

PLATHO - a simulation model of resource allocation in the plant-soil system

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**!!! The documentation of the
PLATHO-model is still under
construction and will be up-
dated continuously!!!**

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Introduction

Growth of an individual plant is determined by competition with other individuals for the local resources light, water and nutrients. As plants in their natural environments are almost always submitted to biotic (e.g. pathogens) and abiotic stresses (e.g. elevated atmospheric ozone), plants in general are situated in an internal conflict: should they invest their available assimilates into growth to increase the capacity for further uptake of external resources or should they invest into defensive compounds to minimize possible damages caused by biotic or abiotic stresses?

In order to get a tool for testing hypotheses concerning the trade off between growth and defence on the level of single plants and to assess susceptibility against stress under field conditions on the level of canopies, a new model was developed that links concepts from existing plant growth simulation models and a mechanistic approach to simulate environmental effects on secondary metabolite concentrations. This model was called PLATHO (PLAnts as Tree and Herb Objects), as it considers the general processes common to all plants and handles different herbaceous and woody species solely as special cases of the class of plants. The long-term objective of model development is to get a tool that makes it possible to minimize risks of biotic and abiotic stress and to reduce management requirements in economic plant systems.

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1 Model overview

PLATHO (PLAnts as Tree and Herb Objects) is a generic plant growth model, which simulates C- and N-fluxes in shoot and mycorrhizosphere. It considers the general processes common to all plants and handles different species solely as special cases of the class of plants. Functionally equivalent plant species can be simulated by model reparameterisation using only different species-specific parameters. Differences in physiological and ecological principles between plant classes (e.g. annuals and trees) are represented by modifications of single process formulations, without changing the overall model structure. Thus, PLATHO was developed independent of a species to emphasize similarities between trees and field crops.

PLATHO works on the level of physiological processes, which are integrated up to the level of a single plant. It combines a new mechanistic approach to simulate environmental effects on synthesis of secondary metabolites on the whole plant level with concepts from other, well established plant growth simulation models, mainly SPASS (Wang 1997; Wang and Engel 2000; Gayler et al. 2002), CERES (Ritchie et al. 1987), SUCROS (Rabbinge et al.) and TREEDYN (Bossel 1996). Starting from single plant individuals, each characterized by an own parameter set, interactions of plants in a canopy are simulated. Several plant species can be simulated simultaneously during one simulation run. In each time step, a pool of assimilates available for growth, respiration and defense is calculated, separately for each individual. The gain of resources resulting from photosynthesis and retranslocation from storage organs and dying biomass as well as resource consumption for growth, respiration and defense are calculated in units of glucose. In parallel, water- and nitrogen uptake by roots are simulated.

All processes simulated by PLATHO are related to temperature and the availability of the resources light, water and nitrogen. The model requires input data for climate (daily values of radiation, minimum and maximum temperature, rainfall resp. irrigation and relative air humidity), soil properties and data relating to fertilisation.

The model can be used to simulate growth of

1. single plant individuals without competition by neighbours
2. plant individuals competing for resources in canopies which are composed of

- identical individuals (intraspecific competition)
- different individuals of one or more species (inter- or intraspecific competition)

Plant individuals can differ in species, ecophysiological and genetic parameters and in the start values of their state variables. Plant individuals are arranged in a rectangular grid with periodical boundary conditions (boundary effects are not considered). The distance between the individuals is determined by canopy density. Different plant individuals are simulated simultaneously. Competition effects are simulated considering interactions with the four next neighbours of each individual (see figure 1).

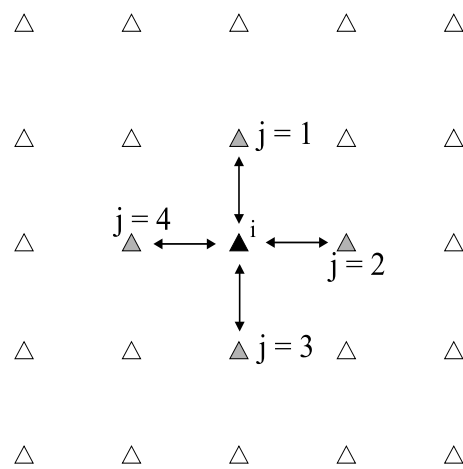


Figure 1: Arrangement of plant individuals in a rectangular grid and symbols used for calculating interaction with the next neighbours.

To simulate competition and genetic variation in canopies, more than one individual must be defined in the input files. These individuals are grouped together in an elementary grid which is periodically continued on the boundaries. For practical simulation purposes it is useful to consider only a few different plant individuals (e.g. two species in a mixed canopy, where all individuals of one species have identical parameters and start values, or a monoculture with small and tall individuals). Figures 2 and 3 show examples for elementary grids with three and four different individuals. The degree of competition between individuals depends on canopy density. If only a single plant individual is defined in the input files, a grid of identical individuals is simulated. Depending on canopy density there will be either competition or no competition.

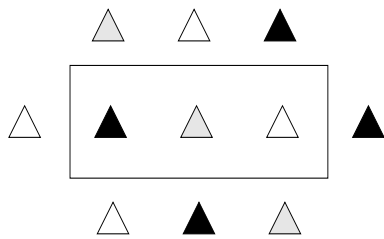


Figure 2: Example for periodical boundary conditions in a 3 species (individuals) simulation

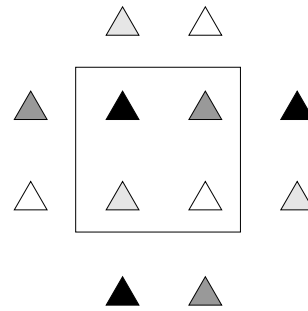


Figure 3: Example for periodical boundary conditions in a 4 species (individuals) simulation

2 Technical realization

The model structure of PLATHO is highly modular. It is implemented in C within the development tool Expert-N (Engel and Priesack 1993; Baldioli et al. 1995; Stenger et al. 1999). Expert-N consists of several modules for simulating different processes in the soil-plant-atmosphere system, which can be coupled together in various combinations. Plant processes simulated in PLATHO are governed by climate and soil processes, which can be simulated using modules from Expert-N. The link between PLATHO modules (plant process) and other modules of Expert-N (soil processes) is realized by defined interfaces. This model structure makes PLATHO to be a useful research instrument, because it allows to test several hypothesis for single processes of plant growth by changing single modules.

3 Process description

Processes simulated by PLATHO are morphological development, phenological development, respiration, biomass growth and allocation to biochemical pools, photosynthesis, water uptake, nitrogen uptake, uptake of ozone and senescence, .

3.1 Morphology and canopy structure

Competition for external resources on the level of single plants relates directly to space sequestration of the competing individuals. Therefore a simplified plant morphology is considered within the PLATHO model. It is assumed that all biomass of a plant is located in a cylinder with flexible height to diameter proportion HD [-], where HD depends on development stage and competitive situation of the plant (3.1.3). The base area of this cylinder, A_{Plant} [m^2] (3.1.1), defines the influence zone of the plant individual and is used to calculate competition coefficients $C_{i,j}$ against neighbour individuals (above and below ground, 3.1.2). Vertical distributions of leaf area (3.1.5) and root length (3.1.7) are considered using species specific distribution functions. Plants are assumed to be rotationally symmetric. The symbols used for the calculation of plant morphology are shown in figure 4.

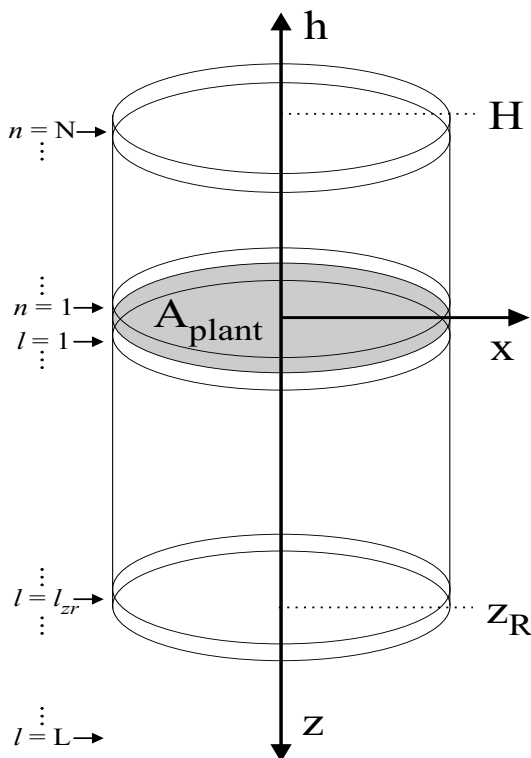


Figure 4: Geometry and symbols used for calculating plant morphology. H [m] is the actual height of the plant, z_R [m] the actual depth of the root system. N simulation layers are considered above ground and L layers below ground. l_{z_R} is the deepest rooted soil layer. h [m] is the height over the ground and z [m] the depth in the soil. The distance x [m] from the center of the plant is used for the calculation of competition coefficients, A_{plant} [m^2] is the basal area of the cylinder and describes the zone that is influenced by the plant individual.

An example for the competitive situation in a mixed canopy (two species with individuals differing in size) shows figure 5.

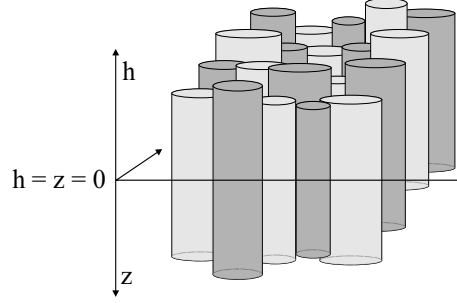


Figure 5: Example for competition between two species

3.1.1 Plant area

The base area A_{Plant} [m²] of the cylinder representing the shape of the plant, is calculated from stem diameter d_S [m] assuming a constant crown-to-stem diameter-ratio $r_{C/S}$ [-]. However, the radius of a plant cannot exceed the distance between two plants.

$$A_{Plant} = \begin{cases} \frac{\pi}{4} \cdot (r_{C/S} \cdot d_S)^2 & \text{if } d_S < \frac{2}{r_{C/S} \cdot \sqrt{\varrho_{Canopy}}} \\ \frac{\pi}{\varrho_{plant}} & \text{if } d_S \geq \frac{2}{r_{C/S} \cdot \sqrt{\varrho_{Canopy}}} \end{cases} \quad (1)$$

where ϱ_{Canopy} [plants · m⁻²] is the density of the canopy.

