{2.0}{\frac{1.0}{\phi_{NO+N_2O,T}} + \frac{1.0}{\phi_{NO+N_2O,wfps}}}$$

with $\phi_{NO+N_2O,T}$ given by:

$$\phi_{NO+N_2O,T} = METRX_F_NIT_NO_N_2O_T_EXP_1 \cdot e^{\frac{T}{METRX_F_NIT_NO_N_2O_T_EXP_2}}$$

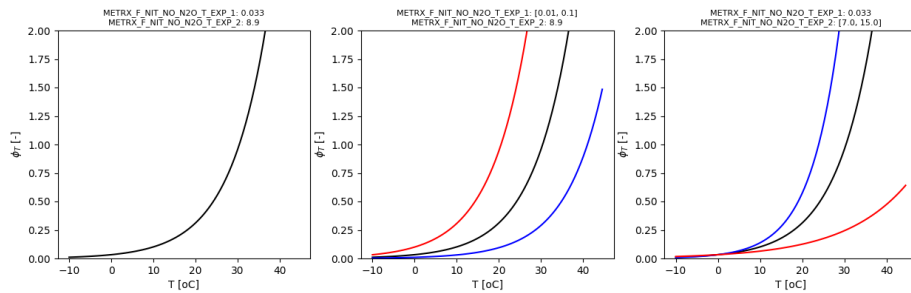


Figure 1.21: NO and N2O production during nitrification depending on soil temperature

and with $\phi_{NO+N_2O,wfps}$ given by:

$$\phi_{NO+N_2O,wfps} = 1 - \frac{1}{1 + e^{(wfps - METRX_F_NIT_NO_N_2O_M_WEIBULL_1) \cdot METRX_F_NIT_NO_N_2O_M_WEIBULL_2}}$$

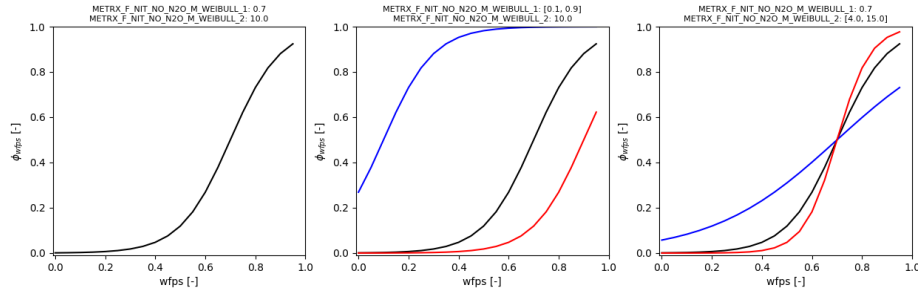


Figure 1.22: NO and N₂O production during nitrification depending on soil water

The fraction of NO depends on soil water:

$$\frac{d(NO)}{dt} = \frac{d(NO + N_2O)}{dt} \cdot \phi_{NO,wfps}$$

with

$$\phi_{NO,wfps} = 1 - \frac{1}{1 + e^{METRX_F_NIT_NO_M_EXP_1 \cdot (wfps - METRX_F_NIT_NO_M_EXP_2)}}$$

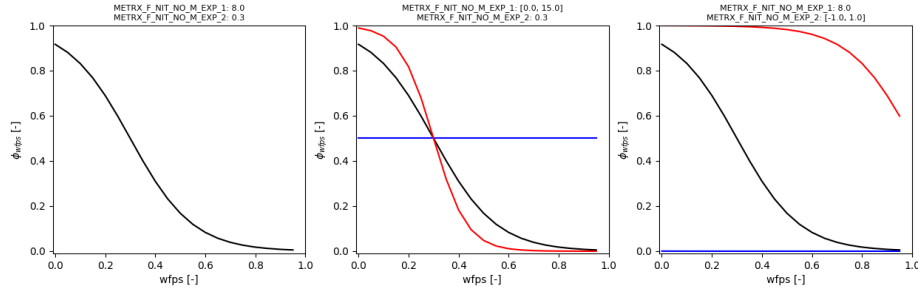


Figure 1.23: NO production during nitrification depending on soil water

No pH effect of ammonia oxidation on N₂O emissions observed (Booth, Stark and Rastetter 2005).

NO₂ nitrification The second step of nitrification is calculated independent of microbial biomass:

$$\frac{dNO_2^-}{dt} = \frac{NO_2^-}{METRX_KMM_NO2_NIT + NO_2^-}$$

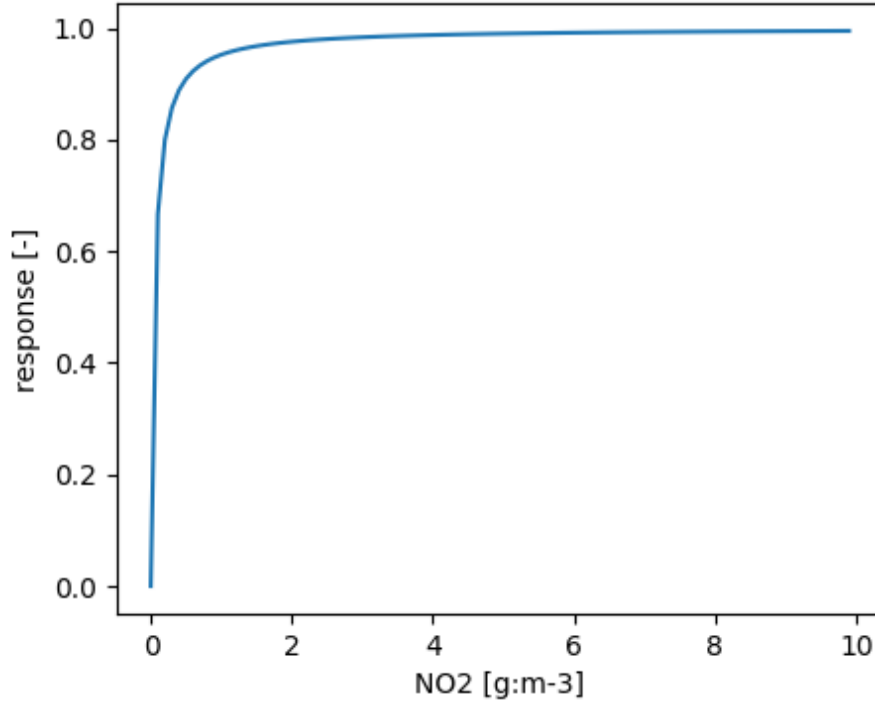
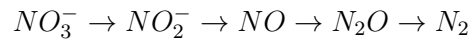


Figure 1.24: Nitrification of NO2 depending on NO2

Denitrification

Microbial denitrification Denitrification is calculated as four-step process including the nitrogen species NO_3^- , NO_2^- , NO and N_2O :



Denitrifier growth All denitrification steps are calculated based on actively denitrifying microbial biomass. The associated activity coefficient of denitrifying microbes a_{mic} is given by a harmonic mean of a soil temperature (ϕ_T) and a soil water (ϕ_{wfps}) depending response coefficient.

$$a_{mic} = \frac{2}{\frac{1}{\phi_T} + \frac{1}{\phi_{wfps}}}$$

with ϕ_T given by:

$$\phi_T = e^{-METRX_F_MIC_T_EXP_1 \cdot \left(1 - \frac{T}{METRX_F_MIC_T_EXP_2}\right)^2}$$

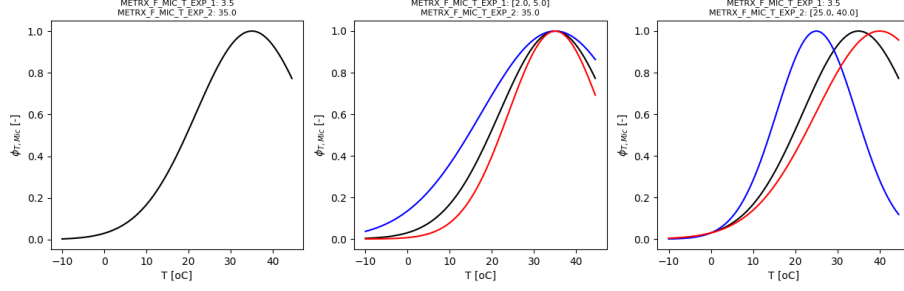


Figure 1.25: Response function depending on temperature

and with ϕ_{wfps} given by:

$$\phi_{wfps} = 1 - \frac{1}{1 + e^{(wfps - METRX_F_MIC_M_WEIBULL_1) \cdot METRX_F_MIC_M_WEIBULL_2}}$$

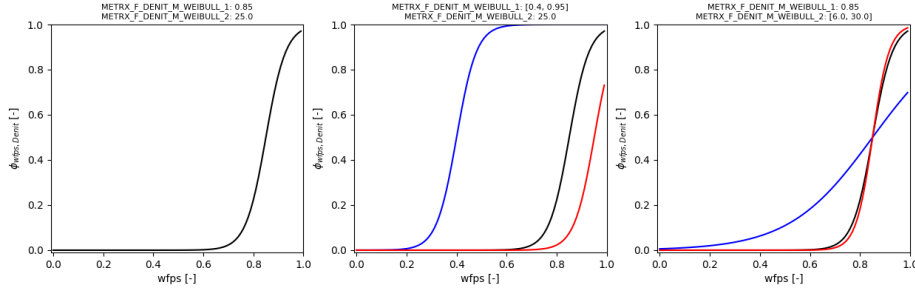


Figure 1.26: Response function depending on soilwater

Microbial growth depends on carbon and nitrogen availability:

$$\begin{aligned} \phi_C &= \frac{DOC}{DOC + METRX_KMM_C_DENIT} \\ \phi_N &= \frac{N_{total}}{N_{total} + METRX_KMM_N_DENIT} \\ \phi_{C,N} &= \frac{2}{\frac{1}{\phi_C} + \frac{1}{\phi_N}} \end{aligned}$$

Microbial enzymes relevant for denitrification are:

- narG and napA: ($\text{NO}_3 \rightarrow \text{NO}_2$)
- nirK and nirS: ($\text{NO}_2 \rightarrow \text{NO}$)
- cnorB and qnorB: ($\text{NO} \rightarrow \text{N}_2\text{O}$)
- nosZ ($\text{N}_2\text{O} \rightarrow \text{N}_2$)

Heterotrophic denitrification decreases with increasing pH (Kool et al. 2010). Low pH inhibits all enzymes but especially nosZ. The general pH influence on microbial denitrifier growth influencing all enzymes is given by:

$$\phi_{pH} = 1 - \frac{1}{1 + e^{\frac{ph - METRX_F_DENIT_PH_1}{METRX_F_DENIT_PH_2}}}$$

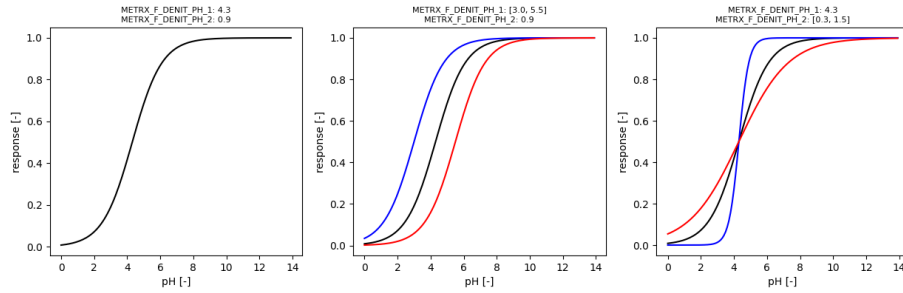


Figure 1.27: Response function of denitrification depending on pH

The pH factor specifically for nosZ influencing denitrification of N_2O is given by:

$$\phi_{pH,nosZ} = 1 - \frac{1}{1 + e^{\frac{ph - METRX_F_DENIT_N2O_PH_1}{METRX_F_DENIT_N2O_PH_2}}}$$

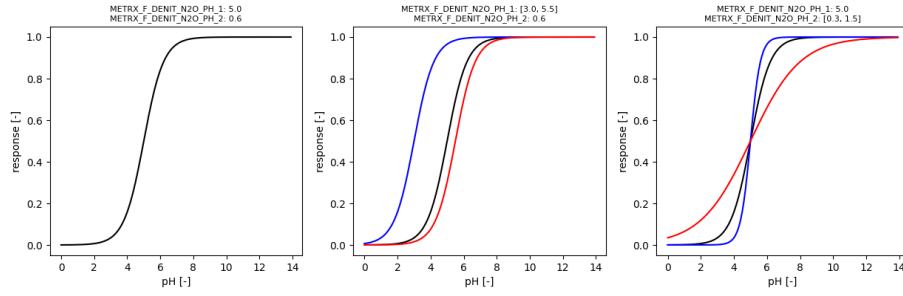


Figure 1.28: Response function of denitrification of N2O depending on pH

Total microbial carbon demand includes assimilation and dissimilation:

$$\begin{aligned}
 C_{demand} &= c_{mic} \mu_{mic} a_{mic} \frac{1.0}{Y_{denit}} \phi_{C,N} \phi_{pH} \\
 C_{demand,assi} &= C_{demand} Y_{denit} \\
 C_{demand,diss} &= C_{demand} (1 - Y_{denit})
 \end{aligned}$$

The denitrification efficiency is constant:

$$Y_{denit} = METRX_MIC_EFF_ANAEROBIC_RESPIRATION$$

Denitrifier nitrogen use Denitrification of N_x depends on their relative abundance using associated scaling factors:

$$\begin{aligned}
 \psi_{NO_3^-} &= \frac{NO_3^-}{NO_3^- + NO_2^- + NO + N_2O} \\
 \psi_{NO_2^-} &= (1 - \psi_{NO_3^-}) \cdot \frac{NO_2^-}{NO_2^- + NO + N_2O} \\
 \psi_{NO} &= (1 - \psi_{NO_3^-}) \cdot \frac{NO}{NO_2^- + NO + N_2O} \\
 \psi_{N_2O} &= (1 - \psi_{NO_3^-}) \cdot \frac{N_2O}{NO_2^- + NO + N_2O}
 \end{aligned}$$

N_x can be denitrified a single step or multiple steps before it is released from the denitrifying microbial organism to the soil environment. The fraction of N_x , which is completely

denitrified to N_2 within the same organism depends on the soil anaerobic volume (assuming denitrification enzymes are more developed under anaerobic conditions):

$$\phi_{anvf,1} = METRX_F_DENIT_N2_1 \cdot METRX_F_DENIT_N2_2 + V_{an} \cdot METRX_F_DENIT_N2_3$$

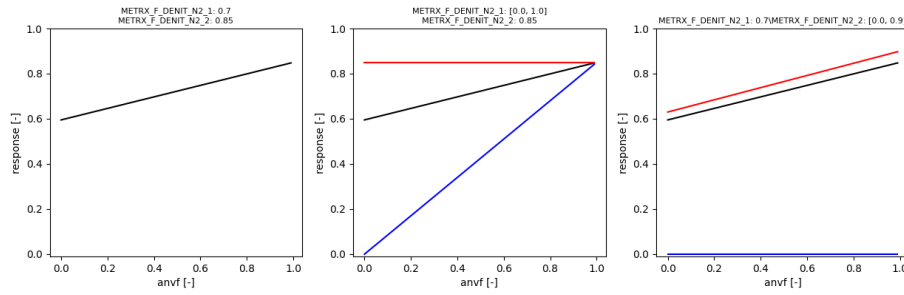


Figure 1.29: Response function of denitrification depending on anaerobicity

Stoichiometry between dissimilative nitrogen and carbon demand is based on succinate ($CH_{1.8}O_{0.5}N_{0.2}$) (Kampschreur et al. 2012):

- $C_4H_4O_4 + 3.23NO_3 + 1.64H + 0.36NH_4 \rightarrow 1.8CH_{1.8}O_{0.5}N_{0.2} + 3.23NO_2 + 2.2CO_2 + 1.92H_2O$
- $C_4H_4O_4 + 6.45NO_2 + 8.09H + 0.36NH_4 \rightarrow 1.8CH_{1.8}O_{0.5}N_{0.2} + 6.45NO + 2.2CO_2 + 5.15H_2O$
- $C_4H_4O_4 + 6.45NO + 1.64H + 0.36NH_4 \rightarrow 1.8CH_{1.8}O_{0.5}N_{0.2} + 3.23NO + 2.2CO_2 + 1.92H_2O$

Denitrification of NO_3^- Currently, it is assumed that after denitrification of NO_3^- , NO_2^- is always released to the environment:

$$\begin{aligned} \frac{dNO_3^-}{dt} &= \psi_{NO_3^-} \cdot C_{demand} \cdot \Xi_{CN,NO_3^-} \\ \Xi_{CN,NO_3^-} &= \xi_{CN,NO_3^- \rightarrow NO_2^-} \\ \frac{dNO_3^-}{dt} &= \frac{dNO_{3 \rightarrow NO_2}^-}{dt} \end{aligned}$$

Denitrification of NO_2^- Denitrified NO_2^- is partly transferred to NO , N_2O and N_2 depending on the anaerobicity of the soil. The associated carbon demand is given by:

$$\begin{aligned}\frac{dC_{\text{NO}_2^-}}{dt} &= \psi_{\text{NO}_2^-} \frac{C_{\text{denit}}}{dt} \\ \frac{dC_{\text{NO}_2^- \rightarrow \text{N}_2}}{dt} &= \frac{dC_{\text{NO}_2^-}}{dt} \cdot \phi_{\text{anvf},1} \cdot \phi_{\text{pH},\text{nosZ}} \\ \frac{dC_{\text{NO}_2^- \rightarrow \text{NO}}}{dt} &= \frac{dC_{\text{NO}_2^-}}{dt} \cdot (1 - \phi_{\text{anvf},1}) \cdot \phi_{\text{anvf},2} \\ \frac{dC_{\text{NO}_2^- \rightarrow \text{N}_2\text{O}}}{dt} &= \frac{dC_{\text{NO}_2^-}}{dt} - \frac{dC_{\text{NO}_2^- \rightarrow \text{N}_2}}{dt} - \frac{dC_{\text{NO}_2^- \rightarrow \text{NO}}}{dt}\end{aligned}$$

The stoichiometry between carbon and nitrogen is given by:

$$\begin{aligned}\frac{d\text{NO}_{2,\text{NO}_2^- \rightarrow \text{N}_2}^-}{dt} &= \xi_{\text{CN},\text{NO}_2^- \rightarrow \text{N}_2} \frac{dC_{\text{NO}_2^- \rightarrow \text{N}_2}}{dt} \\ \frac{d\text{NO}_{2,\text{NO}_2^- \rightarrow \text{NO}}^-}{dt} &= \xi_{\text{CN},\text{NO}_2^- \rightarrow \text{NO}} \frac{dC_{\text{NO}_2^- \rightarrow \text{NO}}}{dt} \\ \frac{d\text{NO}_{2,\text{NO}_2^- \rightarrow \text{N}_2\text{O}}^-}{dt} &= \xi_{\text{CN},\text{NO}_2^- \rightarrow \text{N}_2\text{O}} \frac{dC_{\text{NO}_2^- \rightarrow \text{N}_2\text{O}}}{dt}\end{aligned}$$

Denitrification of NO Denitrified NO is partly transferred to N_2O and N_2 depending on the anaerobicity of the soil. The associated carbon demand is given by:

$$\begin{aligned}\frac{dC_{\text{NO}}}{dt} &= \psi_{\text{NO}} \frac{C_{\text{denit}}}{dt} \\ \frac{dC_{\text{NO} \rightarrow \text{N}_2}}{dt} &= \frac{dC_{\text{NO}}}{dt} \cdot \phi_{\text{anvf},1} \cdot \phi_{\text{pH},\text{nosZ}} \\ \frac{dC_{\text{NO} \rightarrow \text{N}_2\text{O}}}{dt} &= \frac{dC_{\text{NO}}}{dt} - \frac{dC_{\text{NO} \rightarrow \text{N}_2}}{dt}\end{aligned}$$

The stoichiometry between carbon and nitrogen is given by:

$$\begin{aligned}\frac{d\text{NO}_{\text{NO} \rightarrow \text{N}_2}}{dt} &= \xi_{\text{CN},\text{NO} \rightarrow \text{N}_2} \frac{dC_{\text{NO} \rightarrow \text{N}_2}}{dt} \\ \frac{d\text{NO}_{\text{NO} \rightarrow \text{N}_2\text{O}}}{dt} &= \xi_{\text{CN},\text{NO} \rightarrow \text{N}_2\text{O}} \frac{dC_{\text{NO} \rightarrow \text{N}_2\text{O}}}{dt}\end{aligned}$$

Denitrification of N₂O The associated carbon demand is given by:

$$\frac{dC_{N_2O}}{dt} = \psi_{N_2O} \frac{C_{denit}}{dt}$$

The stoichiometry between carbon and nitrogen is given by:

$$\frac{dN_2O}{dt} = \xi_{CN,N_2O} \frac{dC_{N_2O}}{dt}$$

Chemodenitrification At low pH (<4.5) N₂O can be produced via chemical decomposition of hydroxylamine (NH₂OH), nitroxyl hydride (HNO) or NO₂⁻, which are intermediate products of ammonia oxidation (Zumft 1997; Wragge et al. 2001).

Temperature dependency of chemodenitrification:

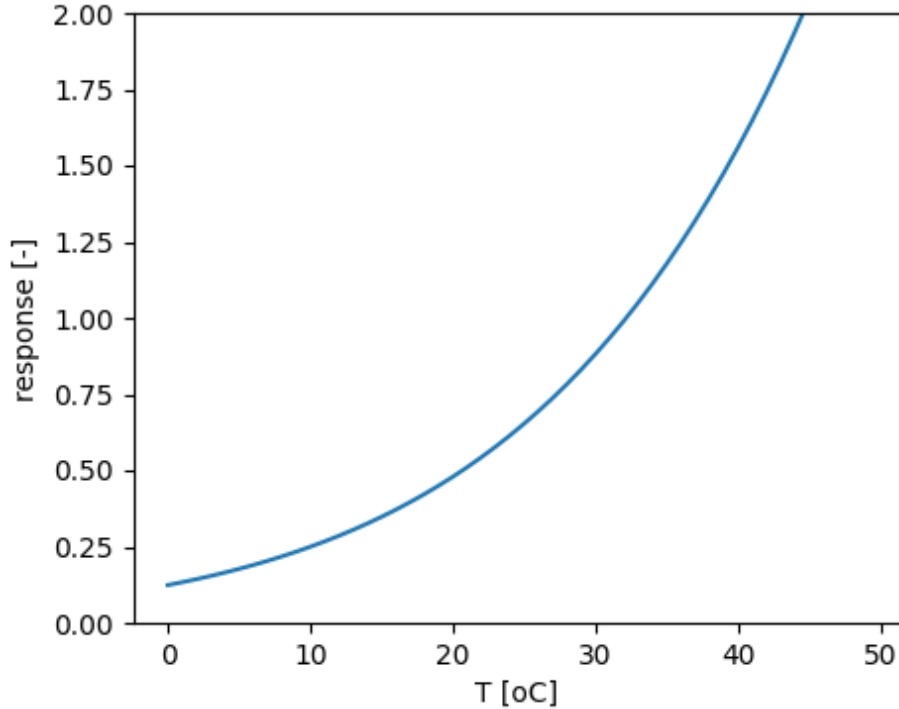


Figure 1.30: Response function depending on temperature

pH dependency of chemodenitrification:

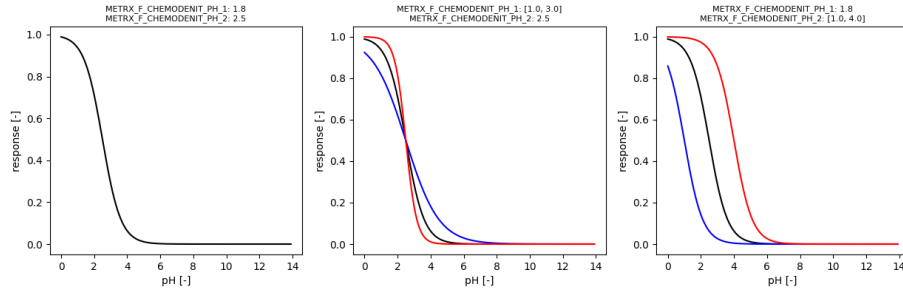


Figure 1.31: Response function depending on pH

Fermentation and syntrophy Under anaerobic conditions acetate and hydrogen are produced, which may serve as substrate for iron reducing and methanogenic bacteria.

Temperature dependency of microbial activity:

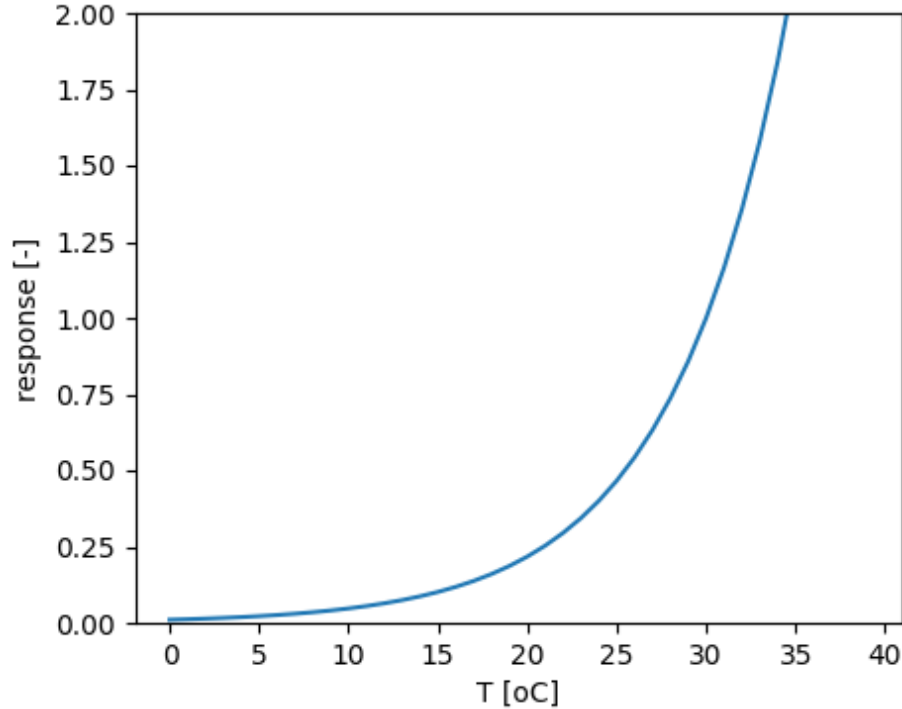
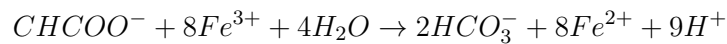
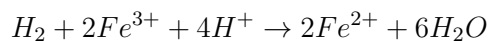


Figure 1.32: Response function depending on temperature

Iron reduction The stoecheometry of iron reduction via aceate is given by::



The stoecheometry of iron reduction via aceate is given by::



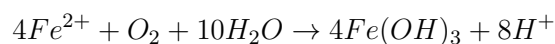
Iron reduction via acetate and hydrogen depends on the amount of Fe3+ and the amount of either acetate or hydrogen each modeled using a Michaelis Menten kinetic. Further influencing factors are temperature, NO3 and O2:

$$\frac{dFe^{3+}}{dt} = -METRX_MUEMAX_C_FE_RED \cdot \phi_T \cdot \phi_{NO3} \cdot \phi_{O2} \cdot \phi_{Fe3+} \cdot \phi_{AC/H2}$$

The dependy on NO3 is given by:

$$\phi_{NO3} = 1 - \frac{NO3}{NO3 + NO3_MOLAR_MAX_FE_RED}$$

Iron oxidation The stoecheometry of iron oxidation is given by::



$$\frac{dFe^{2+}}{dt} = -METRX_KR_OX_FE \cdot Fe^{2+} \cdot \phi_{O2}$$

The dependy on O2 is given by:

$$\phi_{O2} = \frac{O_2}{O_2 + METRX_KMM_O2_FE_OX}$$

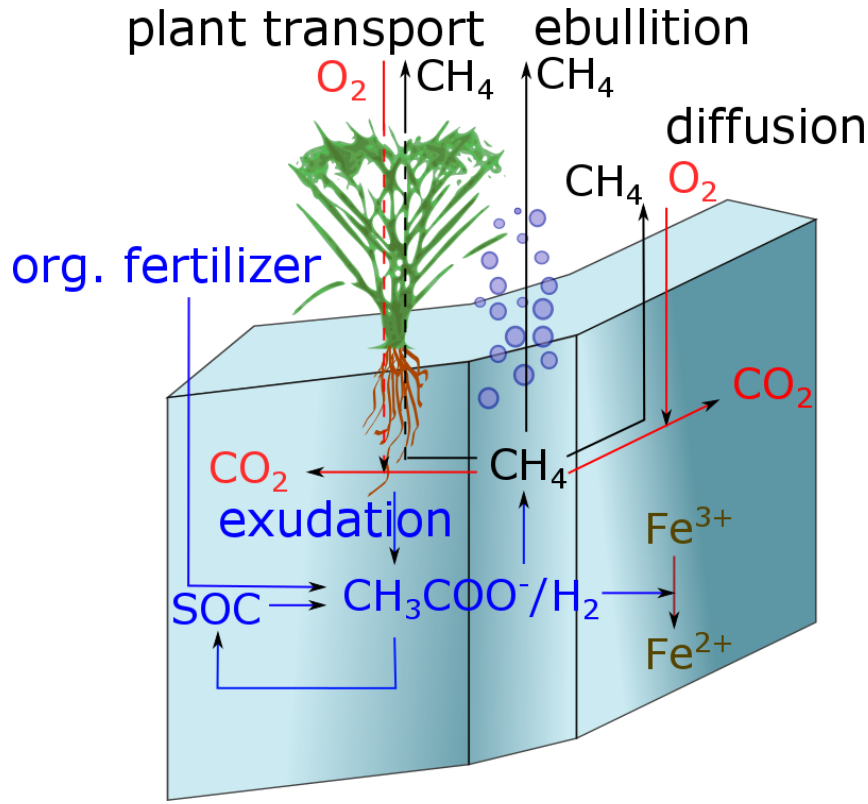


Figure 1.33: Scheme of methane related processes

Methane production Methane production takes first place after large fraction of total iron has been reduced:

$$Fe^{3+} < METRX_FRAC_FE_CH4_PROD \cdot (Fe^{3+} + Fe^{2+})$$

Methane production depends on temperature and pH:

$$\phi_T = \frac{METRX_F_CH4_PRODUCTION_T_EXP_1}{\left(1 - \frac{1}{METRX_F_CH4_PRODUCTION_T_EXP_2}\right)^2}$$

$$\phi_{pH} = \frac{1}{1 + \left(\frac{|pH-7|}{2}\right)^{3.4}}$$

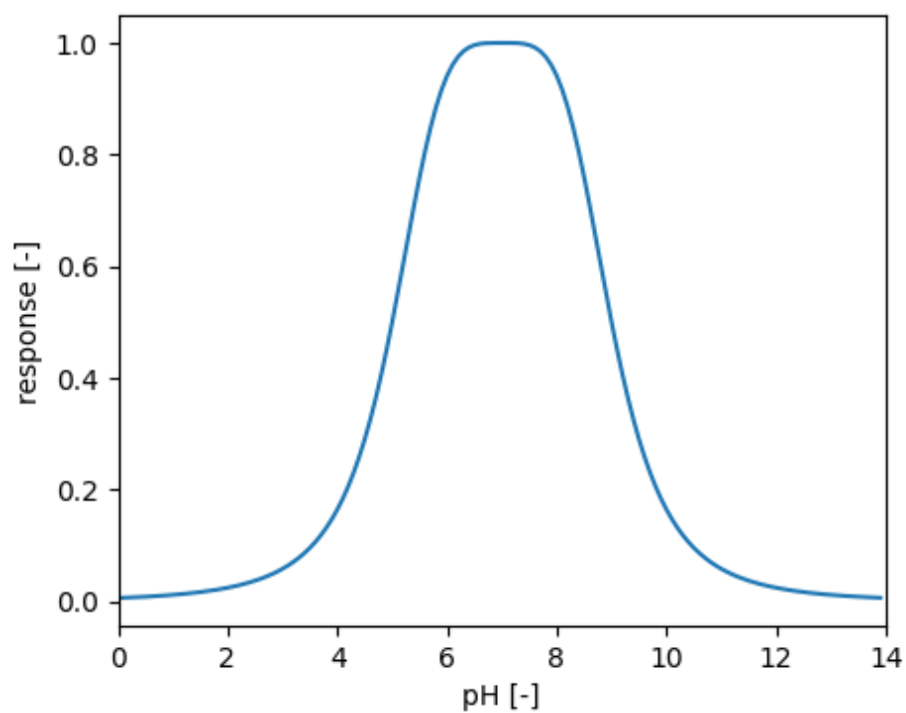


Figure 1.34: pH dependency of methane production

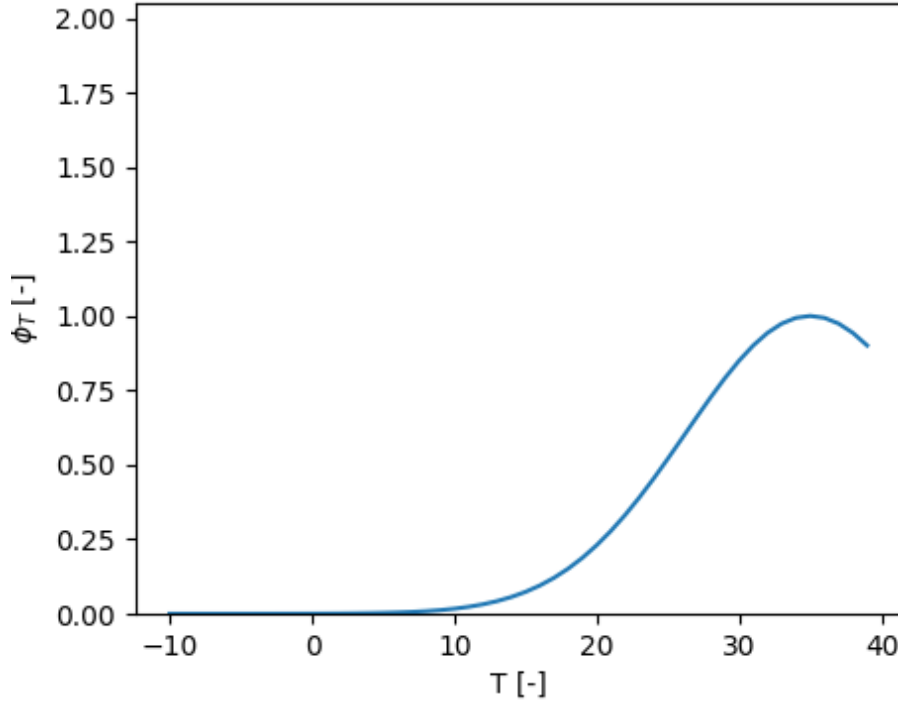
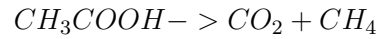