3.1.2 Calculation of competition coefficients

Plant areas of two individuals i and j are overlapping if the distance d [m] between the individuals is lower than the sum of both radii r_i [m] and r_j [m].

The competition coefficient between two (competing) individuals i and j is given by equation 2, where $A_{i,j}$ (equation 3) is the cross section of both plant areas and $x = \xi$ (see figure 6) is given by equation 4.

$$C_{i,j} = \begin{cases} 0 & \text{if } r_i + r_j \leq d \\ \frac{A_{i,j}}{r_i^2 \cdot \pi} & \text{if } (r_i + r_j > d) \wedge (r_j - r_i < d) \\ 1 & \text{if } r_j - r_i \geq d \end{cases} \quad (2)$$

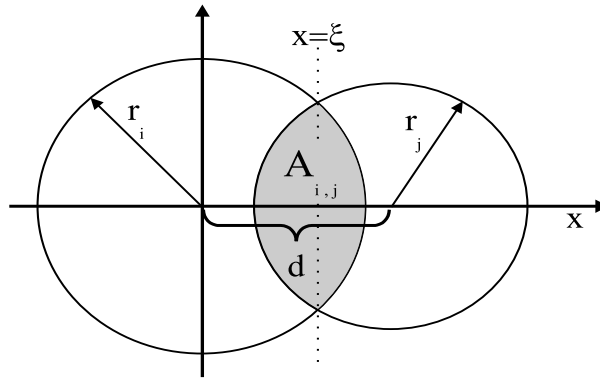


Figure 6: Geometry and symbols used for the calculation of competition coefficient between individuals i and j . r_i is the radius of the zone influenced by individual i , d the distance between individuals and $A_{i,j}$ the intersection of both plant areas. x is the distance from individual i towards individual j .

with

$$A_{i,j} = 2 \cdot \left(\int_{\xi}^{r_i} \sqrt{r_i^2 - x^2} dx + \int_{d-r_j}^{\xi} \sqrt{r_j^2 - (r_j - x')^2} dx' \right) \quad (3)$$

and

$$\xi = \frac{r_i^2 + d^2 - r_j^2}{2 \cdot d} \quad (4)$$

3.1.3 Plant height growth

The calculation of the increment in stem height follows Bossel (1996). Under light competition ($C_L > 0$), plants are assumed to grow in height until they reach the maximum height-to-diameter ratio HD_{max} [-]. If HD_{max} has been reached, further growth will continue at $HD = HD_{max}$. If there is no competition for light ($C_L = 0$), plants are assumed to pursue diameter growth until their minimum height-to-diameter HD_{min} [-] has been reached. A single plant without light competition grows at height-to-diameter ratio $HD = HD_{min}$. For annual plants, HD_{max} depends on actual height of the plant. For trees, HD_{max} is constant during the simulation period. The light competition factor C_L [-] is calculated from the competition factors $C_{i,j}$ [-] (see equation 2), the actual leaf area index LAI_j [$\text{m}^2(\text{leaf}) \cdot \text{m}^{-2}(\text{soil})$] (see equation 12) and the actual heights H_j [m] of

the next neighbours:

$$C_L = \frac{\sum_{j=1}^4 C_{i,j} \cdot LAI_j \cdot \min \{1, H_i/H_j\}}{\sum_{j=1}^4 LAI_j} \quad (5)$$

Case 1 (only diameter growth):

$$\frac{dH}{dt} = 0 \quad \text{if} \quad HD > HD_{max} \quad \text{or} \quad C_L = 0 \wedge HD > HD_{min} \quad (6)$$

Case 2 (only height growth):

$$\frac{dH}{dt} = \frac{4 \cdot \frac{dW_S}{dt}}{\pi \cdot \rho_S \cdot d_S^2} \quad \text{if} \quad HD < HD_{min} \quad \text{or} \quad C_L > 0 \wedge HD < HD_{max} \quad (7)$$

Case 3 (height/diameter is constant):

$$\frac{dH}{dt} = \frac{4 \cdot \frac{dW_S}{dt}}{3\pi \cdot \rho_S \cdot d_S^2} \quad \text{if} \quad C_L = 0 \wedge HD = HD_{min} \quad \text{or} \quad C_L > 0 \wedge HD = HD_{max} \quad (8)$$

HD is calculated from actual plant height H [m] and stem diameter d_S [m]:

$$HD = \frac{H}{d_S} \quad (9)$$

3.1.4 Stem diameter

Stems are assumed to be cylinders having the same height as the plant. Thus stem diameter d_S [m] can be calculated from stem weight W_S [kg] and stem density ρ_S [kg · m⁻³]:

$$d_S = \sqrt{\frac{4 \cdot W_S}{\pi \cdot H \cdot \rho_S}} \quad (10)$$

where H [m] is the actual plant height.

3.1.5 Leaf area and leaf area distribution

Total (living) plant leaf area A_L [m²] is calculated from actual leaf weight W_L [kg], assuming a mean specific leaf weight, λ_{Lw}^* [kg · m⁻² (leaf)]:

$$A_L = W_L / \lambda_{Lw}^* \quad (11)$$

For calculating the leaf area index LAI [m²(leaf) · m⁻²(soil)], total plant leaf area is divided by the area, which can be potentially covered by the plant:

$$LAI = \begin{cases} A_L / A_{Plant} & \text{if } A_{Plant} \geq \varrho_{Canopy}^{-1} \\ A_L \cdot \varrho_{Canopy} & \text{if } A_{Plant} < \varrho_{Canopy}^{-1} \end{cases} \quad (12)$$

where A_{Plant} [m²] is the base of the cylinder representing the shape of the plant and ϱ_{Canopy} is [m⁻²] is the number of plant individuals per square meter.

The cumulative leaf area $A_{L,cum}$ [m²] over height h [m] is assumed to follow a species specific leaf area distribution function:

$$A_{L,cum}(h) = \alpha_L + \frac{\beta_L}{1 + e^{-4 \cdot (h/H - p_L)}}$$

with

$$\begin{aligned} \beta_L &= A_L \cdot \frac{(e^{-4 \cdot (1-p_L)} + 1) \cdot (e^{4 \cdot p_L} + 1)}{e^{-4 \cdot (1-p_L)} - e^{4 \cdot p_L}} \\ \alpha_L &= \frac{-\beta_L}{e^{-4 \cdot (1-p_L)} + 1} \end{aligned} \quad (13)$$

where H [m] is the actual plant height and p_L [-] is an input parameter that describes the relative height of maximum leaf area density. The species specific form of leaf area distribution is approximated using different values of p_L .

The cumulated leaf area index LAI_{cum} [m²(leaf) · m⁻²(soil)] above h (equation 14) and leaf area density a_L [m²(leaf) · m⁻¹] at height h (equation 15) are derived from $A_{L,cum}(h)$:

$$LAI_{cum}(h) = \frac{A_{L,cum}(h)}{A_{Plant}} \quad (14)$$

$$a_L(h) = \frac{d}{dh} A_{L,cum}(h) \quad (15)$$

3.1.6 Specific leaf weight

Specific leaf weight depends strongly on light availability and nitrogen availability within leaves. In the model it is assumed that in deeper leaf layers, where incoming radiation is low, plants compensate this scarcity by thinner leaves (increased leaf area per unit leaf biomass, i.e. decreased specific leaf weight). Further it is assumed that plants compensate also low nitrogen concentrations in leaves by decreasing the specific leaf weight to maximize photosynthetic capacity per unit nitrogen in leaves. Therefore the mean specific leaf weight, λ_{Lw}^* [$\text{kg} \cdot \text{m}^{-2}$ (leaf)], is estimated from actual leaf area index LAI , [$\text{m}^2(\text{leaf}) \cdot \text{m}^{-2}(\text{soil})$] and the mean nitrogen concentration in leaves, $\nu_{L,act}$ [$\text{kg}(\text{N}) \cdot \text{kg}$]. The dependency of specific leaf weight from height h is assumed to follow an exponential distribution function.

$$\lambda_{Lw}^* = \max \{ \lambda_{Lw,max} \cdot (1 - \alpha_N \cdot LAI); \lambda_{Lw,min}^* \}$$

with

$$\alpha_N = \frac{2 \cdot \nu_{L,opt} - \nu_{L,act} - \nu_{L,min}}{4 \cdot \nu_{L,opt} \cdot LAI_{crit}} \quad (16)$$

where α_N is a function of $\nu_{L,act}$ which provides $\lambda_{Lw}^* = \lambda_{Lw,min}^*$ in case of pessimal nitrogen of leaves ($\nu_{L,act} = \nu_{L,min}$) and $LAI \geq LAI_{crit}$. λ_{Lw}^* is used to calculate total leaf area from actual leaf weight (equation 11). The minimal value of mean specific leaf weight is estimated from minimal and optimal leaf nitrogen concentrations:

$$\lambda_{Lw,min}^* = \frac{\lambda_{Lw,max}}{2} \cdot \frac{\nu_{L,opt} + \nu_{L,min}}{\nu_{L,opt}} \quad (17)$$

The actual specific leaf weight of leaves at height h follows from the cumulative leaf area index above h , $LAI_{cum}(h)$ [$\text{m}^2(\text{leaf}) \cdot \text{m}^{-2}(\text{soil})$].

$$\lambda_{Lw}(h) = \lambda_{Lw,max} \cdot e^{-\kappa \cdot LAI_{cum}(h)} \quad (18)$$

κ [$\text{m}^2(\text{soil}) \cdot \text{m}^{-2}(\text{leaf})$] describes the decrease in specific leaf weight if the cumulative leaf area index LAI_{cum} increases. κ is calculated from the relation

$$\lambda_{Lw}^* = \frac{1}{LAI} \cdot \int_0^{LAI} \lambda_{Lw}(h) dLAI_{cum} = \frac{\lambda_{Lw,max}}{\kappa \cdot LAI} \cdot (1 - e^{-\kappa \cdot LAI}) \quad (19)$$

3.1.7 Root system

The calculation of rooting depth is adapted from the CERES model family (Jones and Kiniry; Villalobos and Hall 1989; Wang 1997). It is assumed that root extension growth only occurs if root weight increases. The increase of rooted depth z_R [m] depends on actual temperature, T_{soil} [$^{\circ}C$], and actual soil water content, θ_{act} [$m^3 \cdot m^{-3}$], in the lowest rooted soil layer l_{zR} (see figure 4):

$$\frac{dz_R}{dt} = r_{z_R} \cdot f_T(l_{z_R}) \cdot f_{\theta}(l_{z_R}) \cdot \left(1 - \frac{z_R}{z_{R,max}}\right) \quad (20)$$

where r_{z_R} [$m \cdot d^{-1}$] is the maximal root extension rate and f_T [-] and f_{θ} [-] are factors relating to actual temperature and moisture in soil layer l (equations 27 and 28).