Figure 1.35: Temperature dependency of methane production

The stoecheometric formula for acetate methanogenesis is given by:



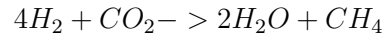
Acetoclastic methanogenesis is given by:

$$\frac{dCH_4}{dt} = METRX_MUEMAX_C_CH4_PROD \cdot \phi_{CH_3COOH} \cdot \phi_T \cdot \phi_{pH} \cdot \phi_{O_2}$$

with ϕ_{CH_3COOH} given by:

$$\phi_{CH_3COOH} = \frac{CH_3COOH}{METRX_KMM_AC_CH4_PROD + CH_3COOH}$$

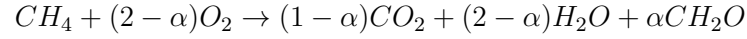
The stoecheometric formula for hydrogenotrophic methanogenesis is given by:



Hydrogenotrophic methanogenesis is given by:

$$\frac{\partial CH_4}{\partial t} = METRX_MUEMAX_H2_CH4_PROD \cdot \phi_{H_2} \cdot \phi_T \cdot \phi_{pH} \cdot \phi_{O_2}$$

Methane oxidation The stoeecheometry of methanotrophy is given by:



Methane oxidation depends on nitrogen, oxygen and methane concentration as well as temperature:

$$\begin{aligned}\phi_N &= (1 - METRX_F_N_CH4_OXIDATION) \\ &\quad METRX_F_N_CH4_OXIDATION \frac{N}{METRX_KMM_N_CH4_OX + N} \\ \phi_{O_2} &= \frac{O_2}{METRX_K_O2_CH4_OX \cdot O_2} \\ \phi_{CH_4} &= \frac{CH_4}{METRX_KMM_CH4_CH4_OX + CH_4} \\ \phi_T &= METRX_F_CH4_OXIDATION_T_EXP_1 \\ &\quad \left(1 - \frac{1}{METRX_F_CH4_OXIDATION_T_EXP_2}\right)^2\end{aligned}$$

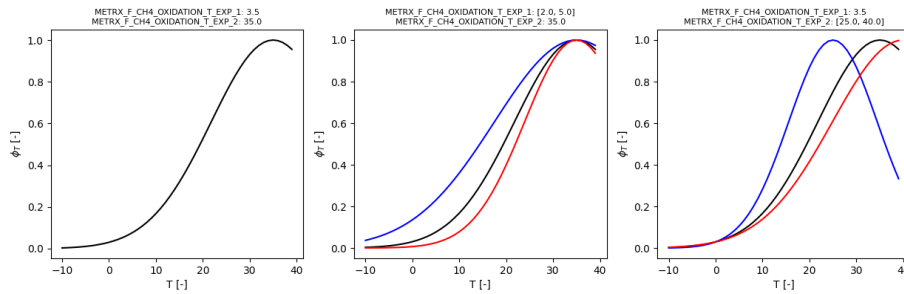


Figure 1.36: Temperature dependency of methane oxidation

Methane oxidation is given by:

$$\frac{dCH_4}{dt} = -METRX_MUEMAX_C_CH4_OX \cdot \phi_N \cdot \phi_{O_2} \cdot \phi_{CH_4} \cdot \phi_T$$

Algae growth Algae growth is only considered if option "algae" is set true.

Algae growth only takes place if ponding water table exists and incoming shortwave radiation directly above soil (below canopy) is greater zero.

Algae growth rate depends on:

- Nitrogen availability:

$$\phi_N = (1.0 - \Phi_{METRX_F_N_ALGAE}) + \Phi_{METRX_F_N_ALGAE} \cdot \frac{N}{\Phi_{METRX_KMM_N_ALGAE} + N}$$

- Temperature:

$$\phi_T = \begin{cases} 0.0 & T \leq 15.0 \\ \frac{T-15.0}{15.0} & 15.0 < T \leq 30.0 \\ 1.0 - \frac{T-30.0}{15.0} & 30.0 < T \leq 45.0 \\ 0.0 & 45.0 > T \end{cases}$$

- Photosynthetic radiation:

$$\phi_P = 1.0 - e^{\frac{-P}{100.0}}$$

Algae growth rate is given by:

$$\mu_g = \Phi_{METRX_MUEMAX_C_ALGAE} \cdot \min(\phi_N, \phi_T, \phi_P)$$

Algae growth changes pH value of the ponding water table:

$$\Delta pH = 3.0 \cdot \phi_N \cdot \phi_T \cdot \phi_P$$

Algae turnover:

$$\mu_d = m_A \cdot \Phi_{METRX_AMAX_ALGAE}$$

Chemistry

NH₃-NH₄ equilibrium The chemical equilibrium between dissolved NH_3 and NH_4 is given by (Sadeghi et al., 1988):

$$\begin{aligned} f_{NH_3} &= \frac{c_{NH_3}}{c_{NH_3} + c_{NH_4}} \\ f_{NH_3} &= \frac{1}{1 + \frac{10^{-pH}}{K_a}} \\ K_a &= 10^{\frac{-2728.3}{T} - 0.094219} \end{aligned}$$

The chemical equilibrium between dissolved NH_3 and NH_4 is calculated for the surface water table and the soil solution.

Ammonium adsorption Ammonium is partly adsorped at the soil surface depending on soil texture.

Dissolution Phase equilibrium between dissolved and gaseous state is calculated throughout the soil profile as well as for the top layer of the surface water table (if existing).

For the following species the phase equilibrium between dissolved and gaseous state is calculated:

- O_2
- CH_4
- CO_2
- NH_3
- NO
- N_2O

For the equilibrium between the partial pressure in the gas phase $p_{i,gas}$ and the concentrations in the dissolved species i , the Henry law is applied:

$$c_{i,liq} = H_i p_{i,gas}$$

Diffusion of gaseous species Gaseous diffusion is calculated for:

- O_2
- N_2O (separately for aerobic and anaerobic species)
- NO (separately for aerobic and anaerobic species)
- CH_4
- CO_2
- NH_3

For the bottom, a Neuman no-flow boundary condition is used and for the top a Dirichlet boundary condition is used.

Diffusion of dissolved species Diffusion of dissolved species is calculated for:

- O_2
- CH_4
- CO_2
- NH_3
- Urea
- NH_4
- NO_3
- DOC

The amount of dissolved matter that leaves the simulated domain is added to the leaching output.

If there is a calculated inflow of matter, there is a following correction of mass. The mass is scaled down throughout the whole profile by the amount of calculated mass inflow.

Ebullition Ebullition is calculated in the soil as well as in the water table. Considered substances are CH_4 , CO_2 , O_2 , NH_3 , NO , N_2O and N_2 .

Gas bubbles can be formed as soon as a critical water filled pore space is reached.

Ebullition occurs as soon as total pressure ($CH_4 + CO_2 + \dots$) exceeds static pressure. Once formed, gas bubbles are transported upwards not being dissolved in upper soil layers as long as water filled pore space is below critical water filled pore space.

If water filled pore space is below critical water filled pore space, gas bubbles are dissolved.

Perturbation

Anaerobic volume MeTrx considers for a subset of carbon and nitrogen species a horizontal (within one soil layer) differentiation between aerobic and anaerobic parts of the soil. The differentiation is based on the oxygen partial pressure, which in turn is mainly determined by the water profile, respiration processes and gaseous diffusion of oxygen.

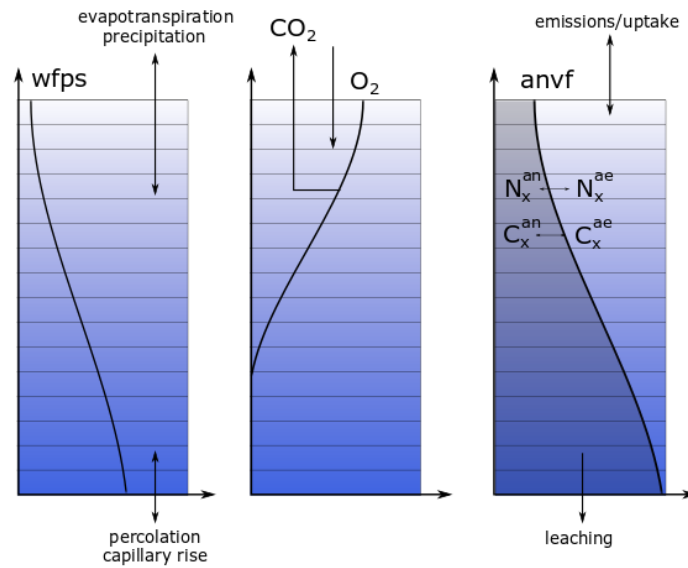


Figure 1.37: Scheme of soil profile anaerobicity

The anaerobic volume V_{an} within one soil layer is given by:

$$V_{an} = e^{-(\tau p_{O_2})^2}$$

wherein p_{O_2} refers to the oxygen partial pressure in bar.

Currently, two different anaerobic volume definitins can be considered:

- a "relaxed" one affecting processes, which are not exclusively subject to strict anaerobic conditions, e.g., decomposition of soil organic matter
- a "strict" one affecting processes, which require rather strict anaerobic condtions, e.g., denitrification

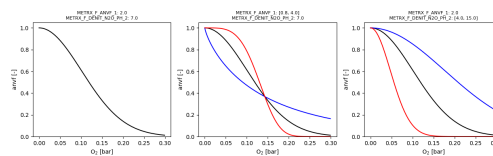


Figure 1.38: Size of the relaxed anaerobic volume fraction depending on partial pressure of oxygen

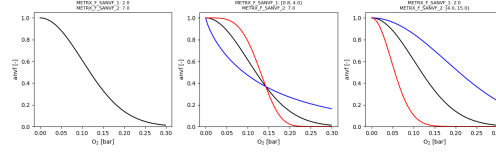


Figure 1.39: Size of the strict anaerobic volume fraction depending on partial pressure of oxygen

A change of the size of the anaerobic volume induces redistribution of the aerobic and anaerobic part of carbon and nitrogen species.

Redistribution occurs by:

- Relative change of the size of the anaerobic volume
- Active transport between aerobic and anaerobic volume

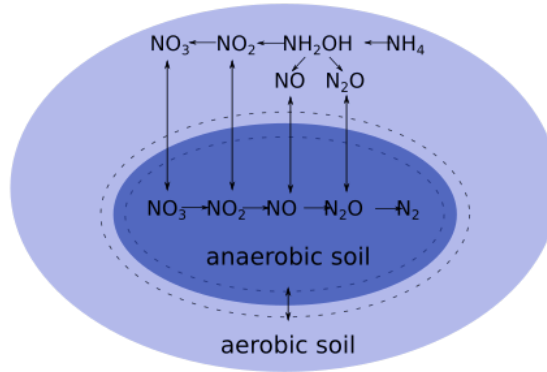


Figure 1.40: Scheme of (an-)aerobic soil fractions

The relative change of a species c_x only takes place if the share between aerobic and anaerobic volume changes:

$$\frac{\partial c_{x,an}}{\partial t} = \frac{c_{x,an}}{V_{an}} \frac{\partial V_{an}}{\partial t}$$

$$\frac{\partial c_{x,ae}}{\partial t} = - \frac{\partial c_{x,an}}{\partial t}$$

The active transport of a species c_x is given by:

$$\frac{\partial c_{x,an}}{\partial t} = T^* \left(c_{x,an} - c_{x,tot} \frac{V_{an}}{V_{tot}} \right)$$

$$\frac{\partial c_{x,ae}}{\partial t} = - \frac{\partial c_{x,an}}{\partial t}$$

The transport coefficient T^* is determined by the two parameters:

– *METRX_KR_ANVF_DIFF_GAS*

– *METRX_KR_ANVF_DIFF_LIQ*

for gaseous and dissolved species, respectively.

Field management

Fertilization MeTrx considers the following list of synthetic fertilizer:

- NH_4NO_3
- NH_3
- NO_3
- NH_4
- NH_4SO_4
- SO_4
- Urea
- CRNF (controlled release fertilizer)
- NI (Nitrification inhibitor)

Manuring MeTrx considers the following list of organic fertilizer:

- slurry
- farmyard
- compost
- straw
- green manure

Tilling Within the given tilling depth, the following effects are considered:

- stubble and aboveground raw litter are incorporated to soil litter pools.
- all C- and N-pools are homogenized
- decomposition is stimulated

Urea hydrolysis Urea from fertilizer or manure is dissolved to ammonium in soil and/or in the surface water table depending on temperature:

$$\frac{dNH_4^+}{dT} = N_{urea}\phi_T$$

$$\frac{dN_{urea}}{dT} = -\frac{dNH_4^+}{dT}$$

Depending on the rate of urea hydrolysis, the pH value from of the respective soil layer or water table layer is increased:

$$pH = pH_i + \frac{\frac{dN_{urea}}{dT}}{METRX_KMM_PH_INCREASE_FROM_UREA}$$

with p_i representing the basi pH value that has been defined as model input.