The calculation of root length distribution, $l_R(l)$ [m] is also based on the concept of CERES-models: actually formed biomass of roots (see equation 66) is converted into root length using a specific root length factor λ_{lR} [$m \cdot kg^{-1}$] and subsequently distributed to soil layers (equation 22). The distribution of newly formed root length to rooted soil layers depends on the species specific root length distribution function $w(l)$ (equation 25) and on actual distribution of moisture, $f_{\theta}(l)$ (equation 28) and nitrogen, $f_N(l)$ (equation 29), in the soil. In addition, in the PLATHO model this concept is extended considering underground competition for space sequestration between neighbour individuals by introducing a further stress factor, C_{RLD} [-], which is estimated from actual root length density of all individuals present in the respective soil disk (equation 24). The maximal value of root length density $K_{lR} = 3 \cdot 10^4 m/m^3$ is taken from Adiku et al. (1996).

The actual loss of root biomass (due to rhizodeposition and senescence, see equation 66 and section 3.7) is also converted to root length and subsequently distributed to rooted soil layers (equation 23). The die off of roots occurs preferably in soil layers with unfavourable moisture and nitrogen conditions.

$$\frac{d l_R(l)}{dt} = l_R^+(l) - l_R^-(l) \quad (21)$$

where

$$l_R^+(l) = \frac{G_{WR}}{\xi_{WR}} \cdot \lambda_{lR} \cdot \frac{w(l) \cdot \min\{f_{\theta}(l), f_N(l)\} \cdot C_{RLD}(l)}{\sum_{l=1}^{l_{zR}} [w(l) \cdot \min\{f_{\theta}(l), f_N(l)\} \cdot C_{RLD}(l)]} \quad (22)$$

$$l_R^-(l) = \lambda_R \cdot W_R \cdot \lambda_{lR} \cdot \frac{l_R(l) \cdot \max\{1 - f_\theta(l), 1 - f_N(l)\}}{\sum_{l=1}^{l_{ZR}} [l_R(l) \cdot \max\{1 - f_\theta(l), 1 - f_N(l)\}]} \quad (23)$$

$$C_{RLD}(l) = \left(1 - \frac{l_{R,i}(l) + \sum_{j=1}^4 C_{j,i} \cdot l_{R,j}}{K_{lR} \cdot A_{plant} \cdot (z_l - z_{l-1})} \right) \quad (24)$$

and

$$w(l) = \frac{\alpha_R}{\beta_R} \cdot \int_{z_{l-1}}^{z_l} \left(\frac{z}{\beta_R} \right)^{(\alpha_R-1)} \cdot e^{-(z/\beta_R)^{\alpha_R}} dz$$

with

$$\alpha_R = 1 + 2 \cdot p_R$$

$$\beta_R = \begin{cases} \frac{z_R}{2} & \text{if } p_R = 0 \\ \frac{p_R \cdot z_R}{\left(\frac{\alpha_R-1}{\alpha_R}\right)^{\frac{1}{\alpha_R}}} & \text{else} \end{cases} \quad (25)$$

z_L [m] denotes the depth of the bottom of soil layer l . Species specific forms of root distribution are approximated by different values of the parameter p_R , which describes the relative position of maximal root density.

The root surface in soil layer l , $a_R(l)$ [m²], is calculated from root length in layer l , $l_R(l)$, root density, ϱ_R [kg · m⁻³], and specific root length, λ_R [kg · m⁻¹]:

$$a_R(l) = \sqrt{\frac{4\pi}{\varrho_R \cdot \lambda_{lR}}} \cdot l_R(l) \quad (26)$$

Reduction functions

Reduction functions relating to soil temperature, soil moisture and mineral nitrogen concentration in soil are adapted from the modelling approach used in the SPASS model (Wang 1997). Dependency of root depth growth on **temperature** in the lowest rooted soil layer, $T_{soil}(l_{z_R})$ [°C] is calculated by help of an optimum function with three cardinal temperatures $T_{rt,min}$, $T_{rt,opt}$ and $T_{rt,max}$.

$$f_T = \begin{cases} 0 & \text{if } T_{soil}(l_{z_R}) < T_{rt,min} \vee T_{soil}(l_{z_R}) > T_{rt,max} \\ \frac{2 \cdot (T_{mm} \cdot T_{om})^\alpha - T_{mm}^{2\alpha}}{T_{om}^{2\alpha}} & \text{if } T_{rt,min} \leq T_{soil}(l_{z_R}) \leq T_{rt,max} \end{cases} \quad (27)$$

$$T_{mm} = T_{soil}(l_{zR}) - T_{rt,min}$$

with

$$T_{mm} = T_{soil}(l_{zR}) - T_{rt,min}$$

$$T_{om} = T_{rt,opt} - T_{rt,min}$$

$$T_{xm} = T_{rt,max} - T_{rt,min}$$

and

$$\alpha = \frac{\ln 2 \cdot T_{om}}{T_{xm}}$$

The increase in rooting depth as well as root length growth is reduced, if **water** content in the respective soil layer, $\theta_{act}(l)$ [$\text{m}^3 \cdot \text{m}^{-3}$], decreases below the quarter of the available field capacity:

$$f_{\theta}(l) = \begin{cases} 0 & \text{if } \theta_{act}(l) < \theta_{pwp}(l) \\ \frac{4 \cdot (\theta_{act}(l) - \theta_{pwp}(l))}{\theta_{fc}(l) - \theta_{pwp}(l)} & \text{if } 0 \leq \theta_{act}(l) - \theta_{pwp}(l) \leq \frac{1}{4} \cdot (\theta_{fc}(l) - \theta_{pwp}(l)) \\ 1 & \text{if } \theta_{act}(l) - \theta_{pwp}(l) > \frac{1}{4} \cdot (\theta_{fc}(l) - \theta_{pwp}(l)) \end{cases} \quad (28)$$

Root length growth is also reduced depending on mineral **nitrogen** concentration, $c_N(l)$ [$\text{mg} \cdot \text{kg}^{-1}$] in soil:

$$f_N(l) = \begin{cases} 0.01 & \text{if } c_N(l) < 1.11 \text{ mg} \cdot \text{kg}^{-1} \\ 1 - 1.17 \cdot e^{-0.15 \cdot c_N(l)} & \text{if } c_N(l) \geq 1.11 \text{ mg} \cdot \text{kg}^{-1} \end{cases} \quad (29)$$

3.2 Phenological development

The development of plants depends strongly on environmental factors. In this model, the influences of temperature, length of the photoperiod and atmospheric ozone concentration are considered. Six development stages are distinguished (see table 1). Development stage i is reached, when the biological time t_B [-] (equation 30) exceeds a threshold sum of development days D_i ($D_{i+1} > D_i$). Biological time is the sum of development days multiplied with the factors delaying phenological development. One day of biological time corresponds to one real day with optimal temperature and optimal length of the light period.

Table 1: Definition of development stages for herbs and trees

	Herbs	Trees
$0 \leq t_B < D_1$	before germination	dormance
$D_1 \leq t_B < D_2$	germination - emergence	breaking of the buds
$D_2 \leq t_B < D_3$	vegetative growing	complete unfolding of the leaves
$D_3 \leq t_B < D_4$	begin of fructification	maximal efficiency of leaves
$D_4 \leq t_B < D_5$	only seeds/tubers are growing	leaf fall
$D_5 \leq t_B < D_6$	maturity	leaf and fruit fall

$$t_B = \sum_{d=1}^{d_{act}} \min \{f_{T,dev} \cdot f_{ph}\} \quad (30)$$

where $f_{T,dev}(T_m, T_{dev,min}, T_{dev,opt}, T_{dev,max})$ and $f_{ph}(ph)$ are the temperature and daylength response functions of phenological development (equations 33 and 34). At the end of each year, t_B is set to zero. The actual development rate r_{dev} [d^{-1}] is given by

$$r_{dev} = \frac{f_{T,dev} \cdot f_{ph}}{\Delta D} \quad (31)$$

where

$$\Delta D = D_{i+1} - D_i, \quad i = 0, \dots, 5 \quad (32)$$

is the number of development days in the actual development stage ($D_0 = 0$).