Nitrogen fertilizer release

MeTrx Output

entity name	decription	unit
anvf	Anaerobic volume fraction averaged over the complete soil profile	[-]
pore_connectivity	Pore connectivity averaged over the complete soil profile	[-]
permeability	Permeability averaged over the complete soil profile	[-]
wfps	Water filled pore space averaged over the complete soil profile	[-]
air	Water filled pore space averaged over the complete soil profile	[-]
root_conductivity	Root conductivity averaged over the complete soil profile	[m2s-1]
o2	Sum of oygen mass over the complete soil profile	[kg ha-1]
t_eff_crnf	...	[oC]
n_release_fraction_crnf	...	[-]
nitrification_inhibition	Inhibition of nitrification	[-]
urease_inhibition	Inhibition of urease hydrolysis	[-]
carbon_use_efficiency	Carbon use efficiency	[-]

entity name	decription	unit
N_don	Sum of dissolved organic nitrogen mass over the complete soil profile	[kgha-1]
N_nh4	Sum of ammonium mass over the complete soil profile	[kgha-1]
N_nh4_clay	Sum of ammonium adsorbed to clay minerals mass over the complete soil profile	[kgha-1]
N_urea	Sum of urea mass over the complete soil profile	[kgha-1]
N_no2_ae	Sum of aerobic NO2 mass over the complete soil profile	[kgha-1]
N_no2_an	Sum of anaerobic NO2 mass over the complete soil profile	[kgha-1]
N_no3_ae	Sum of aerobic NO3 mass over the complete soil profile	[kgha-1]
N_no3_an	Sum of anaerobic NO3 mass over the complete soil profile	[kgha-1]
N_n2o_ae	Sum of aerobic N2O mass over the complete soil profile	[kgha-1]
N_n2o_an	Sum of anaerobic N2O mass over the complete soil profile	[kgha-1]
N_no_ae	Sum of aerobic NO mass over the complete soil profile	[kgha-1]
N_no_an	Sum of anaerobic NO mass over the complete soil profile	[kgha-1]
N_nh3_gas	Sum of gaseous ammonia mass over the complete soil profile	[kgha-1]
N_nh3_liq	Sum of dissolved ammonia mass over the complete soil profile	[kgha-1]
C_doc_ae	Dissolved organic carbon (aerobic soil volume)	[kgCha-1]
C_doc_an	Dissolved organic carbon (anaerobic soil volume)	[kgCha-1]
C_acetate	Acetate	[kgCha-1]
C_ch4_gas	Methane in gas phase	[kgCha-1]
C_ch4_liq	Dissolved methane	[kgCha-1]
C_aorg	Amount of carbon in active organic material pool	[kgCha-1]

entity name	decription	unit
N_aorg	Amount of carbon in active organic material pool	[kgNha-1]
C_micro_1	Amount of carbon in microbial pool 1	[kgCha-1]
C_micro_2	Amount of carbon in microbial pool 2	[kgCha-1]
C_micro_3	Amount of carbon in microbial pool 3	[kgCha-1]
N_micro_1	Amount of nitrogen in microbial pool 1	[kgNha-1]
N_micro_2	Amount of nitrogen in microbial pool 2	[kgNha-1]
N_micro_3	Amount of nitrogen in microbial pool 3	[kgNha-1]
C_humus_1	Amount of carbon in humus pool 1	[kgCha-1]
C_humus_2	Amount of carbon in humus pool 2	[kgCha-1]
C_humus_3	Amount of carbon in humus pool 3	[kgCha-1]
N_humus_1	Amount of nitrogen in humus pool 1	[kgNha-1]
N_humus_2	Amount of nitrogen in humus pool 2	[kgNha-1]
N_humus_3	Amount of nitrogen in humus pool 3	[kgNha-1]
C_litter_soil_1	Amount of carbon in soil litter pool 1	[kgCha-1]
C_litter_soil_2	Amount of carbon in soil litter pool 2	[kgCha-1]
C_litter_soil_3	Amount of carbon in soil litter pool 3	[kgCha-1]
N_litter_soil_1	Amount of nitrogen in soil litter pool 1	[kgNha-1]
N_litter_soil_2	Amount of nitrogen in soil litter pool 2	[kgNha-1]
N_litter_soil_3	Amount of nitrogen in soil litter pool 3	[kgNha-1]
C_algae	Amount of carbon in algae pool	[kgCha-1]
N_algae	Amount of nitrogen in algae pool	[kgNha-1]
C_litter_stubble	Amount of nitrogen in stubble pool	[kgCha-1]
N_litter_stubble	Amount of nitrogen in stubble pool	[kgNha-1]

entity name	decription	unit
C_total	Total soil organic carbon	[kgCha-1]
N_total	Total soil organic nitrogen	[kgNha-1]
soc_20cm	Soil organic carbon content in the top 20 cm soil horizon	[%]
soc_40cm	Soil organic carbon content in the top 40 cm soil horizon	[%]
totn_20cm	Total nitrogen content in the top 20 cm soil horizon	[%]
totn_40cm	Total nitrogen content in the top 40 cm soil horizon	[%]
fe2_tot	...	□
fe3_tot	...	□
till_fact	...	□
freeze_thaw_fact	...	□
height_litter	Height of the surface litter layer	[m]
ph_watertable	...	□
ph_soil_surface	...	□
dN_no3_groundwater	...	□
dN_assi	...	□
dN_nit_nh4_no2	...	□
dN_nit_no2_no3	...	□
dN_nit_no2_no	...	□
dN_nit_no2_n2o	...	□
dN_denit_no3_no2	...	□
dN_denit_no2_no	...	□
dN_denit_no2_n2o	...	□
dN_denit_no2_n2	...	□
dN_denit_no_n2o	...	□
dN_denit_no_n2	...	□
dN_denit_n2o_n2	...	□
dN_chemodenit_no2_no	...	□
dC_ch4_oxidation	...	[kgCha-1]
dC_ch4_production_hydrogen	...	[kgCha-1]
dC_ch4_production_acetate	...	[kgCha-1]
dC_floor_ch4_plant_diffusion	...	[kgCha-1]
dC_floor_ch4_soil_diffusion	...	[kgCha-1]

entity name	decription	unit
dC_floor_ch4_water_diffusion	...	[kgCha-1]
dC_floor_ch4_bubbling	...	[kgCha-1]
dC_leach_ch4	...	[kgCha-1]
dO_floor_o2_plant_diffusion	...	[]
dC_litter_above	...	[kgCha-1]
dC_litter_below	...	[kgCha-1]
dC_fix_algae	...	[kgCha-1]
dN_fix_algae	...	[]
dC_decomp_litter	...	[kg:ha-1]
dC_co2_prod_mic_1_growth	...	[kgCha-1]
dC_co2_prod_mic_1_↔ maintenance	...	[kgCha-1]
dC_co2_prod_mic_2	...	[kgCha-1]
dC_co2_prod_mic_3_acetate_↔ prod	...	[kgCha-1]
dC_co2_prod_mic_3_acetate_↔ cons	...	[kgCha-1]
dC_co2_prod_ch4_prod	...	[kgCha-1]
dC_co2_prod_ch4_cons	...	[kgCha-1]
dH_hydrogen_prod	...	[]
dC_acetate_prod	...	[kgCha-1]
dC_acetate_cons_fe3	...	[kgCha-1]
dH_hydrogen_cons_fe3	...	[]
dC_doc_prod_litter	...	[kgCha-1]
dC_doc_prod_humus	...	[kgCha-1]
dC_doc_prod_aorg	...	[kgCha-1]
dC_doc_prod_plant	...	[kgCha-1]
dC_doc_prod_total	...	[kgCha-1]
dC_humify_mic_hum_2	...	[kgCha-1]
dC_humify_hum_1_hum_2	...	[kgCha-1]
dC_humify_hum_2_hum_3	...	[kgCha-1]

MeTrx output (daily)

entity name	decription	unit
N_nh4	Ammonium	[kgNm-2]
N_no3	Nitrate	[kgNm-2]
C_doc	Dissolved organic carbon	[kgCm-2]
sC_ch4_ebul	CH4 emissions via ebullition	[kgCm-2]
sC_ch4_plant	CH4 emissions via plant mediated diffusion	[kgCm-2]
sC_ch4_soil	CH4 emissions via soil surface	[kgCm-2]
sC_ch4_water	CH4 emissions via surface water table	[kgCm-2]
sC_ch4_leach	CH4 leaching	[kgCm-2]
sC_ch4_prod	CH4 production	[kgCm-2]
sC_ch4_ox	CH4 oxidation	[kgCm-2]
sC_acetate_prod	Acetate production	[kgCm-2]
sC_doc_prod	DOC production	[kgCm-2]
sN_no3_denit	NO3 denitrification	[kgNm-2]
sN_n2o_ebul	N2O emissions via ebullition	[kgNm-2]
sN_n2o_plant	N2O emissions via plant mediated diffusion	[kgNm-2]
sN_n2o_soil	N2O emissions via soil surface	[kgNm-2]
sN_n2o_water	N2O emissions via surface water table	[kgNm-2]
sN_no_ebul	NO emissions via ebullition	[kgNm-2]
sN_no_plant	NO emissions via plant mediated diffusion	[kgNm-2]
sN_no_soil	NO emissions via soil surface	[kgNm-2]
sN_no_water	NO emissions via surface water table	[kgNm-2]
sN_nh3_ebul	NH3 emissions via ebullition	[kgNm-2]
sN_nh3_plant	NH3 emissions via plant mediated diffusion	[kgNm-2]
sN_nh3_soil	NH3 emissions via soil surface	[kgNm-2]
sN_nh3_water	NH3 emissions via surface water table	[kgNm-2]
sO_plant_o2_cons	Oxygen consumption by roots	[kgOm-2]
sO_plant_o2_prod	Oxygen release by roots	[kgOm-2]
sO_algae_o2_prod	Oxygen release by algae	[kgOm-2]
ph_watertable	Mean pH value in the surface water table	[-]
ph_soil_surface	Mean pH value in the soil	[-]
anvf	Anaerobic volume fraction	[%]

Subdaily output

entity name	decription	unit
layer	Soil layer	[-]
level	Soil layer level (positive from soil surface upwards)	[m]
extension	extension	[m]
pH	pH value	[-]
pore_connectivity	Connectivity of pores	[0-1]
relative_permeability	Relative permeability of gaseous diffusion	[0-1]
aerenchym_permeability	Aerenchym permeability	[...]

MeTrx layer output (daily) "cfdd[oC]", water_content | Water content | [0-1] air↔_content | Air content | [0-1] porosity | Porosity | [0-1] fe2 | Iron Fe2+ [kg:ha-1] fe3 | Iron Fe3+ | [kg:ha-1] C_co2 | CO2 content | [kg:ha-1] C_ch4 | CH4 content | [kg↔:ha-1] dC_ch4_bubbling | CH4 transport via ebullition | [kg:ha-1] dC_ch4_production | CH4 production | [kg:ha-1] dC_ch4_oxidation | CH4 oxidation | [kg:ha-1] dC_doc↔_production | DOC production | [kg:ha-1] dC_acetate_production | Acetate production | [kg:ha-1] dC_microbial_death | Microbial death | [kg:ha-1] C_doc | Dissolved organic carbon | [kg:ha-1] C_acetate | Acetate | [kg:ha-1] N_no3 | NO3 | [kg:ha-1] N_nh4 | NH4 | [kg:ha-1] N_urea | IUrea | [kg:ha-1] N_nh3 | NH3 | [kg:ha-1] o2 | Oxygen partial pressure | [bar] N_no | NO content | [kg:ha-1] N_n2o | N2O content | [kg:ha-1] C_humus_1 | Humus pool 1 | [kg:ha-1] C_humus_2 | Humus pool 2 | [kg:ha-1] C_humus_3 | Humus pool 3 | [kg:ha-1] dN_no3_cons_denit | Denitrification of NO3 | [kg:ha-1] denit_factor↔_c | Factor of denitrification dependency on carbon availability | [0-1] denit_factor_n | Factor of denitrification dependency on nitrogen availability | [0-1] dN_no3_prod_nit | NO3 production from nitrification | [kg:ha-1] dN_no3_transport | Downward transport of NO3 | [kg:ha-1]

entity name	decription	unit
C_surface	Surface C-litter	[kgCm-2]
C_soil_20cm	Total soil carbon in 20 cm topsoil	[kgCm-2]
C_humus_1_20cm	Carbon in humus pool 1 in 20 cm topsoil	[kgCm-2]
C_humus_2_20cm	Carbon in humus pool 1 in 20 cm topsoil	[kgCm-2]
C_humus_3_20cm	Carbon in humus pool 1 in 20 cm topsoil	[kgCm-2]
C_litter_20cm	Carbon in litter pools in 20 cm topsoil	[kgCm-2]
C_aorg_20cm	Carbon aorg pool in 20 cm topsoil	[kgCm-2]

Yearly output

1.0.5.3 SoilchemistryDNDC - Denitrification and Decomposition

The soilchemistry model SoilchemistryDNDC has been developed in order to predict GHG emissions from forest and agricultural ecosystems

Litter allocation Plant litter is distributed into very labile, labile, and resistant compartments across the soil profile according to its nitrogen content.

Incoming plant is litter is characterized by:

- foliage
- fine roots
- storage organs
- stubble
- above- and belowground wood
- root exsudation
- dung and urine

Nitrification During the first step of nitrification ($NH_4^+ \rightarrow NO_2$) some fraction is converted to N_2O and NO :

$$\frac{dNO}{dt} = -\psi_{KNO} \cdot \phi_{TM,NO} \cdot \phi_{pH,NO} \cdot \frac{dNH_4}{dt} \frac{dN_2O}{dt} = -\psi_{KN_2O} \cdot \phi_{TM,N_2O} \cdot \frac{dNH_4}{dt}$$

The temperature (T) moisture (θ) factor $\phi_{TM,NO}$ is given by

$$\phi_{TM,NO} = \frac{1}{\frac{1}{\Psi_{TF_NUP_NO1} e^{\frac{T}{\Psi_{TF_NUP_NO2}}}} + \frac{1}{1 - \frac{\Psi_{M_FACT_P1}}{1 + e^{\theta - \Psi_{M_FACT_P2}}}}}$$

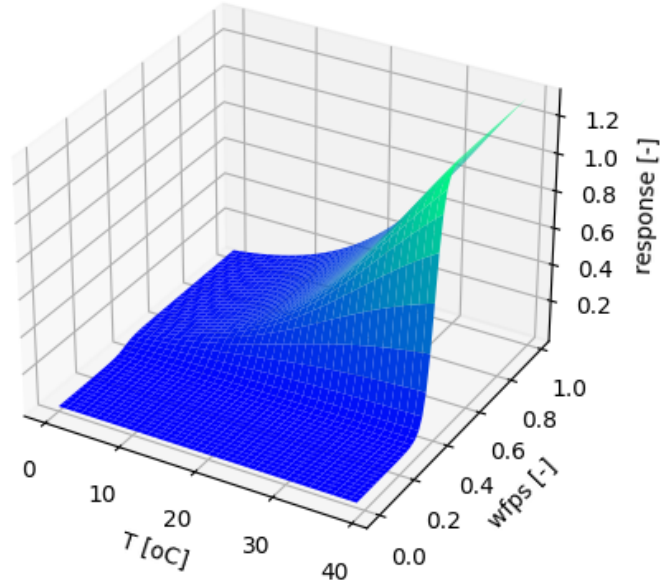


Figure 1.41: Temperature moisture dependency of N₂O production during nitrification

The pH factor is given by

$$\phi_{pH,NO} = \Psi_{PH_FACT_P2} - \Psi_{PH_FACT_P3} \cdot pH$$

The temperature (T) moisture (θ) factor ϕ_{TM,N_2O} is given by

$$\phi_{TM,N_2O} = \frac{1}{\frac{1}{\Psi_{TF_NUP_N2O1} e^{\frac{T}{\Psi_{TF_NUP_N2O2}}}} + \frac{1}{1 - \frac{\Psi_{M_FACT_P3}}{1 + e^{-\theta - \Psi_{M_FACT_P4}}}}}$$

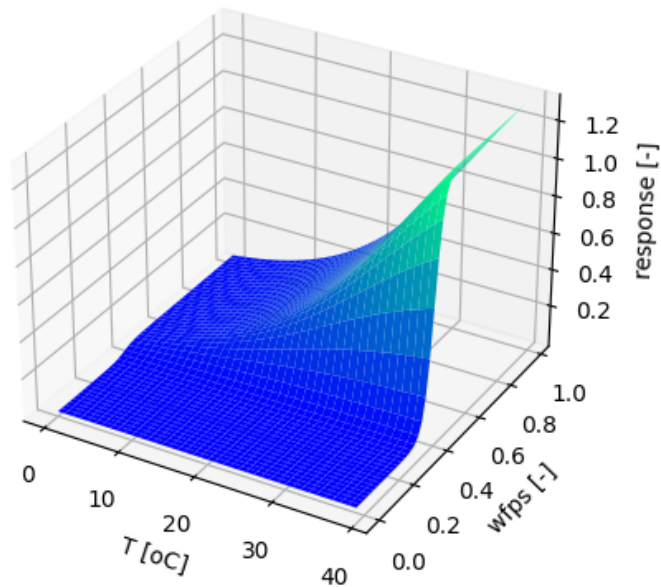


Figure 1.42: Temperature moisture dependency of NO production during nitrification

1.0.5.4 soillibs

Fertilization If surface water is present at fertilization, and defined fertilizer depth equals zero, fertilizer is equally added in surfacebulk layers.

Fertilizer application can be placed heterogeneously, e.g., crop-specific in multi-cropping systems. The amount of fertilizer that is placed at a specific location is implemented as fraction of total fertilized nitrogen. For now, different N-species (e.g., NH_4 , NO_3 , DON) are not distinguished but only considered as total N.