3.2.1 Influence of air temperature

In order to consider the influence of daily mean air temperature T_m [°C] on the actual development rate, a response factor $f_{T,dev}$ [-] is introduced. $f_{T,dev}$ describes an optimum function, where the shape of this function is determined by the minimal temperature for phenological development, $T_{dev,min}$ [°C], the optimal temperature, $T_{dev,opt}$ [°C], and the maximal temperature, $T_{dev,max}$ [°C].

$$f_{T,dev} = \begin{cases} 0 & \text{if } T_m < T_{dev,min} \vee T_m > T_{dev,max} \\ \frac{2 \cdot (T_{mm} \cdot T_{om})^\alpha - T_{mm}^{2\alpha}}{T_{om}^{2\alpha}} & \text{if } T_{dev,min} \leq T_m \leq T_{dev,max} \end{cases} \quad (33)$$

with

$$\alpha = \frac{\ln 2 \cdot T_{om}}{T_{xm}}$$

and

$$T_{mm} = T_m - T_{dev,min}$$

$$T_{om} = T_{dev,opt} - T_{dev,min}$$

$$T_{xm} = T_{dev,max} - T_{dev,min}$$

3.2.2 Influence of light

Another factor that affects the rate of development is actual length of the photoperiod. According to the type of the photoperiodic response, short-day plants, long-day plants and day-neutral plants are distinguished in PLATHO.

$$f_{ph} = \begin{cases} 1 & \text{for "day-neutral" plants} \\ \frac{1 - e^{-\omega \cdot (ph - ph_{opt} + \frac{4}{\omega})}}{1 - e^{-4}} & \text{for "long day" plants} \\ \frac{1 - e^{\omega \cdot (ph - ph_{opt} + \frac{-4}{\omega})}}{1 - e^{-4}} & \text{for "short day" plants} \end{cases} \quad (34)$$

where ω is a photoperiod sensitivity coefficient.

3.2.3 Influence of atmospheric ozone concentration

High atmospheric ozone concentrations can accelerate senescence. In PLATHO therefore the biological time of the begin of leaf fall, D_4 is decreased under high ozone concentrations. The effect is assumed to be cumulative and only ozone concentrations above a critical value $c_{O_3,crit}$ [ppb] contribute to the acceleration of senescence.

$$D_4 = \max \left\{ D_{4,0} \cdot f_{O_3}, \frac{1}{2} \cdot (D_{4,0} + D_3) \right\} \quad (35)$$

where

$$f_{O_3} = 1 - \alpha_{O_3} \cdot I_{O_3} \quad (36)$$

$D_{4,0}$ is the number of development days before leaf fall without the effect of ozone, α_{O_3} is a ozone sensitivity coefficient and I_{O_3} [-] is actual ozone stress intensity (see equation 153).

3.3 Growth and allocation to biochemical pools

Four aggregated biochemical pools are considered (see figure 7): *assimilates* (temporarily existing products of photosynthesis and reserve remobilisation, handled as glucose), which are immediately available for growth and maintenance processes, *reserves*, which can be mobilized if required, *defensive compounds* (phenylpropanoids in case of apple trees) and *structural biomass*. Structural biomass is divided in fine roots, gross roots, stem, branches, leaves and fruits in case of trees and roots, stem leaves and fruits in case of herbs. Rates of material fluxes between these pools depend on the actual plant internal availability of carbon and nitrogen and on the actual demand for growth and defence, which are calculated every time step. All conversion processes are calculated in units of glucose using biochemical knowledge about energetics and stoichiometries of the dominating reaction pathways. The amount of assimilates, A_{av} [kg(glucose)], which are available to fulfill the demands of all energy consuming processes during a time step Δt [d] is calculated from actual photosynthesis rate P_{act} [kg(glucose) · d⁻¹], potential remobilisation from reserves R [kg] and the assimilate surplus remaining from the time step before A_{old} [kg(glucose)]. Maintenance processes take priority over all other processes. Thus, the amount of assimilates, which are available for synthesising structural biomass and defensive compounds results from

$$A_{av} = (P_{act} + R \cdot \tau_R) \cdot \Delta t - D_M + A_{old} \quad (37)$$

where D_M [kg(glucose)] is the amount of assimilates required for maintenance processes and τ_R [d⁻¹] is the reserves remobilisation rate.

3.3.1 Maintenance

Estimation of the glucose demand for maintenance follows the concepts outlined by Penning de Vries et al. (1989) and Thornley and Johnson (1990). In the model it is assumed, that maintenance respiration rate is independent of plant tissue growth. The glucose requirement for maintenance comprises all energy demands to maintain the functional and compositional status quo of the plant tissue. Three components of maintenance are distinguished: turnover of proteins and lipids, maintenance of ion concentrations across membranes and a component related to metabolic activity.

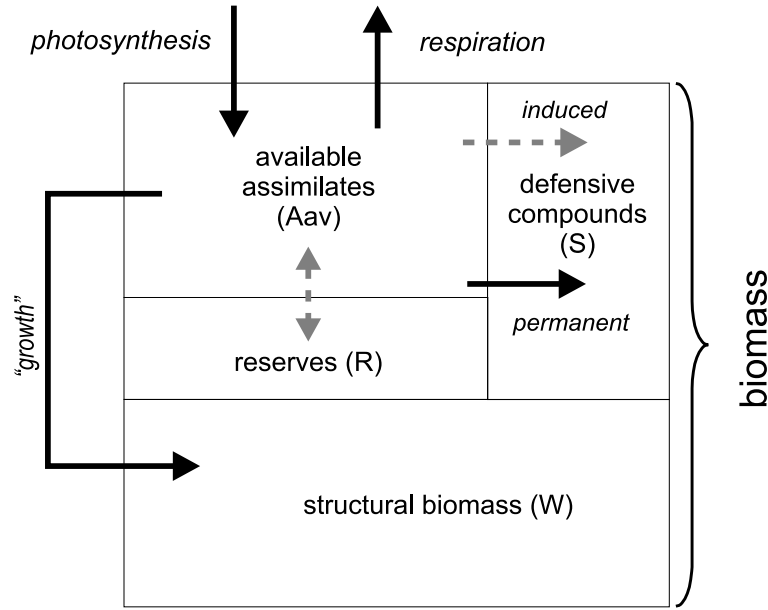


Figure 7: Fluxes between aggregated biochemical pools that are considered in the PLATHO model

The amount of glucose $m_{tu,k}$ [$\text{kg}(\text{glucose}) \cdot \text{d}^{-1}$] that is required to resynthesise proteins and lipids in organ i follows from the fractions $f_{p,k}$ [-] and $f_{l,k}$ [-] of proteins and lipids in organ k , the turnover rates k_p [d^{-1}] and k_l [d^{-1}] of both pools and the actual weight of organ k , W_k [kg]:

$$m_{tu,k} = \frac{180}{36} \cdot \left(f_{p,k} \cdot k_p \cdot \frac{c_{ATP,p}}{MW_p} + f_{l,k} \cdot k_l \cdot \frac{c_{ATP,l}}{MW_l} \right) \cdot W_k \quad (38)$$

where $c_{ATP,p} = 4$ ATP per peptide bond is the ATP cost of protein synthesis from amino acids and $c_{ATP,l} = 7$ ATP per tryglyceride is the ATP cost of lipid resynthesis from glycerol and free fatty acids. $MW_p = 120$ [$\text{g} \cdot \text{mol}^{-1}$] and $MW_l = 900$ [$\text{g} \cdot \text{mol}^{-1}$] are the average molecular weights of one amino acid residue and one lipid respectively. The factor $180/36$ considers the glucose equivalent of one mol ATP.

Costs to maintain concentrations of ions across membranes, m_{ion} [$\text{kg}(\text{glucose}) \cdot \text{d}^{-1}$], are estimated in a similar way:

$$m_{ion,k} = \frac{180}{36} \cdot f_{ion,k} \cdot k_{ion} \cdot \frac{c_{ATP,ion}}{MW_{ion}} \cdot W_k \quad (39)$$

where $f_{ion,k}$ [-] is the fraction of minerals in organ k , k_{ion} [d^{-1}] is the average ion leakage rate through membranes, $c_{ATP,ion} = 1$ ATP per ion transported is the ATP cost for ion

transport and $MW_{ion} = 40$ [g · mol⁻¹] is the average relative molecular mass of minerals. Values of c_{ATP} and MW are taken from Thornley and Johnson (1990).

Gross photosynthesis, P_{act} [kg(CO₂) · d⁻¹], is assumed to be a measure for the estimation of the component of maintenance respiration, m_{met} [kg(glucose) · d⁻¹], that is due to metabolic activity:

$$m_{met} = \mu_{met} \cdot P_{act} \quad (40)$$

where μ_{met} [-] is the fraction of photosynthetic products that is used for metabolic processes. The total demand for maintenance processes in a given time step Δt than follows from

$$D_M = \left(\sum_i (m_{tu,i} + m_{ion,i}) + m_{met} \right) \cdot 2^{\frac{T-20}{10}} \cdot \Delta t \quad (41)$$

3.3.2 Growth and allocation of assimilates to plant organs

Two factors can limit the actual growth rate of the plant: the potential growth rate of the plant or the plant internal availability of assimilates, φ_C (equation 49), and nitrogen, φ_N (equation 50). The potential growth of total biomass, G_{pot} [kg(glucose)], is calculated by means of equations 42 and 43. The actual usage of assimilates for synthesizing structural biomass, G_W [kg(glucose)], is calculated by equation 48, the actual usage for the synthesis of defensive compounds, G_S [kg(glucose)] by means of equation 67). G_{pot} depends on the actual biological time, t_B (equation 30) of the plant:

Herbs:

$$G_{pot} = \begin{cases} 0 & \text{if } 0 \leq t_B < D_1 \\ r_{dev} \cdot W_{seed} \cdot f_T \cdot \Delta t & \text{if } D_1 \leq t_B < D_2 \\ r_{max} \cdot W \cdot f_T \cdot \Delta t & \text{if } D_2 \leq t_B < D_3 \\ \varrho_F \cdot W_{V2} \cdot f_T \cdot \Delta t & \text{if } D_3 \leq t_B < D_5 \end{cases} \quad (42)$$