Author

David Kraus

Date

Dec, 2017

Cation exchange capacity

Authors

- Khaledian Khaledian et al. (2017)
- David Kraus (implementation into LandscapeDNDC)

Cation exchange capacity (CEC) describes the capacity of soils to hold positively charged ions such as:

- Calcium (Ca^{2+})
- Magnesium (Mg^{2+})
- Potassium (K^+)
- Sodium (Na^+)
- Hydrogen (H^+)
- Aluminium (Al^{3+})
- Iron (Fe^{2+})
- Manganese (Mn^{2+})
- Zinc (Zn^{2+})

E.g., clay and soil organic matter (SOM) are negatively charged and are major contributors to total soil CEC. The CEC of SOM depends on the soil pH value (increasing with pH). The CEC of soil can be expressed in mol positive charge per soil mass ($\frac{cmol_c}{kg}$). Sandy soil with low SOM have low CEC ($< 3 \frac{cmol_c}{kg}$), while clayey and SOM-enriched soils have high CEC ($> 20 \frac{cmol_c}{kg}$).

The ecosystem type specific pedotransfer functions of soil CEC are taken from Khaledian et al. (2017).

- Arable ecosystems $41.025 + 1.091 * clay + 0.512 * silt + 0.159 * sand - 10.087 * ph + 0.494 * som$
- Grassland ecosystems $-64.880 + 1.365 * clay + 0.992 * silt + 0.864 * sand - 2.453 * ph + 0.282 * som$
- Forest ecosystems $10.973 + 0.427 * clay - 0.379 * silt - 0.436 * sand + 4.313 * ph + 6.963e - 2 * som$

Enhanced efficiency nitrogen fertilizers

Authors

- David Kraus (implementation into LandscapeDNDC)

Controlled-release nitrogen fertilizer The cumulative fraction of N release [0-1] is given by:

Nitrification inhibition

$$1 - (1 - \beta_3) \cdot \min \left(e^{-\beta_1 T_{cum} + \beta_2 cwf + \beta_0}, 1 \right)$$

Height of litter layer

Authors

- Ruediger Grote
- David Kraus

Update litter height depending on soil organic matter and bulk density.

1.0.6 Global State

1.0.7 Standard outputs

LandscapeDNDC will write simulation results into several output files. These files are in default mode plain text files using the line endings according to the platform where the simulations have been performed. Be aware that, for example, Windows and Unix/Linux do not have identical line endings in text files.

The standard outputs are classified according to the ecosystem compartments / process functionalities:

- Soilchemistry output
Soil items, e.g., soil organic carbon and nitrogen pools, fluxes of various carbon and nitrogen species in and out of the soil system
- Vegetation physiology output
Vegetation items such as biomasses, photosynthesis and respiration rates, stress indicators, ...

- Vegetation structure output
Structural components of the vegetation such as stem diameter and height, crown width. Majorly used for forest simulations.
- Microclimate output
This holds everything with regard to temperature and radiation within the canopy and soil.
- Management output
...
- Watercycle output
This holds everything regarding hydrology, e.g., water contents in different depths, water fluxes in and out of the system, ...
- Ecosystem output
...
- Inventory output
...
- GGCM output
...
- DSS output
...
- Surrogateoutput output
...

Nearly all ecosystem standard sinks offer outputs for the three major timemodes:

- subdaily output (by default having suffix subdaily)
- daily output (by default having suffix daily)
- yearly output (by default having suffix yearly)

For more detailed output LandscapeDNDC provides for most ecosystem standard sinks 'layer-sinks' writing entities reflecting internal discretization.

In the following all output files are described in detail. Each data record in all files contains information about the kernel associated to the record and the simulation time of the record:

- **id**
The ID of the kernel (e.g. grid cell) that produced the output record. Note that currently the source identifier associated with a kernel (i.e. cell) is not written to the output sinks. This means, that reading kernel setups from more than one source may cause ambiguous outputs, if IDs are not unique.
- **year**
The simulation year of the output record
- **day**
The simulation Julian day of the output record (only day and subday sinks)
- **subday**
The simulation subday of the output record (only subday sinks)
- **layer**
The soil layer of the output record (only 'layer-sinks')

1.0.7.1 Nomenclature

- Fluxes may contain a leading symbol in lowercase letters expressing the reference time period. The temporal dimension in the unit may then be omitted:
s: subdaily
d: daily
a: annual
Examples:
dN_no3_leach[kg:ha-1] -> daily leaching of NO3
aN_no3_leach[kg:ha-1] -> yearly leaching of NO3
- Masses of complex matter may be given in reduced form in capital letters:
C: mass of carbon
N: mass of nitrogen
DW: mass of dry matter
Examples:
dN_no3_leach[kg:ha-1] -> daily mass of leached nitrogen in form of NO3 (not including mass of oxygen)
d_no3_leach[kg:ha-1] -> daily mass of leached NO3 (including mass of nitrogen and oxygen)
- The two optional indications of reference time period and reduced form of complex matter are given without delimiter:
dN_no3_leach[kg:ha-1] -> correct
d_N_no3_leach[kg:ha-1] -> incorrect

- Descriptive components are delimited by underscores. Arithmetic symbols are not allowed (e.g., "+", "-", "/", "*")
- Units are given at the end in square brackets: dN_no3_leach[kg:ha-1] -> correct
dN_no3[kg:ha-1]_leach -> incorrect
- Components of units may be optional delimited by a colon to avoid ambiguity:
[m:m-2] -> m per square meter
[mm-2] -> per square millimeter
- There is no delimiter before the unit
dN_no3_leach[kg:ha-1] -> correct
dN_no3_leach_[kg:ha-1] -> incorrect

1.0.7.2 Soilchemistry output

Soilchemistry output (daily) xml-based module selection in project's setup:

```
< module id="output:soilchemistry:daily" />
```

entity name	decription	unit
dC_ch4_emis	Daily methane flux	[kgCha-1]
dC_co2_emis_auto	Daily autotrophic (fine roots) soil respiration	[kgCha-1]
dC_co2_emis_hetero	Daily heterotrophic soil respiration	[kgCha-1]
dC_doc_leach	Daily dissolved organic carbon leaching	[kgCha-1]
dN_don_leach	Daily dissolved organic nitrogen leaching	[kgNha-1]
dN_no3_leach	Daily nitrate leaching	[kgNha-1]
dN_nh4_leach	Daily ammonium leaching	[kgNha-1]
dN_no_emis	Daily nitric oxide flux	[kgNha-1]
dN_n2o_emis	Daily nitrous oxide flux	[kgNha-1]
dN_n2_emis	Daily molecular nitrogen flux	[kgNha-1]
dN_nh3_emis	Daily ammonia flux	[kgNha-1]
dN_n2_fix	Daily molecular nitrogen fixation by soil microor- ganisms	[kgNha-1]

entity name	decription	unit
dC_co2_fix	Daily carbon fixation by soil microorganisms	[kgNha-1]
dS_so4_leach	Daily sulfate leaching	[kgSha-1]
dC_litter_above	Daily carbon above ground litter input	[kgCha-1]
dC_litter_below	Daily carbon below ground litter input	[kgCha-1]
dN_litter_above	Daily nitrogen above ground litter input	[kgNha-1]
dN_litter_below	Daily nitrogen below ground litter input	[kgNha-1]
dN_deposition	Daily nitrogen deposition from the atmosphere	[kgNha-1]
dN_plant_uptake	Daily nitrogen uptake by plants	[kgNha-1]
dN_immobilise	Daily nitrogen immobilisation via microbial as-similation	[kgNha-1]
dN_mineral	Daily nitrogen mineralization rate	[kgNha-1]
dN_nitrify	Daily nitrification to NO3	[kgNha-1]
dN_denitrify	Daily denitrification of NO3	[kgNha-1]
dN_chemo	Daily chemodenitrification of NO2	[kgNha-1]
C_soil	Total soil organic carbon (humus + microbes (living and necromass) + litter (raw and fragmented) + dissolved carbon). NO wood material included	[kgCha-1]
C_soil_20cm	Total soil organic carbon (see: C_soil for composition) in the first 20 cm	[kgCha-1]
C_soil_30cm	Total soil organic carbon (see: C_soil for composition) in the first 30 cm	[kgCha-1]
C_aorg	Total active soil organic carbon	[kgCha-1]
C_litter_raw	Total above and belowground carbon in raw litter	[kgCha-1]
C_litter	Carbon stored in litter pools	[kgCha-1]
C_mic	Microbial biomass carbon	[kgCha-1]
C_sol	Dissolved organic carbon	[kgCha-1]
C_wood	Wood carbon	[kgCha-1]
N_soil	Total non-dissolved organic nitrogen	[kgNha-1]
N_soil_20cm	Total non-dissolved organic nitrogen in the first 20 cm	[kgNha-1]
N_soil_30cm	Total non-dissolved organic nitrogen in the first 30 cm	[kgNha-1]
N_aorg	Total active soil organic nitrogen	[kgCha-1]
N_litter_raw	Total above and belowground nitrogen in raw litter	[kgNha-1]
N_litter	Nitrogen stored in litter pools	[kgNha-1]
N_mic	Microbial biomass nitrogen	[kgNha-1]

entity name	decription	unit
N_sol	Dissolved organic + inorganic nitrogen	[kgNha-1]

Soilchemistry output (horizons/daily) xml-based module selection in project's setup:

```
< module id="output:soilchemistry-horizons:daily" />
```

entity name	decription	unit
dN_no3_leach_10cm[kgNm-2]	Daily NO3 leaching in 10 cm soil depth	[kgNm-2]
dN_no3_leach_20cm[kgNm-2]	Daily NO3 leaching in 10 cm soil depth	[kgNm-2]
dN_no3_leach_30cm[kgNm-2]	Daily NO3 leaching in 10 cm soil depth	[kgNm-2]
dN_no3_leach_50cm[kgNm-2]	Daily NO3 leaching in 50 cm soil depth	[kgNm-2]
dN_no3_leach_100cm[kgNm-2]	Daily NO3 leaching in 100 cm soil depth	[kgNm-2]

Soilchemistry output (layer/daily) xml-based module selection in project's setup:

```
< module id="output:soilchemistry-layer:daily" />
```

entity name	decription	unit
layer	Soil layer	[-]
height	Soil layer height	[m]
extension	extension	[m]
som	Total soil organic matter	[kgDWha-1]
min	Mineral fraction	[kgDWha-1]
C_hum	Carbon in soil humus pool	[kgCha-1]
C_aorg	Carbon in active organic matter pool	[kgCha-1]
C_litter_1	Carbon of very labile litter pool	[kgCha-1]
C_litter_2	Carbon of labile litter pool	[kgCha-1]

entity name	decription	unit
C_litter_3	Carbon of recalcitrant litter pool	[kgCha-1]
C_mic_1	Carbon of microbial pool 1	[kgCha-1]
C_mic_2	Carbon of microbial pool 2	[kgCha-1]
C_mic_3	Carbon of microbial pool 3	[kgCha-1]
C_doc	Dissolved organic carbon	[kgCha-1]
N_hum	Nitrogen in soil humus pool	[kgNha-1]
N_aorg	Active organic nitrogen	[kgNha-1]
N_litter	Nitrogen in soil litter	[kgNha-1]
N_mic	Total microbial nitrogen	[kgNha-1]
N_nh4_clay	Ammonium adsorbed on clay minerals	[kgNha-1]
N_nh4	Ammonium	[kgNha-1]
N_nh3	Ammonia	[kgNha-1]
N_no3	Nitrate	[kgNha-1]
N_no2	Nitrite	[kgNha-1]
N_no	Nitric oxide	[kgNha-1]
N_n2o	Nitroux oxide	[kgNha-1]
N_don	Dissolved organic nitrogen	[kgNha-1]
ph [-]	pH value	[-]
anvf	Anaerobic volume fraction	[-]
o2	Oxygen partial pressure	[bar]
dN_mineral	Daily mineralization rate	[kgNha-1]
dN_nitrify	Daily nitrification rate	[kgNha-1]
dN_denitrify	Daily denitrification rate	[kgNha-1]

Soilchemistry output (layer/subdaily) xml-based module selection in project's setup:

```
< module id="output:soilchemistry-layer:subdaily" />
```

entity name	decription	unit
layer	Soil layer	[-]
height	Soil layer height	[m]

entity name	decription	unit
extension	extension	[m]
C_doc	Dissolved organic carbon	[kgCha-1]
C_microbes	Carbon of microbial biomass	[kgCha-1]
N_nh4	Ammonium	[kgNha-1]
N_nh3	Ammonia	[kgNha-1]
N_no3	Nitrate	[kgNha-1]
N_no2	Nitrite	[kgNha-1]
N_no	Nitric oxide	[kgNha-1]
N_n2o	Nitroux oxide	[kgNha-1]
N_don	Dissolved organic nitrogen	[kgNha-1]
anvf	Anaerobic volume fraction	[-]
o2	Oxygen partial pressure	[bar]

entity name	decription	unit
sC_co2_emis	Soil CO2 emissions	[kgCm-2]
sC_co2_prod_auto	Autotrophic soil repiration	[kgCm-2]
sC_co2_prod_hetero	Heterotrophic soil repiration	[kgCm-2]
sC_doc_leach	Leaching of dissolved carbon	[kgCm-2]

Soilchemistry output (subdaily)

entity name	decription	unit
aC_ch4_emis	Annual methane emissions	[kgCha-1]
aC_co2_emis_auto	Annual autotrophic (fine roots) respiration	[kgCha-1]
aC_co2_emis_hetero	Annual heterotrophic soil respiration	[kgCha-1]
aC_doc_leach	Annual dissolved organic carbon leaching	[kgCha-1]
aC_litter_above	Annual carbon in leave-litter fall	[kgCha-1]
aC_litter_below	Annual rhizodeposited carbon (root exudates and root decay)	[kgCha-1]
aC_fertilize	Annual carbon input via fertilization/manuring	[kgCha-1]
aC_fixation	Annual carbon fixation from atmosphere	[kgCha-1]
aN_no_emis	Annual nitric oxide emissions	[kgNha-1]
aN_n2o_emis	Annual nitroux oxide emissions	[kgNha-1]
aN_n2_emis	Annual molecular nitrogen emissions	[kgNha-1]

entity name	decription	unit
aN_nh3_emis	Annual ammonia emissions	[kgNha-1]
aN_no3_leach	Annual nitrate leaching	[kgNha-1]
aN_nh4_leach	Annual ammonium leaching	[kgNha-1]
aN_don_leach	Annual dissolved organic nitrogen leaching	[kgNha-1]
aN_plant_uptake	Annual nitrogen uptake by plants	[kgNha-1]
aN_litter_above	Annual nitrogen (from the litter)	[kgNha-1]
aN_litter_below	Annual rhizodeposited nitrogen (from the litter)	[kgNha-1]
aN_fertilize	Annual nitrogen input via fertilization/manuring	[kgNha-1]
aN_fixation	Annual nitrogen fixation from atmosphere	[kgNha-1]
aN_deposition_no3	Annual nitrate deposition	[kgNha-1]
aN_deposition_nh4	Annual amonium deposition	[kgNha-1]
aN_mineral	Annual nitrogen mineralization	[kgNha-1]
aN_nitrify	Annual nitrification	[kgNha-1]
aN_chemodenitrify	Annual chemodenitrification	[kgNha-1]
aN_denitrify	Annual microbial denitrification	[kgNha-1]
C_stubble	Carbon stored in stubbles at the end of year	[kgCha-1]
C_wood_above	Carbon stored in aboveground wood at the end of year	[kgCha-1]
C_wood_below	Carbon stored in belowground wood at the end of year	[kgCha-1]
C_soil	Total soil organic carbon at the end of year of the complete soil profile. Note, stubble and wood are excluded, microbial and dissolved carbon are included	[kgCha-1]
C_soil_20cm	Total soil organic carbon at the end of year of the first 20cm of the soil	[kgCha-1]
C_soil_30cm	Total soil organic carbon at the end of year of the first 30cm of the soil	[kgCha-1]
C_mic	Microbial carbon at the end of year of the complete soil profile	[kgCha-1]
C_sol	Dissolved organic carbon at the end of year of the complete soil profile	[kgCha-1]
N_stubble	Nitrogen stored in stubbles at the end of year	[kgNha-1]
N_wood_above	Nitrogen stored in aboveground wood at the end of year	[kgNha-1]
N_wood_below	Nitrogen stored in belowground wood at the end of year	[kgNha-1]

entity name	decription	unit
N_soil	Total soil organic nitrogen at the end of year of the complete soil profile. Note, stubble and wood are excluded, , microbial and dissolved nitrogen are included	[kgNha-1]
N_soil_20cm	Total soil organic nitrogen at the end of year of the first 20cm of the mineral soil. Note, the litter layer is not included	[kgNha-1]
N_soil_30cm	Total soil organic nitrogen at the end of year of the first 30cm of the mineral soil. Note, the litter layer is not included	[kgNha-1]
N_mic_total	Microbial nitrogen at the end of year of the complete soil profile	[kgNha-1]
N_sol_total	Dissolved organic nitrogen at the end of year of the complete soil profile	[kgNha-1]
aC_change	Annual change of all nitrogen pools	[kgCha-1]
aN_change	Annual change of all nitrogen pools	[kgNha-1]