Trees:

$$G_{pot} = \begin{cases} 0 & \text{if } 0 \leq t_B < D_1 \\ r_{max} \cdot W \cdot f_T \cdot \Delta t & \text{if } D_1 \leq t_B < D_4 \\ r_{max} \cdot W \cdot f_{AT} \cdot f_T \cdot \Delta t & \text{if } D_4 \leq t_B < D_6 \end{cases} \quad (43)$$

r_{dev}	actual development rate [d^{-1}] (equation 32)
r_{max}	maximal growth rate of the plant [$kg(\text{glucose}) \cdot kg^{-1} \cdot d^{-1}$]
W_{seed}	seed weight in units of glucose [$kg(\text{glucose})$]
W	actual structural biomass of the plant [kg]
f_T	temperature response function [-]
ϱ_F	fruit flush rate [$kg(\text{glucose}) \cdot kg^{-1} \cdot d^{-1}$]
W_{V2}	vegetative structural biomass at the end of stage 2 [kg]
f_{AT}	(= $(D_6 - t_B)/2$) factor relating to growth reduction in autumn [-]

G_{pot} is divided into demand for growth of structural biomass D_W [$kg(\text{glucose})$] and demand for defence D_S [$kg(\text{glucose})$], similar to the model approach of Coley et al. (1985):

$$D_W = G_{pot} \cdot (1 - \sigma) \quad (44)$$

$$D_S = G_{pot} \cdot \sigma \quad (45)$$

with

$$\sigma = \sigma_0 + \sigma_I \quad (46)$$

σ [-] is the potential defence investment, which consists of a permanent part σ_0 and an induced part σ_I . σ_I is assumed to be greater than zero only in case of actual stress like a pathogen attack or if the plant internal ozone concentration exceeds the threshold value of ozone tolerance. σ_I is a function of stress intensity.

$$\sigma_I = a_I \cdot I^\alpha \quad (47)$$

In the PLATHO model, the demand for growth processes takes priority over that for defence. Assimilates are only allocated to defence either if their available amount exceeds growth demand, or if availability of nitrogen is lower than the demand required for growth processes (see section 3.3.3). The actual amount of assimilates, which are used for growth

of structural biomass results from plant internal availability of assimilates, φ_C [-], and nitrogen, φ_N [-]:

$$G_W = D_W \cdot \varphi_C \cdot \varphi_N \quad (48)$$

where

$$\varphi_C = \min \left\{ 1, \frac{A_{av}}{D_W} \right\} \quad (49)$$

and

$$\varphi_N = \min \left\{ 1, \frac{N_{av}}{N_{dem,grw}} \right\} \quad (50)$$

where N_{av} [kg(N)] is the amount of plant internal nitrogen, which is potentially available for growth processes (equation 65) and $N_{dem,grw}$ [kg(N)] is the demand for nitrogen required to realise the potential plant organ growth (equation 123).

In a second step, G_W is partitioned to the single plant organs k , where the index k denotes roots (R), leaves (L), stem (S) and fruits (F) in case of herbaceous plants, and fine roots (FR), gross roots (GR), leaves (L), branches (B), stem (S) and fruits (F) in case of trees respectively (equation 51). The partitioning factors f_k ($\sum f_k = 1$) depend on actual biological time t_B of the plant (equations 54 – 63). Due to the endeavour of the plant to compensate shortages in assimilates or in nitrogen, additional weighting factors $w_{C,k}$ and $w_{N,k}$ are introduced to consider regulation in the allocation pattern.

$$G_{W_k} = G_W \cdot \frac{f_k \cdot w_{C,k} w_{N,k}}{\sum_k f_k \cdot w_{C,k} w_{N,k}} \quad (51)$$

where

$$w_{C,k} = \begin{cases} \gamma_C^{1-\varphi_C} & \text{if } k = \text{L, S, B} \\ \gamma_C^{\varphi_C-1} & \text{if } k = \text{R, FR, GR} \\ 1 & \text{if } k = \text{F} \end{cases} \quad (52)$$

$$w_{N,k} = \begin{cases} \gamma_N^{1-\varphi_N} & \text{if } k = R, FR \\ \gamma_N^{\varphi_N-1} & \text{if } k = S, B, GR \\ 1 & \text{if } k = L, F \end{cases} \quad (53)$$

γ_C and γ_N are parameters which characterise the ability of the plant to regulate the allocation pattern. If no regulation is considered, these factors are set to 1.

Calculation of partitioning coefficients (herbs):

$$f_R = \begin{cases} \frac{f_{RL} \cdot f_{LS}}{f_{RL} \cdot f_{LS} + f_{LS+1}} & \text{if } D_1 \leq t_B < D_2 \\ \frac{\varrho_R \cdot (K_R - W_R)}{r_{max} \cdot W} & \text{if } D_2 \leq t_B < D_3 \\ \frac{\varrho_R \cdot (K_R - W_R) \cdot f_{AH}}{\varrho_F \cdot W_{V2}} & \text{if } D_3 \leq t_B < D_4 \\ 0 & \text{if } D_4 \leq t_B < D_5 \end{cases} \quad (54)$$

$$f_L = \begin{cases} \frac{f_{LS}}{f_{RL} \cdot f_{LS} + f_{LS+1}} & \text{if } D_1 \leq t_B < D_2 \\ \frac{\varrho_L \cdot (K_L - W_L)}{r_{max} \cdot W} & \text{if } D_2 \leq t_B < D_3 \\ \frac{\varrho_L \cdot (K_L - W_L) \cdot f_{AH}}{\varrho_F \cdot W_{V2}} & \text{if } D_3 \leq t_B < D_4 \\ 0 & \text{if } D_4 \leq t_B < D_5 \end{cases} \quad (55)$$

$$f_S = \begin{cases} \frac{1}{f_{RL} \cdot f_{LS} + f_{LS+1}} & \text{if } D_1 \leq t_B < D_2 \\ 1 - f_R - f_L & \text{if } D_2 \leq t_B < D_3 \\ \frac{r_{max} \cdot W \cdot f_{AH}}{\varrho_F \cdot W_{V2}} - f_R - f_L & \text{if } D_3 \leq t_B < D_4 \\ 0 & \text{if } D_4 \leq t_B < D_5 \end{cases} \quad (56)$$

$$f_F = \begin{cases} 0 & \text{if } D_1 \leq t_B < D_2 \\ 0 & \text{if } D_2 \leq t_B < D_3 \\ 1 - f_S - f_R - f_L & \text{if } D_3 \leq t_B < D_4 \\ 1 & \text{if } D_4 \leq t_B < D_5 \end{cases} \quad (57)$$

Calculation of partitioning coefficients (trees):

$$f_{FR} = \begin{cases} \frac{\varrho_{FR} \cdot (K_{FR} - W_{FR})}{r_{max} \cdot W} & \text{if } D_1 \leq t_B < D_6 \\ 0 & \text{else} \end{cases} \quad (58)$$

$$f_{GR} = f_{Wood} \cdot f_{ugwd} \quad (59)$$

$$f_S = f_{Wood} \cdot (1 - f_{ugwd}) \cdot (1 - f_{brf}) \quad (60)$$

$$f_B = f_{Wood} \cdot (1 - f_{ugwd}) \cdot f_{brf} \quad (61)$$

$$f_L = \begin{cases} \frac{\varrho_L \cdot (K_L - W_L)}{r_{max} \cdot W} & \text{if } D_1 \leq t_B < D_6 \\ 0 & \text{else} \end{cases} \quad (62)$$

$$f_F = \begin{cases} \frac{\varrho_F \cdot (K_F - W_F)}{r_{max} \cdot W} & \text{if } D_1 \leq t_B < D_6 \\ 0 & \text{else} \end{cases} \quad (63)$$

where

$$f_{Wood} = \begin{cases} 1 - f_{FR} - f_L - f_F & \text{if } D_1 \leq t_B < D_6 \\ 0 & \text{else} \end{cases} \quad (64)$$

f_{RL}	allometric root to leaf ratio [d ⁻¹]
f_{LS}	allometric leaf to stem ratio [d ⁻¹]
ϱ_R	root flush rate [kg(glucose) · kg ⁻¹ · d ⁻¹]
ϱ_{FR}	fine root flush rate [kg(glucose) · kg ⁻¹ · d ⁻¹]
ϱ_L	leaf flush rate [kg(glucose) · kg ⁻¹ · d ⁻¹]
ϱ_F	fruit flush rate [kg(glucose) · kg ⁻¹ · d ⁻¹]
K_R	growth capacity of roots [kg] (equation 75)
K_{FR}	growth capacity of fine roots [kg] (equation 75)
K_L	growth capacity of leaves [kg] (equation 72)
K_F	growth capacity of fruits [kg] (equation 76)
W	actual structural biomass of the plant [kg]
W_R	actual structural biomass of roots [kg]
W_{FR}	actual structural biomass of fine roots [kg]
W_L	actual structural biomass of leaves [kg]
W_F	actual structural biomass of fruits [kg]
r_{max}	maximal growth rate of the plant [kg(glucose) · kg ⁻¹ · d ⁻¹]

W_{V2} vegetative structural biomass at the end of stage 2 [kg]
 f_{AH} ($= D_4 - t_B$) factor relating to growth reduction in autumn [-]

The amount of nitrogen, which is potentially available for growth processes, N_{av} [kg], is the sum of potential nitrogen uptake from soil $N_{upt,pot}$ [kg] and potential nitrogen mobilisation from nitrogen reserve pool N_{mob} [kg]:

$$N_{av} = N_{upt,pot} + N_{mob} \quad (65)$$

where $N_{upt,pot}$ (equation 127) is calculated from actual root surface, soil nitrogen availability and soil moisture conditions. N_{mob} (equation 137) results from the difference between actual and minimal nitrogen concentration in plant organs. The demand for nitrogen, $N_{dem,grw}$ [kg], is derived from the amount of nitrogen required to realize potential plant organ growth (equation 123).

The total change of structural biomass W_k [kg] of organ k results from G_{W_k} and the actual loss rate of living biomass of the respective organ λ_k [d⁻¹]:

$$\Delta W_k = \frac{1}{\xi_{W_k}} \cdot G_{W_k} - \lambda_k(I) \cdot W_k \cdot \Delta t \quad (66)$$

where the ξ_{W_k} [kg(glucose)·kg⁻¹] are factors considering the conversion of glucose into structural biomass of organ k . λ_k is a function of actual stress intensity I [-] ($0 < I \leq 1$) and the effectivity of plant defence. The effectivity of plant defence is a function of the concentration s_k of defensive compounds in organ k (see section 3.7).

3.3.3 Defensive compounds

After fulfilling the demand for growth, the conversion of assimilates to defensive compounds can take place. We assume that the formation of defensive compounds, even if they contain no nitrogen (e.g. phenylpropanoids), depends on the plant internal nitrogen availability factor φ_N , due to the nitrogen requirements of precursory compounds and

enzymatic activity. The amount of assimilates converted to defensive compounds, G_S [kg(glucose)], is derived from

$$G_S = \begin{cases} D_S \cdot \varphi_N^\delta & \text{if } A_{av} \geq G_W + D_S \\ (A_{av} - G_W) \cdot \varphi_N^\delta & \text{if } A_{av} < G_W + D_S \end{cases} \quad (67)$$

where

$$G_W = \sum_k G_{W_k} \quad (68)$$

and δ [-] is a form parameter, which allows the consideration of non-linear relations between defensive compounds formation and plant internal nitrogen availability. The total change of the pool of defensive compound, S [kg], results from G_S , the turnover rate of defensive compounds τ_S [d⁻¹] and the actual loss of living biomass.

$$\Delta S = \frac{1}{\xi_S} \cdot G_S - \tau_S \cdot S \cdot \Delta t - \sum \lambda_k \cdot s_k \cdot W_k \cdot \Delta t \quad (69)$$

where ξ_S [g(glucose)·g] considers the conversion of glucose to the respective defensive compound.

3.3.4 Reserves pool

In a final procedure it is checked whether the reserves pool, R [kg((starch))], must be depleted to meet all demands, or if assimilates are still remaining and can be used to refill the reserves pool. We assume that all the assimilate surplus from the prior time step, as well as the actual gain resulting from photosynthesis will be first used. Mobilisation of reserves will then occur only if the actual demand exceeds these amounts:

$$\Delta R = \begin{cases} \frac{1}{\xi_R} \cdot (P_{act} \cdot \Delta t + A_{old} - D_M - G_W - G_S) \cdot r_R \cdot \Delta t & \text{if } \chi \leq 1 \\ P_{act} \cdot \Delta t + A_{old} - D_M - G_W - G_S & \text{if } \chi > 1 \end{cases}$$

with

$$\chi = \frac{D_M + G_W + G_S}{A_{old} + P_{act} \cdot \Delta t} \quad (70)$$

where ξ_R [$\text{kg}(\text{glucose}) \cdot \text{kg}(\text{starch})^{-1}$] is the conversion factor from glucose to starch and r_R [d^{-1}] is the relative reserves growth rate.

The new value of A_{old} [$\text{kg}(\text{glucose})$] follows from the difference between the actual input into the assimilates pool and the output for assimilate consuming processes (equation 71).

If $\chi > 1$, no assimilates will remain in the assimilates pool.

$$\Delta A_{old} = P_{act} \cdot \Delta t - D_M - G_W - G_S - \Delta R \quad (71)$$

3.3.5 Growth capacities

If simulation starts, maximal biomass of leaves, fine roots and, in case of trees, fruits are calculated. Maximal leaf weight, K_L [kg] is estimated from the maximal leaf area index of the plant, LAI_{max} [-], the maximal specific leaf weight, $\lambda_{L,max}$ [$\text{kg} \cdot \text{m}^{-2}$] and the potential area per single plant, $A_{Plant,max}$ [m^2]:

$$K_L = LAI_{max} \cdot \lambda_{Lw,max} \cdot A_{Plant,max} \quad (72)$$

with

$$A_{Plant,max} = \min \left\{ \frac{\pi}{\varrho_{plant}}, \left(\frac{H_{max}}{HD_{min}} \cdot r_{C/S} \right)^2 \cdot \frac{\pi}{4} \right\} \quad (73)$$

where ϱ_{plant} [$\text{plants} \cdot \text{m}^{-2}$] is the canopy density, H_{max} [m] the maximal height of the plant, HD_{min} [-] the minimal plant height to stem diameter ratio and $r_{C/S}$ [-] the crown diameter to stem diameter of the plant. In case of trees, $r_{C/S}$ is an input parameter; in case of herbs, $r_{C/S}$ is calculated from the coefficient f_{LS} [-], which gives the maximal leaf to stem weight ratio:

$$r_{C/S} = \sqrt{\frac{f_{LS} \cdot H_{max} \cdot \varrho_S}{LAI_{max} \cdot \lambda_{Lw,max}}} \quad (74)$$

where ϱ_S [$\text{kg} \cdot \text{m}^{-3}$] is the density of stem tissue (dry weight). LAI_{max} is an input parameter. Maximal weight of fine roots, K_R [kg] and K_{FR} [kg] respectively, and, in case of

trees, maximal weight of fruits are estimated from allometric coefficients f_{RL} [-] and f_{FL} [-]:

$$K_{(F)R} = K_L \cdot f_{RL} \quad (75)$$

$$K_F = K_L \cdot f_{FL} \quad (76)$$

In case of herbs, growth of compartment stem is also limited:

$$K_S = \min \left\{ \frac{\pi \cdot H_{max}^3 \cdot \rho_S}{4 \cdot HD_{min}^2}; \frac{K_L}{f_{LS}} \right\} \quad (77)$$

3.4 Photosynthesis

Three steps are performed to calculate gross photosynthesis rate of the plant:

1. simulation of light distribution in the canopy (section 3.4.1)
2. calculation of radiation absorption per leaf layer and calculation of CO₂ assimilation (section 3.4.2)
3. integration of CO₂ assimilation over plant height

Actual photosynthetic capacity per leaf layer in response to external environmental and plant internal factors is in the last section of this chapter (section 3.4.3).

3.4.1 Light distribution

The calculation of light distribution in a canopy takes place according to the method described by Kropff and Laar and Wang (1997). It is assumed that photosynthetic active radiation, ϕ_{PAR} [$\text{W}\cdot\text{m}^{-2}$], reaching the top of the canopy, accounts for 50% of global radiation, ϕ_g [$\text{W}\cdot\text{m}^{-2}$], at this site (input value).

$$\phi_{PAR} = 0.5 \cdot \phi_g \quad (78)$$

One part of the photosynthetic active radiation reaches the canopy as direct radiation, $\phi_{PAR,dir}$ [$\text{W}\cdot\text{m}^{-2}$], the other part reaches the canopy in the form of diffuse radiation, $\phi_{PAR,dif}$ [$\text{W}\cdot\text{m}^{-2}$].

$$\phi_{PAR,dir} = \phi_{PAR} \cdot (1 - f_{dif}) \quad (79)$$

$$\phi_{PAR,dif} = \phi_{PAR} \cdot f_{dif} \quad (80)$$

The fraction of diffuse radiation, f_{dif} [-] (equation 81), is estimated from the actual transmissivity of the atmosphere, τ_A [-] (equation 82)

$$f_{dif} = \begin{cases} 0.23 & \text{if } \tau_A < 0.75 \\ 1.33 - 1.46 \cdot \tau_A & \text{if } \tau_A \leq 0.75 \wedge \tau_A > 0.35 \\ 1.0 - 2.3 \cdot (\tau_A - 0.07)^2 & \text{if } \tau_A \leq 0.35 \wedge \tau_A > 0.07 \\ 1 & \text{if } \tau_A \leq 0.07 \end{cases} \quad (81)$$

where τ_A is derived from the ratio of global radiation ϕ_g at the top of the canopy and the actual value of extra-terrestrial radiation, ϕ_e [$\text{W}\cdot\text{m}^{-2}$].

$$\tau_A(t) = \frac{\int_{t-\frac{\Delta t}{2}}^{t+\frac{\Delta t}{2}} \phi_g(t') dt'}{\int_{t-\frac{\Delta t}{2}}^{t+\frac{\Delta t}{2}} \phi_e(t') dt'} \quad (82)$$

ϕ_e at solar time t [d] during a day d of the year, counted from January 1th, is derived from the solar constant, $\phi_s = 1370$ [$\text{W}\cdot\text{m}^{-2}$] (considering the eccentricity of the orbit of earth) and the actual height of the sun, β [degree]:

$$\phi_e(t) = 1370 \cdot \sin \beta \cdot \left[1 + 0.033 \cdot \cos \frac{2\pi \cdot (d + 10)}{365} \right] \quad (83)$$

where $\beta(t, d)$ depends on the latitude λ [degree] of the geographic location of the plant and the actual declination δ_s [degree] of the sun:

$$\sin \beta(t, d) = \sin \lambda \cdot \sin \delta_s(d) + \cos \lambda \cdot \cos \delta_s(d) \cdot \cos 2\pi (t - 0.5) \quad (84)$$

$$\delta_s(d) = -\arcsin \left[\sin \frac{2\pi \cdot 23.45}{360} \cos \frac{2\pi (d + 10)}{365} \right] \quad (85)$$

If daily input values of global radiation, ϕ_G [$\text{W}\cdot\text{m}^{-2}$] are used instead of actual values ϕ_g , the distribution of actual global radiation over the day is calculated from the course of solar height:

$$\phi_g(t) = \phi_G \cdot \frac{\sin \beta(t) \cdot (1 + \sin \beta(t))}{\int_0^1 \sin \beta(t) \cdot (1 + \sin \beta(t)) dt} \quad (86)$$

Within the canopy, radiation fluxes attenuate exponentially with the cumulative LAI_{cum} (equation 14), countered from the top of the plant downwards.