Soilchemistry output (yearly)

1.0.7.3 Vegetation physiology output

Physiology output (daily) xml-based module selection in project's setup:

```
< module id="output:physiology:daily" />
```

entity name	decription	unit
species	Abbreviated name of species	[-]
day_emergence	Day of emergence	[-]
gdd	Accumulated growing degree days	[oC]
pds_gdd	Phenological development stage based on accumulated growing degree days	[-]
pds_zadok	Phenological development stage based on Zadok	[-]
dvs_flush	Plant development stage (in forest simulations: relative state of foliage flushing)	[-]

entity name	decription	unit
dvs_mort	Relative state of foliage senescence	[-]
dN_don_upt	Plant uptake of soil organic nitrogen	[kgN m-2 ts-1]
dN_nh4_upt	Plant uptake of soil ammonium	[kgN m-2 ts-1]
dN_no3_upt	Plant uptake of soil nitrate	[kgN m-2 d-1]
dN_nh3_upt	Plant uptake of soil ammonia	[kgN m-2 d-1]
dN_nox_upt	Uptake of NOx	[kgN m-2 d-1]
dN_n2_fix	Nitrogen fixation by plants	[kgN m-2 d-1]
dC_fol_grow	Daily increase of foliages carbon	[kgC m-2 d-1]
dC_fru_grow	Daily increase of fruit carbon	[kgC m-2 d-1]
dC_frt_grow	Daily increase of (fine) roots carbon	[kgC m-2 d-1]
dC_lst_grow	Daily increase of living structural matter (carbon)	[kgC m-2 d-1]
dC_fac_grow	Daily carbon allocated to pool available substrate	[kgC m-2 d-1]
dC_fol_resp	Foliar respiration	[kgC m-2 d-1]
dC_fru_resp	Fruit respiration	[kgC m-2 d-1]
dC_frt_resp	Fine roots respiration	[kgC m-2 d-1]
dC_lst_resp	Living structural matter respiration	[kgC m-2 d-1]
dC_maintenance_resp	Total residual respiration	[kgC m-2 d-1]
dC_transport_resp	Total transport and uptake respiration	[kgC m-2 d-1]
dC_growth_resp	Total growth respiration	[kgC m-2 d-1]
dC_co2_upt	Carbon uptake-Photosynthesis rate	[kgC m-2 d-1]
f_Fac	Relative state of free available carbon	[-]
DW_fol	Living foliar biomass	[kgDW m-2]
DW_dfol	Dead foliar biomass	[kgDW m-2]
DW_fru	Fruit biomass	[kgDW m-2]
DW_frt	Fine roots biomass	[kgDW m-2]
DW_lst	Living structural matter (e.g., young wood) biomass	[kgDW m-2]
DW_dst	Dead structural matter (e.g., old wood) biomass	[kgDW m-2]
DW_above	Total aboveground biomass	[kgDW m-2]
DW_below	Total belowground biomass	[kgDW m-2]
lai	Leaf area index	[m2 m-2]
specific_leaf_area	Specifc leaf area	[m-2 kg-1]
n_ret	Retention of nitrogen	[kgN m-2]

entity name	decription	unit
NC_fol	Nitrogen content in the foliage	[kgN kgDW-1]
NC_frt	Nitrogen content in the fine roots	[kgN kgDW-1]
NC_fru	Nitrogen content in the fruit	[kgN kgDW-1]
NC_lst	Nitrogen content in living structural matter (e.g., young wood)	[kgN kgDW-1]
NC_dst	Nitrogen content in dead structural matter (e.g., old wood)	[kgN kgDW-1]
N_total	Total plant nitrogen	[kgN m-2]
dDW_fol_sen	Foliage senescence	[kgDW m-2 d-1]
dDW_fru_sen	Fruit senescence	[kgDW m-2 d-1]
dDW_frt_sen	Fine roots senescence	[kgDW m-2 d-1]
dDW_lst_sen	Living structural matter (e.g., young wood) senescence	[kgDW m-2 d-1]
dDW_dst_sen	Dead structural matter (e.g., old wood) senescence	[kgDW m-2 d-1]
dC_exsudates	Root exsudates losses	[kgC m-2 d-1]
dN_lit_fol	Nitrogen in the foliage-litter	[kgN m-2 d-1]
dN_lit_fru	Nitrogen in the Fruit-litter	[kgN m-2 d-1]
dN_lit_frt	Nitrogen in the fine roots-litter	[kgN m-2 d-1]
dN_lit_ldst_below	Nitrogen in aboveground living and dead structural matter	[kgN m-2 d-1]
dN_lit_ldst_above	Nitrogen in belowground living and dead structural matter	[kgN m-2 d-1]
drought_rel	Species specific drought stress factor	[-]
heat_damage_longterm	Longterm heat damage	[-]
conduct_rel	Relative stomatal conductance	[-]
vc_act_25	Activity state of rubisco at 25 degrees celsius	[umol m-2 d-1]
iso_act	Activity state of isoprene synthase	[umol m-2 d-1]
mono_act	Activity state of monoterpene synthase	[umol m-2 d-1]
d_iso_emis	Isoprene emission from plants	[umol m-2 d-1]
d_mono_emis	Monoterpene emission from plants	[umol m-2 d-1]
d_mono_storage_emis	Monoterpene emission from plant storage	[umol:m-2]
d_ovoc_emis	OVOC emission from plant storage	[umol:m-2]
dN_nh4_throughf	Ammonium deposition through rainfall	[kgN L-1]
dN_no3_throughf	Nitrate deposition throug rainfall	[kgN L-1]

entity name	decription	unit
-------------	------------	------

Physiology output (layer/daily) xml-based module selection in project's setup↵
:

```
< module id="output:physiology-layer:daily" />
```

entity name	decription	unit
layer	Canopy/soil layer	[-]
level	Level height	[m]
extension	Height	[m]
DW_fol/DW_frt	Foliage (living and dead) / fine roots biomass	[kgDW m-2]
lai	Leaf area index	[-]
dN_upt_nh3	Nitrogen uptake	[kgN]
dN_upt_nox	Nitrogen gasses uptake	[kgN]
dC_co2_upt	Carbon dioxide uptake	[kgN]
vc_act_25	Activity state of rubisco at 25 degrees celsius	[umol m-2 s-1]
vc_max	Actual activity state of rubisco	[umol m-2 s-1]
j_max	Maximum rate of electron transport	[umol m-2 s-1]
j_pot	Potential rate of electron transport	[umol m-2 s-1]
ci	Intercellular concentration of CO2	[umol m-2 s-1]
iso_act	Activity state of isoprene synthase	[nmol m-2 s-1]
mono_act	Activity state of monoterpene synthase	[nmol m-2 s-1]
iso_emis	Isoprene emission from plants	[umol m-2 s-1]
mono_emis	Monoterpene emission from plants	[umol m-2 s-1]
rootlength	root length	[m]

Physiology output (subdaily) xml-based module selection in project's setup↵
:

```
< module id="output:physiology:subdaily" />
```

entity name	decription	unit
day_emerg	Day of emergence	[day]
temp_cum	Growing degree days	[gdd]
dvs_flush	Relative state of foliage flushing in forest simulations	[-]
dvs_mort	Relative state of foliage senescence	[-]
dN_don_upt	Plant uptake of soil organic nitrogen	[kgN m-2 ts-1]
dN_nh4_upt	Plant uptake of soil ammonium	[kgN m-2 ts-1]
dN_no3_upt	Plant uptake of soil nitrate	[kgN m-2 ts-1]
dN_nh3_upt	Plant uptake of soil ammonia	[kgN m-2 ts-1]
dN_nox_upt	Uptake of NOx	[kgN m-2 ts-1]
dN_n2_fix	Nitrogen fixation by plants	[kgN m-2 ts-1]
dC_fol_grow	Increase of foliages carbon	[kgC m-2 ts-1]
dC_frt_grow	Increase of (fine) roots carbon	[kgC m-2 ts-1]
dC_lst_grow	Increase of living structural tissue carbon	[kgC m-2 ts-1]
dC_fru_grow	Increase of fruit (buds) carbon	[kgC m-2 ts-1]
dC_fac_grow	Carbon allocated to pool available substrate	[kgC m-2 ts-1]
dC_fol_resp	Foliar respiration	[kgC m-2 ts-1]
dC_frt_resp	Fine roots respiration	[kgC m-2 ts-1]
dC_lst_resp	Young living structural tissue respiration	[kgC m-2 ts-1]
dC_fru_resp	Fruit (buds) respiration	[kgC m-2 ts-1]
dC_maintenance_resp	Total residual respiration	[kgC m-2 ts-1]
dC_transport_resp	Total transport and uptake respiration	[kgC m-2 ts-1]
dC_growth_resp	Total growth respiration	[kgC m-2 ts-1]
dC_co2_upt	Carbon uptake-Photosynthesis rate	[kgC m-2 ts-1]
f_Fac	Relative state of free available carbon	[-]
DW_fol	Foliar mass	[kgDW m-2]
DW_frt	Fine roots mass	[kgDW m-2]
DW_lst	Living structural tissue mass	[kgDW m-2]
DW_dst	Dead structural tissue mass	[kgDW m-2]
DW_fru	Fruit (buds) mass	[kgDW m-2]
lai	Leaf area index	[-]
sla	Leaf area index	[m-2 kg-1]
n_ret	Retention of nitrogen	[kgN m-2]

entity name	decription	unit
NC_fol	Nitrogen content in the foliage	[kgN kgDW-1]
NC_frt	Nitrogen content in the fine roots	[kgN kgDW-1]
NC_lst	Nitrogen content in the living structural tissue	[kgN kgDW-1]
NC_dst	Nitrogen content in the dead structural tissue	[kgN kgDW-1]
NC_fru	Nitrogen content in the fruit	[kgN kgDW-1]
dC_fol_sen	Foliage senescence	[kgDW m-2 ts-1]
dC_frt_sen	Fine roots senescence	[kgDW m-2 ts-1]
dC_lst_sen	Living structural tissue senescence	[kgDW m-2 ts-1]
dC_fru_sen	Fruit (buds) senescence	[kgDW m-2 ts-1]
dC_exsudates	Root exsudates losses	[kgC m-2 ts-1]
N_lit_fol	Nitrogen in the foliage-litter	[kgN m-2]
N_lit_frt	Nitrogen in the fine roots-litter	[kgN m-2]
N_lit_lst	Nitrogen in the living structural tissue-litter	[kgN m-2]
N_lit_fru	Nitrogen in the fruit-litter	[kgN m-2]
drought_rel	Species specific drought stress factor	[-]
conduct_rel	Conductance rel	[-]
vc_act_25	Activity state of rubisco at 25 degrees cel-sius	[umol m-2 s-1]
iso_act	Activity state of isoprene synthase	[umol m-2 s-1]
mono_act	Activity state of monoterpene synthase	[umol m-2 s-1]
iso_emis	Isoprene emission from plants	[umol m-2 s-1]
mono_emis	Monoterpene emission from plants	[umol m-2 s-1]
dN_nh4_throughf	Ammonium deposition through rainfall	[kgN L-1]
dN_no3_throughf	Nitrate deposition throug rainfall	[kgN L-1]

Physiology output (yearly) xml-based module selection in project's setup:

```
< module id="output:physiology:yearly" />
```

entity name	decription	unit
aN_n2_fix	Annual nitrogen fixation	[kgN m-2]
DW_fol	Foliage biomass	[kgDW m-2]
DW_frt	Fine roots biomass	[kgDW m-2]
DW_lst	Living structural biomass	[kgDW m-2]
DW_dst	Dead structural biomass	[kgDW m-2]
DW_fru	Fruit (grain, storage) biomass	[kgDW m-2]
DW_above	Aboveground biomass	[kgDW m-2]
DW_below	Belowground biomass	[kgDW m-2]
NC_fol	Nitrogen content in the foliage	[kgN kgDW-1]
NC_frt	Nitrogen content in the fine roots	[kgN kgDW-1]
NC_fru	Nitrogen content in the fruit	[kgN kgDW-1]
NC_lst	Nitrogen content in living structural matter (e.g., young wood)	[kgN kgDW-1]
NC_dst	Nitrogen content in dead structural matter (e.g., old wood)	[kgN kgDW-1]
N_total	Total plant nitrogen	[kgN m-2]

1.0.7.4 Vegetation structure output

Vegetation structure output (daily) xml-based module selection in project's setup:

```
< module id="output:vegstructure:daily" />
```

entity name	decription	unit
area_cover	Area cover	[-]
area_fraction	Area fraction	[-]
n_tree	Number of plants	[-]
vol_tree	Volume of plants	[m3ha-1]
h_max	maximal Height of plants	[m]
h_min	minimal Height of plants	[m]
diam_ground	Stem diameter at ground	[m]
diam_breast	Stem diameter at breast height	[m]

entity name	decription	unit
depth	Depth	[m]
sla	Specific leaf area	[m ² kg ⁻¹]
lai	Leaf area index	[-]
crown_diam_ratio	Crown diameter ratio	[-]
sap_fol_ratio	Sapwood foliage ratio	[-]
branch_fraction	Branch fraction	[-]
DW_stem_wood	Stem wood	[kg m ⁻²]
DW_branch_wood	Branch wood	[kg m ⁻²]
DW_root_wood	Root wood	[kg m ⁻²]

Vegetation structure output (horizons,daily) xml-based module selection in project's setup:

```
< module id="output:vegstructure-horizons:daily" />
```

entity name	decription	unit
lai_canopy_top	Leaf area index at canopy top	[m ² m ⁻²]
lai_canopy_middle	Leaf area index at canopy middle	[m ² m ⁻²]
lai_canopy_bottom	Leaf area index at canopy bottom	[m ² m ⁻²]
root_length_density_10cm	Root length density in 10 cm soil depth	[mm ⁻³]
root_length_density_20cm	Root length density in 20 cm soil depth	[mm ⁻³]
root_length_density_40cm	Root length density in 40 cm soil depth	[mm ⁻³]
root_length_density_60cm	Root length density in 60 cm soil depth	[mm ⁻³]
root_length_density_80cm	Root length density in 80 cm soil depth	[mm ⁻³]
root_length_density_120cm	Root length density in 120 cm soil depth	[mm ⁻³]
root_length_density_150cm	Root length density in 150 cm soil depth	[mm ⁻³]

Vegetation structure output (layer,daily) xml-based module selection in project's setup:

```
< module id="output:vegstructure-layer:daily" />
```

entity name	decription	unit
level	Level height	[m]
extension	Height	[m]
lai	Leaf area index	[-]
sla	Specific leaf area	[m2 kg-1]
fol_fraction	Foliage fraction	[0-1]
frt_fraction	Fine roots fraction	[0-1]

Vegetation structure output (layer,yearly) xml-based module selection in project's setup:

```
< module id="output:vegstructure-layer:yearly" />
```

entity name	decription	unit
level	Level height	[m]
extension	Height	[m]
sla	Specific leaf area	[m2 kg-1]
fol_fraction	Foliage fraction	[0-1]
frt_fraction	Fine roots fraction	[0-1]

Vegetation structure output (yearly) xml-based module selection in project's setup:

```
< module id="output:vegstructure:yearly" />
```

entity name	decription	unit
area_cover	Area cover	[-]
area_fraction	Area fraction	[-]

entity name	decription	unit
n_tree	Number of plants	[-]
vol_tree	Volume of plants	[m ³ ha ⁻¹]
h_max	maximal Height of plants	[m]
h_min	minimal Height of plants	[m]
diam_ground	Stem diameter at ground	[m]
diam_breast	Stem diameter at breast height	[m]
depth	Depth	[m]
lai	Leaf area index	[-]
crown_diam_ratio	Crown diameter ratio	[-]
sap_fol_ratio	Sapwood foliage ratio	[-]
branch_fraction	Branch fraction	[-]
DW_stem_wood	Stem wood	[kg m ⁻²]
DW_branch_wood	Branch wood	[kg m ⁻²]
DW_root_wood	Root wood	[kg m ⁻²]