$$\phi_{PAR}(h) = (1 - \varrho) \cdot \phi_{PAR}(0) \cdot e^{-k \cdot \sum LAI_{cum}(h)} \quad (87)$$

where ϱ [-] is the reflexion coefficient of the canopy, k [-] the extinction coefficient of ϕ_{PAR} and $\sum LAI_{cum}(h)$ the total cumulative leaf area index over height h . In the model, three

components of radiation fluxes are distinguished: the diffuse flux ϕ_{dif} [$\text{W}\cdot\text{m}^{-2}$], the total direct flux $\phi_{dir,tot}$ [$\text{W}\cdot\text{m}^{-2}$] and the direct component of the direct flux (total direct flux minus scattered light) $\phi_{dir,dir}$ [$\text{W}\cdot\text{m}^{-2}$]. Each form of radiation flux has its own extinction coefficient (equations 91–92). The different light profiles are described in equations 88–90:

$$\phi_{dif}(h) = \phi_{PAR,dif} \cdot (1 - \varrho_{dif}) \cdot e^{-\left(k_{dif} \cdot LAI_{cum}(h) + \sum_{j=1}^4 C_{i,j} \cdot k_{dif,j} \cdot LAI_{cum,j}(h)\right)} \quad (88)$$

$$\phi_{dir,tot}(h) = \phi_{PAR,dir} \cdot (1 - \varrho_{dir}) \cdot e^{-\left(k_{dir,tot} \cdot LAI_{cum}(h) + \sum_{j=1}^4 C_{i,j} \cdot k_{dir,tot,j} \cdot LAI_{cum,j}(h)\right)} \quad (89)$$

$$\phi_{dir,dir}(h) = \phi_{PAR,dir} \cdot (1 - \sigma_s) \cdot e^{-\left(k_{dir,dir} \cdot LAI_{cum}(h) + \sum_{j=1}^4 C_{i,j} \cdot k_{dir,dir,j} \cdot LAI_{cum,j}(h)\right)} \quad (90)$$

where k_{dif} [-] is the extinction coefficient for diffuse radiation (input),

$$k_{dir,tot} = \frac{0.5 \cdot k_{dif}}{0.8 \cdot \sin \beta} \quad (91)$$

is the extinction coefficient for (total) direct radiation,

$$k_{dir,dir} = \frac{0.5 \cdot k_{dif}}{\sin \beta \cdot 0.8 \cdot \sqrt{1 - \sigma_s}} \quad (92)$$

is the extinction coefficient for direct component of direct radiation,

$$\varrho_{dif} = \frac{1 - \sqrt{1 - \sigma_s}}{1 + \sqrt{1 - \sigma_s}} \quad (93)$$

is the reflexion coefficient for diffuse radiation and

$$\varrho_{dir} = \frac{2 \cdot \varrho_{dif}}{1 + 2 \cdot \sin \beta} \quad (94)$$

is the reflexion coefficient for direct radiation. $\sigma_s = 0.2$ [-] is the scattering coefficient of leaves for visible radiation and $C_{i,j}$ are the competition coefficients between the regarded plant i and its neighbours j .

3.4.2 Radiation absorption and CO₂ assimilation

The amount of radiation captured by shaded leaves at height h [m] follows from the derivation of diffuse radiation flux and the scattered component of the direct radiation flux with respect to the cumulative leaf area index, LAI_{cum} [$\text{m}^2(\text{leaf}) \cdot \text{m}^{-2}(\text{soil})$]:

$$\phi_{a,sh}(h) = - \frac{d\phi_{dif}}{dLAI_{cum}} \Big|_h - \left(\frac{d\phi_{dir,tot}}{dLAI_{cum}} \Big|_h - \frac{d\phi_{dir,dir}}{dLAI_{cum}} \Big|_h \right) \quad (95)$$

Sunlit leaves absorb the flux that shaded leaves absorb as well as the direct component of the direct flux. The latter component differs for leaves with different orientation:

$$\phi_{a,su}(h, \beta') = \phi_{a,sh}(h) + (1 - \sigma) \frac{\phi_{PAR,dir}}{\sin \beta} \cdot \sin \beta' \quad (96)$$

where $\sin \beta'$ is the sine of incidence of the direct beam.

The dependency of CO₂ assimilation from light intensity is described by a negative exponential function, following Goudriaan and Laar (1994). This function is characterised by the initial slope (light use efficiency, ε [$\frac{\text{kg}(\text{CO}_2)}{\text{m}^2 \cdot \text{h}} / \frac{\text{J}}{\text{m}^2 \cdot \text{s}}$]) and the asymptote (gross assimilation rate at light saturation, p_{max} [$\text{kg}(\text{CO}_2) \cdot \text{m}^{-2} \cdot \text{h}^{-1}$], (equation 101)). The CO₂ assimilation rate per leaf area of shaded leaves at height h follows from equation 97. Assimilation rate of sunlit leaves is calculated by integration of the rate of radiation absorption over β' (equation 98).

$$p_{sh}(h) = p_{max} \cdot \left[1 - \exp \left(-\varepsilon \cdot \frac{\phi_{a,sh}(h)}{p_{max}} \right) \right] \quad (97)$$

$$p_{su}(h) = p_{max} \cdot \int_0^\pi \omega(\beta') \left(1 - \exp \left(-\varepsilon \cdot \frac{\phi_{a,su}(\beta')}{p_{max}} \right) \right) d\beta' \quad (98)$$

where $\omega(\beta')$ describes the leaf angle distribution (in case of a spherical leaf angle distribution $\omega(\beta') = 1/\pi$).

The fraction of sunlit leaf area at height h , $f_{su}(h)$ [-], is estimated from the extinction coefficient for the direct component of the direct beam, $k_{dir,dir}$ [-], and the cumulative leaf area index above h :

$$f_{su}(h) = e^{-\left(k_{dir,dir} \cdot LAI_{cum} + \sum_{j=1}^4 C_{i,j} \cdot k_{dir,dir,j} \cdot LAI_{cum,j} \right)} \quad (99)$$

The actual gross photosynthesis rate of the plant, $P_{act}(t)$ [kg(glucose) · d⁻¹] follows from integration of p_{sh} and p_{su} over plant height h :

$$P_{act}(t) = 24 \cdot \frac{30}{44} \cdot \int_0^H [f_{su}(h) \cdot p_{su}(h) + (1 - f_{su}(h)) \cdot p_{sh}(h)] \cdot a_L(h) dh \quad (100)$$

The factor 24 considers the conversion of h⁻¹ to d⁻¹, the factor 30/44 considers the conversion from CO₂ into glucose. If daily time steps are used, $P_{act}(t)$ is calculated by integration over one day using the Gaussian integration method (Kropff and Laar).

3.4.3 Photosynthetic capacity of leaves and responses to external and internal factors

In the model, the actual rate of photosynthesis at light saturation, p_{max} [kg(CO₂) · m⁻² · h⁻¹], can be affected by several factors: atmospheric CO₂-concentration, leaf nitrogen content, stomatal aperture, temperature, glucose level. Photosynthetic capacity of leaves can also be reduced in case of damages caused by ozone or leaf pathogens. The model considers these effects by help of response functions (equations 102–113).

$$p_{max} = p_{opt} \cdot \varphi_{CO_2} \cdot \min \{ \varphi_{\nu}, \varphi_{H_2O}, \varphi_T, \varphi_{CH_2O} \} \cdot \varphi_{O_3} \cdot \varphi_{Path} \quad (101)$$

where p_{opt} [kg(CO₂) · m⁻² · h⁻¹] is the photosynthetic capacity under light saturation, ambient CO₂ conditions and optimal physiological conditions.

In the following, the single response factors are explained.

CO₂ effect:

The response of photosynthetic capacity with respect to concentration of atmospheric CO₂ is estimated by equation 102:

$$\varphi_{CO_2} = \min \left(2.3, \frac{c_i - \Gamma_0}{c_{i,amb} - \Gamma_0} \right) \quad (102)$$

with

$$c_i = c_{CO_2} \cdot R_{c_i/c_a} \quad (103)$$

and

$$c_{i,amb} = c_{CO_2,amb} \cdot R_{c_i/c_a} \quad (104)$$

φ_{CO_2}	CO ₂ response factor [-]
c_i	CO ₂ concentration in stomatal cavity [ppm]
$c_{i,amb}$	CO ₂ concentration in stomatal cavity under ambient conditions [ppm]
c_{CO_2}	atmospheric CO ₂ concentration [ppm]
$c_{CO_2,amb}$	(=340) ambient atmospheric CO ₂ concentration [ppm]
Γ_0	CO ₂ compensation point [ppm]
R_{c_i/c_a}	internal/external CO ₂ ratio [-]

Nitrogen:

$$\varphi_\nu(h) = \begin{cases} 1 & : \nu_{act,L}(h) > \nu_{opt,L} \\ \frac{\psi_N(h)^{\gamma \cdot (k+1)}}{\psi_N(h)^{\gamma+k}} & : \nu_{min,L} \leq \nu_{act,L}(h) \leq \nu_{opt,L} \\ 0 & : \nu_{act,L}(h) < \nu_{min,L} \end{cases} \quad (105)$$

where

$$\psi_N(h) = \frac{\nu_{act,L}(h) - \nu_{min,L}}{\nu_{opt,L} - \nu_{min,L}} \quad (106)$$

$\varphi_\nu(h)$	leaf nitrogen response factor at height h [-]
$\nu_{act,L}(h)$	actual leaf nitrogen concentration $\frac{kg(N)}{kg}$
$\nu_{min,L}$	minimal leaf nitrogen concentration $\frac{kg(N)}{kg}$
$\nu_{opt,L}$	optimal leaf nitrogen concentration $\frac{kg(N)}{kg}$
γ	parameter [-]
k	parameter [-]