1.0.7.5 Microclimate output

Microclimate output (daily) xml-based module selection in project's setup:

```
< module id="output:microclimate:daily" />
```

entity name	decription	unit
daylength	Day length	[h]
solar_radiation	Solar radiation	[Wm ⁻²]
sw_rad_above_canopy_in	Incoming short wave radiation above canopy (directed downwards)	[Wm ⁻²]
sw_rad_above_canopy_out	Outgoing short wave radiation above canopy (directed upwards)	[Wm ⁻²]
lw_rad_above_canopy_in	Incoming long wave radiation above canopy (directed downwards)	[Wm ⁻²]
lw_rad_above_canopy_out	Outgoing long wave radiation above canopy (directed upwards)	[Wm ⁻²]
latent_heat_out_top	Latent heat exchange at top of canopy (directed upwards)	[Wm ⁻²]

entity name	decription	unit
latent_heat_out_bottom	Latent heat exchange at botom of soil profile (directed downwards)	[Wm-2]
sensible_heat_out_top	Sensible heat exchange at top of canopy (directed upwards)	[Wm-2]
sensible_heat_out_bottom	Sensible heat exchange at botom of soil profile (directed downwards)	[Wm-2]
energy	Energy content of total ecosystem	[MJm-2]
temp_above_canopy_avg	Mean temperature above canopy	[oC]
temp_above_canopy_min	Minimum temperature above canopy	[oC]
temp_above_canopy_max	Maximum temperature above canopy	[oC]
temp_canopy_top	Temperature at top of canopy	[oC]
temp_canopy_middle	Temperature at middle of canopy	[oC]
temp_canopy_bottom	Temperature at bottom of canopy	[oC]
temp_soil_surface	Temperature at soil surface	[oC]
temp_5cm	Temperature at 5 cm depth	[oC]
temp_10cm	Temperature at 10 cm depth	[oC]
temp_15cm	Temperature at 15 cm depth	[oC]
temp_20cm	Temperature at 20 cm depth	[oC]
temp_30cm	Temperature at 30 cm depth	[oC]
temp_50cm	Temperature at 50 cm depth	[oC]
temp_100cm	Temperature at 100 cm depth	[oC]
vpd	Vapour pressure deficit (weighted by Leaf Area Index if LAI > 0.0)	[mbar]

Microclimate output (layer/daily) xml-based module selection in project's setup:

```
< module id="output:microclimate-layer:daily" />
```

entity name	decription	unit
level	Canopy/soil layer	[-]
extension	extension	[m]
temp_avg	Temperature	[oC]

entity name	decription	unit
temp_max	Maximum temperature	[oC]
temp_min	Minimum temperature	[oC]
sw_rad	Radiation	[Wm-2]
vpd	Vapour pressure defficit	[bar]
windspeed	Wind speed	[ms-1]
sun_fraction	Sun	[-]

Microclimate output (layer/subdaily) xml-based module selection in project's setup:

```
< module id="output:microclimate-layer:subdaily" />
```

entity name	decription	unit
level	Canopy/soil layer	[-]
extension	extension	[m]
temp_avg	Temperature	[oC]
temp_max	Maximum temperature	[oC]
temp_min	Minimum temperature	[oC]
sw_rad	Radiation	[Wm-2]
vpd	Vapour pressure defficit	[bar]
windspeed	Wind speed	[ms-1]
sun_fraction	Sun	[-]

Microclimate output (subdaily) xml-based module selection in project's setup↵
:

```
< module id="output:microclimate:subdaily" />
```

entity name	decription	unit
sw_rad_above_canopy_in	Incoming short wave radiation above canopy (directed downwards)	[Wm-2]
sw_rad_above_canopy_out	Outgoing short wave radiation above canopy (directed upwards)	[Wm-2]
lw_rad_above_canopy_in	Incoming long wave radiation above canopy (directed downwards)	[Wm-2]
lw_rad_above_canopy_out	Outgoing long wave radiation above canopy (directed upwards)	[Wm-2]
latent_heat_out_top	Latent heat exchange at top of canopy (directed upwards)	[Wm-2]
latent_heat_out_bottom	Latent heat exchange at botom of soil profile (directed downwards)	[Wm-2]
sensible_heat_out_top	Sensible heat exchange at top of canopy (directed upwards)	[Wm-2]
sensible_heat_out_bottom	Sensible heat exchange at botom of soil profile (directed downwards)	[Wm-2]
energy	Energy content of total ecosystem	[MJm-2]
temp_above_canopy_avg	Mean temperature above canopy	[oC]
temp_above_canopy_min	Minimum temperature above canopy	[oC]
temp_above_canopy_max	Maximum temperature above canopy	[oC]
temp_canopy_top	Temperature at top of canopy	[oC]
temp_canopy_middle	Temperature at middle of canopy	[oC]
temp_canopy_bottom	Temperature at bottom of canopy	[oC]
temp_soil_surface	Temperature at soil surface	[oC]
temp_5cm	Temperature at 5 cm depth	[oC]
temp_10cm	Temperature at 10 cm depth	[oC]
temp_15cm	Temperature at 15 cm depth	[oC]
temp_20cm	Temperature at 20 cm depth	[oC]
temp_30cm	Temperature at 30 cm depth	[oC]
temp_50cm	Temperature at 50 cm depth	[oC]
temp_100cm	Temperature at 100 cm depth	[oC]
vpd_canopy_avg	Average vapor pressure deficit throughout the canopy	[mbar]

1.0.7.6 Management output

entity name	decription	unit
dC_fru_export	Daily carbon of plant fruits exported from field due to cutting	[KgCha-1]
dC_fol_export	Daily carbon of plant foliage exported from field due to cutting	[KgCha-1]
dC_dfol_export	Daily carbon of dead plant foliage exported from field due to cutting	[KgCha-1]
dC_lst_export	Daily carbon of plant living structural tissue exported from field due to cutting	[KgCha-1]
dC_dst_export	Daily carbon of plant dead structural tissue exported from field due to cutting	[KgCha-1]
dC_above_export	Daily carbon of plant above ground exported from field due to cutting	[KgCha-1]
dC_frt_export	Daily carbon of plant fine roots exported from field due to cutting	[KgCha-1]
dC_fru_remain	Daily carbon of plant fruits remaining at the field after cutting	[KgCha-1]
dC_fol_remain	Daily carbon of plant foliage remaining at the field after cutting	[KgCha-1]
dC_lst_remain	Daily carbon of plant living structural tissue remaining at the field after cutting	[KgCha-1]
dC_dst_remain	Daily carbon of plant dead structural tissue remaining at the field after cutting	[KgCha-1]
dC_frt_remain	Daily carbon of plant fine roots remaining at the field after cutting	[KgCha-1]
dC_fru_litter	Daily carbon of plant fruits allocated to soil due to cutting	[KgCha-1]
dC_fol_litter	Daily carbon of plant foliage allocated to soil due to cutting	[KgCha-1]
dC_lst_litter	Daily carbon of plant living structural tissue allocated to soil due to cutting	[KgCha-1]
dC_dst_litter	Daily carbon of plant dead structural tissue allocated to soil due to cutting	[KgCha-1]
dC_frt_litter	Daily carbon of plant fine roots allocated to soil due to cutting	[KgCha-1]
dN_fru_export	Daily nitrogen of plant fruits exported from field due to cutting	[KgNha-1]
dN_fol_export	Daily nitrogen of plant foliage exported from field due to cutting	[KgNha-1]

entity name	decription	unit
dN_lst_export	Daily nitrogen of plant living structural tissue exported from field due to cutting	[KgNha-1]
dN_dst_export	Daily nitrogen of plant dead structural tissue exported from field due to cutting	[KgNha-1]
dN_above_export	Daily nitrogen of plant above ground exported from field due to cutting	[KgNha-1]
dN_frt_export	Daily nitrogen of plant fineroots exported from field due to cutting	[KgNha-1]
dN_fru_remain	Daily nitrogen of plant fruits remaining at the field after cutting	[KgNha-1]
dN_fol_remain	Daily nitrogen of plant foliage remaining at the field after cutting	[KgNha-1]
dN_lst_remain	Daily nitrogen of plant living structural tissue remaining at the field after cutting	[KgNha-1]
dN_dst_remain	Daily nitrogen of plant dead structural tissue remaining at the field after cutting	[KgNha-1]
dN_frt_remain	Daily nitrogen of plant fine roots remaining at the field after cutting	[KgNha-1]
dN_fru_litter	Daily nitrogen of plant fruits allocated to soil due to cutting	[KgNha-1]
dN_fol_litter	Daily nitrogen of plant foliage allocated to soil due to cutting	[KgNha-1]
dN_lst_litter	Daily nitrogen of plant living structural tissue allocated to soil due to cutting	[KgNha-1]
dN_dst_litter	Daily nitrogen of plant dead structural tissue allocated to soil due to cutting	[KgNha-1]
dN_frt_litter	Daily nitrogen of plant fineroots allocated to soil due to cutting	[KgNha-1]

Cutting output

entity name	decription	unit
dN_fertilizer	Daily nitrogen application in form of different inorganic fertilizers	[kgNha-1]
dN_yearsum	Daily nitrogen application in form of different inorganic fertilizers	[kgNha-1]

Fertilize output

entity name	decription	unit
dC_fru_export	Daily carbon of plant fruits exported from field due to grazing	[KgCha-1]
dC_fol_export	Daily carbon of plant foliage exported from field due to grazing	[KgCha-1]
dC_lst_export	Daily carbon of plant living structural tissue exported from field due to grazing	[KgCha-1]
dC_dst_export	Daily carbon of plant dead structural tissue exported from field due to grazing	[KgCha-1]
dC_above_export	Daily carbon of aboveground plant biomass exported from field due to grazing	[KgCha-1]
dC_frt_export	Daily carbon of plant fine roots exported from field due to grazing	[KgCha-1]
dC_frt_litter	Daily carbon of plant fine roots allocated to soil due to grazing	[KgCha-1]
dC_dung_litter	Daily carbon of dung allocated to soil due to grazing	[KgCha-1]
dN_fru_export	Daily nitrogen of plant fruits exported from field due to grazing	[KgNha-1]
dN_fol_export	Daily nitrogen of plant foliage exported from field due to grazing	[KgNha-1]
dN_lst_export	Daily nitrogen of plant living structural tissue exported from field due to grazing	[KgNha-1]
dN_dst_export	Daily nitrogen of plant dead structural tissue exported from field due to grazing	[KgNha-1]
dN_above_export	Daily nitrogen of aboveground plant biomass exported from field due to grazing	[KgNha-1]
dN_frt_export	Daily nitrogen of plant fineroots exported from field due to grazing	[KgNha-1]
dN_frt_litter	Daily nitrogen of plant fineroots allocated to soil due to grazing	[KgNha-1]
dN_dung_litter	Daily nitrogen of dung allocated to soil due to grazing	[KgNha-1]
dN_urine_litter	Daily nitrogen of urine allocated to soil due to grazing	[KgNha-1]

Grazing output

entity name	decription	unit
dC_fru	Carbon of fruit (yield) at harvest	[KgCha-1]
dC_fru_export	Carbon of fruit (yield) exported after harvest	[KgCha-1]
dC_straw	Carbon of straw at harvest	[KgCha-1]
dC_straw_export	Carbon of straw exported after harvest	[KgCha-1]
dC_rootlitter	Carbon of roots at harvest	[KgCha-1]
dN_fru	Nitrogen of fruit (yield) at harvest	[KgCha-1]
dN_fru_export	Nitrogen of fruit (yield) exported after harvest	[KgNha-1]
dN_straw	Nitrogen of straw at harvest	[KgNha-1]
dN_straw_export	Nitrogen of straw exported after harvest	[KgNha-1]
dN_rootlitter	Nitrogen of roots at harvest	[KgNha-1]

Harvest output

entity name	decription	unit
dN_manure	Daily nitrogen application in form of manure	[kgNha-1]
dN_yearsum	Yearly nitrogen application in form of manure	[kgNha-1]
dC_manure	Daily carbon application in form of manure	[kgCha-1]
dC_yearsum	Yearly carbon application in form of manure	[kgCha-1]

Manure output

1.0.7.7 Watercycle output

Watercycle output (daily) xml-based module selection in project's setup:

```
< module id="output:watercycle:daily" />
```

entity name	decription	unit
precipitation	Precipitation	[mm]
irrigation	Irrigation	[mm]
throughfall	Throughfall	[mm]
pot_evapotranspiration	Potential evapotranspiration	[mm]

entity name	decription	unit
pot_transpiration	Potential transpiration	[mm]
transpiration	Actual transpiration	[mm]
wateruptake	Soilwater uptake by plants (may be stored in plants and not directly transpired)	[mm]
interception_evaporation	Actual evaporation from interception	[mm]
soil_evaporation	Actual evaporation from soil surface	[mm]
surface_evaporation	Actual evaporation from snow/watertable surface	[mm]
runoff	Lateral surface water runoff	[mm]
percolation	Percolation out of last soil layer	[mm]
infiltration	Infiltration into the soil	[mm]
groundwater_access	Water input from groundwater	[mm]
groundwater_loss	Water lost to groundwater	[mm]
capillary_rise	Water input through capillary rise	[mm]
snow_height	Height of snow	[m]
snow	Amount of snow in water equivalents	[mm_H2Oeq]
leafwater	Intercepted leaf water	[mm]
surfacewater	Surface water	[mm]
soilwater	Total soil water	[mm-m3]
soilwater_rooted	Soil water in rooted soil layers	[mm-m3]
soilwater_floor	Soil water in the humus layer	[vol_perc]
soilwater_5cm	Soil water at 5 cm depth	[vol_perc]
soilwater_10cm	Soil water at 10 cm depth	[vol_perc]
soilwater_15cm	Soil water at 15 cm depth	[vol_perc]
soilwater_20cm	Soil water at 20 cm depth	[vol_perc]
soilwater_30cm	Soil water at 30 cm depth	[vol_perc]
soilwater_40cm	Soil water at 40 cm depth	[vol_perc]
soilwater_50cm	Soil water at 50 cm depth	[vol_perc]
soilwater_60cm	Soil water at 60 cm depth	[vol_perc]
soilwater_80cm	Soil water at 80 cm depth	[vol_perc]
soilwater_100cm	Soil water at 100 cm depth	[vol_perc]
soilwater_120cm	Soil water at 120 cm depth	[vol_perc]
capillary_pressure_5cm	Capillary pressure at 5 cm depth	[hPa]
capillary_pressure_10cm	Capillary pressure at 10 cm depth	[hPa]

entity name	decription	unit
capillary_pressure_20cm	Capillary pressure at 20 cm depth	[hPa]
capillary_pressure_30cm	Capillary pressure at 30 cm depth	[hPa]
capillary_pressure_40cm	Capillary pressure at 40 cm depth	[hPa]
capillary_pressure_50cm	Capillary pressure at 50 cm depth	[hPa]
capillary_pressure_100cm	Capillary pressure at 100 cm depth	[hPa]
groundwater	Groundwater depth (depth from which all below layers have a water-filled pore space of at least 0.9)	[m]
irrigation_reservoir	Water available for irrigation	[mm]
plant_waterdeficit	Cumulative water lost from the stem storage	[mm]

Watercycle output (horizons,daily) xml-based module selection in project's setup:

```
< module id="output:watercycle-horizons:daily" />
```

entity name	decription	unit
soilwater_0_10cm	Soil water between 0 - 10 cm depth	[mm]
soilwater_10_20cm	Soil water between 10 - 20 cm depth	[mm]
soilwater_20_40cm	Soil water between 20 - 40 cm depth	[mm]
soilwater_40_60cm	Soil water between 40 - 60 cm depth	[mm]
soilwater_60_80cm	Soil water between 60 - 80 cm depth	[mm]
soilwater_80_120cm	Soil water between 80 - 120 cm depth	[mm]
soilwater_120_150cm	Soil water between 120 - 150 cm depth	[mm]

Watercycle output (subdaily) xml-based module selection in project's setup↵
:

```
< module id="output:watercycle:subdaily" />
```

entity name	decription	unit
precipitation	Precipitation	[mm]
irrigation	Irrigation	[mm]
throughfall	Throughfall	[mm]
pot_evapotranspiration	Potential evapotranspiration	[mm]
pot_transpiration	Potential transpiration	[mm]
transpiration	Actual transpiration	[mm]
wateruptake	Soilwater uptake by plants (may be stored in plants and not directly transpired)	[mm]
interception_evaporation	Actual evaporation from interception	[mm]
soil_evaporation	Actual evaporation from soil surface	[mm]
surface_evaporation	Actual evaporation from snow/watertable surface	[mm]
runoff	Lateral surface water runoff	[mm]
percolation	Percolation out of last soil layer	[mm]
infiltration	Infiltration into the soil	[mm]
snow	Amount of snow in water equivalents	[mm_H2Oeq]
leafwater	Intercepted leaf water	[mm]
surfacewater	Surface water	[mm]
soilwater	Total soil water	[mm-m3]
soilwater_rooted	Soil water in rooted soil layers	[mm-m3]
soilwater_10cm	Soil water at 10 cm depth	[vol_perc]
soilwater_20cm	Soil water at 20 cm depth	[vol_perc]
soilwater_30cm	Soil water at 30 cm depth	[vol_perc]
soilwater_50cm	Soil water at 50 cm depth	[vol_perc]
soilwater_100cm	Soil water at 100 cm depth	[vol_perc]
plant_waterdeficit	Cumulative water lost from the stem storage	[mm]

Watercycle output (yearly) xml-based module selection in project's setup:

```
< module id="output:watercycle:yearly" />
```

entity name	decription	unit
precipitation	Precipitation	[mm]
irrigation	Irrigation	[mm]
throughfall	Throughfall	[mm]
pot_evapotranspiration	Potential evapotranspiration	[mm]
pot_transpiration	Potential transpiration	[mm]
transpiration	Actual transpiration	[mm]
wateruptake	Soilwater uptake by plants (may be stored in plants and not directly transpired)	[mm]
interception_evaporation	Actual evaporation from interception	[mm]
soil_evaporation	Actual evaporation from soil surface	[mm]
surface_evaporation	Actual evaporation from snow/watertable surface	[mm]
runoff	Lateral surface water runoff	[mm]
percolation	Percolation out of last soil layer	[mm]
infiltration	Infiltration into the soil	[mm]

1.0.7.8 Ecosystem output

entity name	decription	unit
dC_gpp	Daily gross primary productivity	[kgCha-1]
dC_ter	Daily total ecosystem respiration	[kgCha-1]
dC_nee	Daily total net ecosystem exchange (C uptake - respiration)	[kgCha-1]
aC_fertilize	Annual carbon input from fertilization	[kgCha-1]
C_total	Total ecosystem carbon	[kgCha-1]
C_soil	Total soil carbon	[kgCha-1]
C_wood_above	Total carbon in aboveground dead wood	[kgCha-1]
C_wood_below	Total carbon in belowground dead wood	[kgCha-1]
C_stand_above	Total carbon in aboveground wood	[kgCha-1]
C_stand_below	Total carbon in belowground wood	[kgCha-1]
N_total	Total ecosystem nitrogen	[kgNha-1]
N_soil	Total soil nitrogen	[kgNha-1]
N_wood_above	Total nitrogen in aboveground dead wood	[kgNha-1]
N_wood_below	Total nitrogen in belowground dead wood	[kgNha-1]
N_stand_above	Total nitrogen in aboveground wood	[kgNha-1]
N_stand_below	Total nitrogen in belowground wood	[kgNha-1]

entity name	decription	unit
ET	Daily total evapotranspiration	[mm]

Ecosystem output (daily)

entity name	decription	unit
aC_gpp	Annual gross primary productivity	[kgCha-1]
aC_ter	Annual total ecosystem respiration	[kgCha-1]
aC_fertilize	Annual carbon input from fertilization	[kgCha-1]
aC_export_harvest	Annual carbon exported from field by harvest and cutting	[kgCha-1]
aC_leach	Annual carbon leached out	[kgCha-1]
C_total	Total ecosystem carbon	[kgCha-1]
C_soil	Total soil carbon	[kgCha-1]
C_wood_above	Total carbon in aboveground dead wood	[kgCha-1]
C_wood_below	Total carbon in belowground dead wood	[kgCha-1]
C_stand_above	Total carbon in aboveground wood	[kgCha-1]
C_stand_below	Total carbon in belowground wood	[kgCha-1]
aN_fertilize	Annual amont of nitrogen fertilizer	[kgNha-1]
aN_export_harvest	Annual nitrogen exported from field by harvest and cutting	[kgNha-1]
aN_deposition	Annual nitrogen input by deposition	[kgNha-1]
aN_fixation	Annual nitrogen fixation	[kgNha-1]
aN_emis	Annual nitrogen loss by gaseous emissions	[kgNha-1]
aN_leach	Annual nitrogen loss by leaching	[kgNha-1]
N_total	Total ecosystem nitrogen	[kgNha-1]
N_soil	Total soil nitrogen	[kgNha-1]
N_wood_above	Total nitrogen in aboveground dead wood	[kgNha-1]
N_wood_below	Total nitrogen in belowground dead wood	[kgNha-1]
N_stand_above	Total nitrogen in aboveground wood	[kgNha-1]
N_stand_below	Total nitrogen in belowground wood	[kgNha-1]

Ecosystem output (yearly)

1.0.7.9 Inventory output

entity name	decription	unit
surfacetemperature	Surface temperature	[oC]
surfacewater	Surface watertable	[mm]
precipitation	Surface watertable	[mm]
percolation	Surface watertable	[mm]
C_soil	Soil organic carbon	[kgm-2]
N_soil	Soil organic nitrogen	[kgm-2]
DW_above	Aboveground biomass dry weight	[kgm-2]
C_stubble	Amount of carbon of stubble	[kgm-2]
DW_fru		[kgm-2]
DW_fru_export		[kgm-2]
C_plant_export		[kgm-2]
C_plant_litter		[kgm-2]
dC_ch4_emis		[kgm-2]
dC_ch4_emis_cropping↵ _season		[kgm-2]
dC_co2_emis_hetero		[kgm-2]", <tr><td>dN↵ _n2o_emis <td> <td> [kgm-2]",
dN_n2o_emis_cropping↵ _season		[kgm-2]", <tr><td>d↵ N_no_emis <td> <td> [kgm-2]",
dN_n2_emis		[kgm-2]", <tr><td>dN↵ _nh3_emis <td> <td> [kgm-2]",
dC_doc_leach		[kgm-2]", <tr><td>dN↵ _no3_leach <td> <td> [kgm-2]",
dN_don_leach		[kgm-2]", <tr><td>d↵ N_fertilizer <td> <td> [kgm-2]",
dC_fertilizer		[kgm-2]",

Inventory output (daily/yearly)

1.0.7.10 GGCM output

entity name	decription	unit
dN_fertilizer	seasonal nitrogen application in form of different inorganic fertilizers	[kgNha-1]

GGCMI Fertilize output

entity name	decription	unit
dW_grain	dry weight of grain at harvest	[kgHa-1]
dW_above_ground	dry weight of above ground biomass at harvest	[kgHa-1]
dW_roots	dry weight of roots at harvest	[kgHa-1]
CN_grain	C:N ratio of grain at harvest	ratio
N_grain_export	Nitrogen of grain exported after harvest	[KgNha-1]
N_straw_export	Nitrogen of straw exported after harvest	[KgNha-1]

GGCMI Harvest output

entity name	decription	unit
dN_manure	seasonal nitrogen application in form of manure	[kgCha-1]

GGCMI Manure output

entity name	decription	unit
crop_flag	no crop = 0, crop = 1	-
dvs	crop maturity (no crop = -1)	-
dC_ch4_emis	Daily methane flux	[kgCha-1]
dC_emis	Daily flux of CH4 and CO2	[kgCha-1]
dN_leach	Daily leaching of nitrate, ammonium and dissolved organic nitrogen	[kgNha-1]
dN_n2o_emis	Daily nitrous oxide flux	[kgNha-1]
dN_n2_emis	Daily molecular nitrogen flux	[kgNha-1]
dN_out	Loss of reactive nitrogen due to leaching (NO3,NH4,DoN) and emission (N2O, NO, N2, NH3)	[kgNha-1]
dN_in	N input from deposition (NH4, NO3) and N2 fixation	[kgNha-1]
dN_up	Daily nitrogen uptake by plants from the litter layer and mineral soil	[kgNha-1]

entity name	decription	unit
AET	Daily sum of evaporation (soil, surface and from interception) and transpiration	[mm]
transpiration	daily transpiration	[mm]
wateruptake	water uptake from the soil	[mm]
evap	Daily evaporation from soil and surface water (not from interception)	[mm]
runoff	Daily lateral run-off	[mm]
irri	Daily addition of irrigation water	[mm]
soilwater	Total water in soil above wilting point	[mm]

Daily GGCM output

entity name	decription	unit
soilwater	Total water in soil above wilting point	[mm]

Monthly GGCM output

entity name	decription	unit
dvs	fractional maturity	-
planting_year	year of planting	-
planting_day	day of year of planting	-
anthesisday_from_planting	number of days after planting of flowering (anthesis)	-
harvestday_from_planting	number of days after planting of harvesting	-
dC_ch4_emis	Seasonal methane flux	[kgCha-1]
dC_emis	Seasonal flux of CH ₄ and CO ₂	[kgCha-1]
dN_leach	Seasonal leaching of nitrate, ammonium and dissolved organic nitrogen	[kgNha-1]
dN_n2o_emis	Seasonal nitrous oxide flux	[kgNha-1]
dN_n2_emis	Seasonal molecular nitrogen flux	[kgNha-1]
dN_out	Loss of reactive nitrogen due to leaching (NO ₃ , NH ₄ , DoN) and emission (N ₂ O, NO, N ₂ , NH ₃)	[kgNha-1]
dN_in	N input from deposition (NH ₄ , NO ₃) and N ₂ fixation	[kgNha-1]

entity name	decription	unit
dN_up	Seasonal nitrogen uptake by plants from the litter layer and mineral soil	[kgNha-1]
AET	Seasonal sum of evaporation (soil, surface and from interception) and transpiration	[mm]
transp	Seasonal transpiration	[mm]
evap	Seasonal evaporation from soil and surface water (not from interception)	[mm]
runoff	Seasonal lateral run-off	[mm]
irri	Seasonal addition of irrigation water	[mm]

Seasonal GGCM output

entity name	decription	unit
dN_n2_emis	Yearly N2 flux	[kgNha-1]
dN_nh3_emis	Yearly NH3 flux	[kgNha-1]
dN_n2o_emis	Yearly N2O flux	[kgNha-1]
dN_no_emis	Yearly NO flux	[kgNha-1]

Yearly GGCM output dN_no3_leach | Yearly leaching of NO3 | [kgNha-1] dN←
_don_leach | Yearly leaching of dissolved organic nitrogen | [kgNha-1] dN_nh4_leach |
Yearly leaching of NH4 | [kgNha-1]

dN_harvest_export | Yearly N export via harvest (grain + exported straw + exported roots) | [kgNha-1]

dN_dep| N input from deposition (NH4, NO3) | [kgNha-1] dN_fix | Yearly nitrogen fixation by plants | [kgNha-1] dN_fert | Yearly nitrogen input via fertiliser and manure | [kgNha-1]

dN_up | Yearly nitrogen uptake by plants from the litter layer and mineral soil | [kgNha-1] dN_litter_above | Yearly return of N to soil from above-ground plant litter | [kgNha-1] dN_litter_below | Yearly return of N to soil from roots (decay and exudation) | [kgNha-1]

dC_co2_hetero_emis | Yearly flux of CO2 from heterotrophic respiration | [kgCha-1] dC_co2_auto_emis | Yearly flux of CO2 from autotrophic respiration associated with roots | [kgCha-1] dC_ch4_emis | Yearly methane flux | [kgCha-1]

dC_leach | Yearly leaching of DOC and CH4 out of soil | [kgCha-1]

dC_fert | Yearly carbon input via manure | [kgCha-1] dC_litter_above | Yearly addition of C to soil from above-ground plant litter | [kgCha-1] dC_litter_below | Yearly addition

of C to soil from roots (decay and exudation) | [kgCha-1] dC_fix | Yearly fixation of C by algae | [kgCha-1]

throughf | Yearly throughfall (water that reaches surface of soil) | [mm] intercep | Yearly evaporation from interception | [mm] transp | Yearly transpiration | [mm] evap | Yearly evaporation from soil and surface water (not from interception) | [mm] runoff | Yearly lateral run-off | [mm] perc | Yearly percolation out of bottom soil layer | [mm] irri | Yearly addition of irrigation water | [mm]

1.0.7.11 DSS output

entity name	decription	unit
aDW_yield_fruit	Annual dry weight of exported fruits from field	[kgDWha-1]
aDW_yield_biomass	Annual dry weight yield exported from field	[kgDWha-1]
aN_yield_fruit	Annual nitrogen yield exported from field	[kgNha-1]
aN_yield_biomass	Annual nitrogen yield exported from field	[kgNha-1]
aN_fert	Annual nitrogen fertilization	[kgNha-1]
aC_soil_change	Annual change of soil organic matter	[kgCha-1]
nitrogen_use_efficiency_total	Nitrogen loss due to gas emissions and leaching in relation to fertilization	[-]
nitrogen_use_efficiency_plant	Nitrogen uptake of plants in relation to fertilization	[-]
aC_ch4_emis	Annual emissiosn of CH4	[kgCha-1]
aN_n2o_emis	Annual emissiosn of N2O	[kgNha-1]
aN_nh3_emis	Annual emissiosn of NH3	[kgNha-1]
aN_no3_leach	Annual leaching of NO3	[kgNha-1]
a_percolation	Annual sum of percolation of water	[Lha-1]
a_precipitation	Annual sum of precipitation	[Lha-1]
a_temperature	Annual mean of air temperature	[oC]

DSS output (yearly)

1.0.7.12 Surrogateoutput output

entity name	decription	unit
aN_n2o_emis	Yearly N2O flux	[kgNha-1]
aN_no3_leach	Yearly leaching of NO3	[kgNha-1]
aC_harvest_export	Yearly C export via harvest (grain + exported straw + exported roots)	[kgCha-1]
aC_pool_change	Yearly C pool changes	[kgCha-1]

Yearly SURROGATE output

Chapter 2

LandscapeDNDC Farm models

2.0.1 User guide

The FarmSystem model is meant to represent a farm that handles a list of field sites. Field sites refer to individual LandscapeDNDC simulation instances. The definition of an explicit farm that manages a field site is meant to:

- replace the static management definitions especially with regard to harvest dates (so far mainly in croplands). This is especially useful for longterm-simulations when climate change may require adjusted growing degree parametrizations and/or growing season lengths.
- establish communication between gridcells/fields (e.g., manure produced in one grid-cell/field can be transported and incorporated into the soil of another gridcell/field)

2.0.1.1 Setup configuration

The FarmSystem model requires two input definitions:

- Path to the json-formatted FarmSystem input: `file="source/to/input/file.farmsystem"`
- FarmSystem identifier, i.e. id that defines the FarmSystem-specific input information↵
: `id="1"`

For *LandscapeDNDC*, the definition of a gridcell/setup including the *MoBiLE* model as well as the *FarmSystem* model looks as follows:

```
<models>
  <model id="FarmSystem"/>
  <model id="_MoBiLE"/>
</models>
<FarmSystem file="%I/regional/testfarm/testfarm.farmsystem" id="1"/>
<mobile>
```

```

    <modulelist>
    ...
  </modulelist>
</mobile>

```

2.0.2 Field site

A field site includes the following attributes:

- *id*: Identifier of the setup/gridcell responsible for the ecosystem simulation
- *name*: A name identifier
- *area*: The size in [m2] of the field (default: one hectare or 10000 m2)
- *dynamic_parametrization*: Integer number 0 (no dynamic parametrization), 1 (one adjustment after first harvest), or larger (continuous)
- *periods*: list of cropping seasons (see below)

2.0.2.1 Sources

2.0.3 Vegetation period

A vegetation period / cropping season includes the following attributes:

- *start*: day of year of the start of the season
- *years*: a list of years in which the defined season should be handled (if not given, season is handled every year)
- *planting*: list of planting attributes (see below)
- *tilling*: list of tilling attributes (see below)
- *fertilizer*: list of fertilizer attributes (see below)
- *manure*: list of manure attributes (see below)
- *irrigation*: list of irrigation attributes (see below)
- *flooding*: list of flooding attributes (see below)

2.0.3.1 Events

Tilling Farmsystem tilling includes:

- day
- days_after_harvest
- depth

Irrigation Farmsystem irrigation includes:

- day
- years
- fraction_dvs_min
- fraction_dvs_max
- fraction_field_capacity
- amount

Flooding Farmsystem flooding includes:

- start_static / start_dynamic
- end_static / end_dynamic
- bundheight
- watertable
- irrigationheight
- percolationrate
- drainage

Fertilization Farmsystem fertilization includes:

- day
- years
- fraction_dvs_min
- fraction_dvs_max
- fraction_gdd
- type
- amount
- depth
- watermanagement
- irrigationheight

Fertilization Farmsystem fertilization includes:

- day

2.0.4 Output

...

2.0.5 Stores

Chapter 3

LandscapeDNDC EcHy3D

3.0.1 Output

...

3.0.2 User guide

...

Chapter 4

LandscapeDNDC ORYZA2000

4.0.1 User guide

...

4.0.2 Output

...

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