Temperature:

$$\varphi_T = \begin{cases} 0 & \text{if } T < T_{ps,min} \vee T > T_{ps,max} \\ \frac{2 \cdot (T_{ps,act} - T_{ps,min})^p \cdot (T_{ps,opt} - T_{ps,min})^p - (T - T_{ps,min})^{2p}}{(T_{ps,opt} - T_{ps,min})^{2p}} & \text{if } T_{ps,min} \leq T \leq T_{ps,max} \end{cases} \quad (107)$$

where

$$p = \frac{\ln 2}{\ln \left(\frac{T_{ps,max} - T_{ps,min}}{T_{ps,opt} - T_{ps,min}} \right)} \quad (108)$$

φ_T	temperature response factor [-]
T	actual atmospheric temperature [°C]
$T_{ps,min}$	temperature minimum for photosynthesis [°C]
$T_{ps,opt}$	temperature optimum for photosynthesis [°C]
$T_{ps,max}$	temperature maximum for photosynthesis [°C]

Water relation:

$$\varphi_{H_2O} = \frac{T_{act}}{T_{pot}} \quad (109)$$

φ_{H_2O}	stomatal aperture response factor [-]
T_{act}	actual transpiration rate [cm ³]
T_{pot}	potential transpiration rate [cm ³]

Accumulation of assimilates:

Photosynthesis can be limited if the concentration of soluble carbohydrates (equivalent to A_{av} in the model) exceeds a critical value l_C . This critical value depends on the nitrogen concentration in the leaves. It will be smaller if nitrogen is in shortage.

$$\varphi_{CH_2O} = \max \left\{ 0; 1 - \left(\frac{A_{av}/(W_L + W_S)}{l_c} \right)^\gamma \right\} \quad (110)$$

$$l_C = 0.2 + \alpha \cdot \varphi_\nu \quad (111)$$

φ_{CH_2O}	soluble carbohydrates response factor [-]
A_{av}	pool of available assimilates (soluble carbohydrates) [kg]
W_L	actual weight of leaves [kg]
W_S	actual weight of stem [kg]
l_C	critical value for soluble carbohydrates in leaves [-]
φ_N	nitrogen response factor [-]
γ	form parameter [-]
α	(= 0.1) parameter [-]

Ozone:

If leaf internal ozone concentration exceeds a critical value, photosynthesis rate is reduced.

$$\varphi_{O_3} = \max \{0; 1 - \beta_{O_3} \cdot I_{O_3}\} \quad (112)$$

φ_{O_3}	ozone response factor [-]
I_{O_3}	leaf internal ozone concentration [$\mu\text{g} \cdot \text{m}^{-3}$] (equation 153)
β_{O_3}	ozone sensitivity parameter [-]

Leaf pathogens:

If infestation of leaves by pathogens exceeds a critical value, photosynthesis rate will be reduced.

$$\varphi_{Path} = \begin{cases} 1 & \text{if } I_{P,L} \leq I_{P,L,crit} \\ \max \{0; 1 - \beta_{Path} \cdot (I_{P,L} - I_{P,L,crit})^{\alpha_{Path}}\} & \text{else} \end{cases} \quad (113)$$

φ_{Path}	response factor [-]
$I_{P,L}$	fraction of infested leaf area [$\text{m}^2(\text{infested leaf area}) \cdot \text{m}^2(\text{total leaf area})$]
$I_{P,L,crit}$	critical fraction of infested leaf area [$\text{m}^2(\text{infested leaf area}) \cdot \text{m}^2(\text{total leaf area})$]

β_{Path} parameter [-]

α_{Path} parameter [-]

3.5 Transpiration and water uptake

Transpiration of a single plant is treated in the model as the actual water uptake by its roots. It is either limited

- by root resistance
- by soil resistance for water transport
- or by climatic conditions.

3.5.1 Root resistance

Limitation by root resistance of water uptake from soil disc l under plant i results from the respective root surface a_R [m^2] of the plants that are present in this disc, and the maximal water uptake rate per root surface, ζ_W [$\text{cm}^3 \cdot \text{m}^{-2} \cdot \text{d}^{-1}$]. The fractions of root surface of the four next neighbours ($j = 1 \dots 4$), that meet disc l under plant i , are calculated using competition factors $C_{j,i}$ (see equation 2). Thus, the maximal water uptake from soil disc l under plant i , $q_{W,max}(l)$ [cm^3], is:

$$q_{W,max}(l) = \left(A_{root,i}(l) \cdot \zeta_{W,i} + \sum_{j=1}^4 A_{root,j}(l) \cdot \zeta_{W,j} \cdot C_{j,i} \right) \cdot \Delta t \quad (114)$$

3.5.2 Soil resistance

Limitation by soil resistance for water transport is introduced using the factor $f_\theta(l)$ [-] that considers the actual water content, $\theta_{act}(l)$ [$\text{cm}^3 \cdot \text{cm}^{-3}$], in soil layer l . If $\theta_{act}(l)$ is greater than permanent wilting point $\theta_{pwp}(l)$ [$\text{cm}^3 \cdot \text{cm}^{-3}$] and lower than field capacity $\theta_{fc}(l)$ [$\text{cm}^3 \cdot \text{cm}^{-3}$], a linear relationship between water uptake rate and actual water content is assumed. Water uptake is not limited, if actual water content is greater than field capacity and lower than water saturation $\theta_{sat}(l)$ [$\text{cm}^3 \cdot \text{cm}^{-3}$]. No water uptake is possible, if actual water content is lower than permanent wilting point. Furthermore, water uptake cannot exceed the amount of water, W_{av} [cm^3], which is actual available for

root water uptake in the soil disc in consideration. Thus, potential water uptake from soil disc l under plant i , $q_{W,pot}(l)$ [cm³], is:

$$q_{W,pot}(l) = \begin{cases} q_{W,max}(l) \cdot f_{\theta}(l) & \text{if } q_{W,max}(l) \cdot f_{\theta}(l) < W_{av}(l) \\ W_{av}(l) & \text{else} \end{cases} \quad (115)$$

where

$$f_{\theta}(l) = \begin{cases} 0 & \text{if } \theta_{act}(l) \leq \theta_{pwp}(l) \\ \frac{\theta_{act}(l) - \theta_{pwp}(l)}{\theta_{fc}(l) - \theta_{pwp}(l)} & \text{if } \theta_{pwp}(l) < \theta_{act}(l) < \theta_{fc}(l) \\ 1 & \text{if } \theta_{fc}(l) \leq \theta_{act}(l) \leq \theta_{sat}(l) \end{cases} \quad (116)$$

and

$$W_{av}(l) = (\theta_{act}(l) - \theta_{pwp}(l)) \cdot A_{plant,i} \cdot \Delta z(l) \cdot 10^6 \text{cm}^3 \cdot \text{m}^{-3} \quad (117)$$

$A_{plant,i}$ [m²] is the basal area of plant i and $\Delta z(l)$ [m] is the thickness of soil layer l .

If the hydraulic relation $\Psi(\theta)$ of the soil is known, the more realistic factor $f_{\Psi}(l)$ [-] can be used instead of $f_{\theta}(l)$:

$$f_{\Psi}(l) = \begin{cases} 0 & \text{if } \Psi_{act}(l) \geq \Psi_{pwp}(l) \\ \frac{\Psi_{act}(l) - \Psi_{pwp}(l)}{\Psi_{fc}(l) - \Psi_{pwp}(l)} & \text{if } \Psi_{fc}(l) < \Psi_{act}(l) < \Psi_{pwp}(l) \\ 1 & \text{if } \Psi_{sat}(l) \leq \Psi_{act}(l) \leq \Psi_{fc}(l) \end{cases} \quad (118)$$

where $\Psi_{act}(l)$ [mm] is the actual water potential in soil layer l and $\Psi_{pwp}(l)$, $\Psi_{fc}(l)$ and $\Psi_{sat}(l)$ [mm] are water potential in soil layer l at wilting point, at field capacity and at saturation respectively.

3.5.3 Influence of climatic conditions

Limitation by climatic conditions occurs, if potential water uptake from all soil discs under plant i is greater than potential transpiration, T_{pot} [cm³]. In this case, water uptake from each disc is reduced by the same factor.

$$q_{W,act}(l) = \begin{cases} q_{W,pot}(l) & \text{if } T_{pot} > \sum_l q_{W,pot}(l) \\ q_{W,pot}(l) \cdot \frac{T_{pot}}{\sum_l q_{W,pot}(l)} & \text{if } T_{pot} \leq \sum_l q_{W,pot}(l) \end{cases} \quad (119)$$

Potential transpiration results from the difference between potential evapotranspiration and actual evaporation. For calculation of both, potential evapotranspiration and actual evaporation, Expert-N provides several modules (e.g. Penman-Monteith equation), which can be linked to the PLATHO model. For calculating the fraction of actual transpiration, $T_{i,act}$ [cm³], which is caused by plant i , the actual water uptake from each soil disc is divided between plant i and the neighbours present in the soil disc according to the respective water uptake capacity:

$$T_{i,act} = \sum_{l=1}^L q_{W,act}(l) \cdot C_W(l) \quad (120)$$

where the root competition factor for water uptake in soil layer l is:

$$C_W(l) = \frac{A_{root,i}(l) \cdot \zeta_{W,i}}{A_{root,i}(l) \cdot \zeta_{W,i} + \sum_{j=1}^4 A_{root,j}(l) \cdot \zeta_{W,j} \cdot C_{j,i}} \quad (121)$$

3.6 Nitrogen uptake

- nitrogen demand of the plant
- nitrogen uptake capacity of roots
- nitrogen supply of the soil in root zone.

3.6.1 Nitrogen demand

The total nitrogen demand of a plant, N_{dem} [kg(N)], is divided into two parts: the first part, $N_{dem,grw}$ [kg(N)], is due to the nitrogen requirement for growth processes, the second part, $N_{dem,opt}$ [kg(N)], accounts for the effort of the plant to optimise the nitrogen equipment of their organs:

$$N_{dem} = N_{dem,grw} + N_{dem,opt} \quad (122)$$

where

$$N_{dem,grw} = \sum \frac{1}{\xi_{W_k}} \cdot G_{W_k} \cdot \nu_{opt,k} \quad (123)$$

and

$$N_{dem,opt} = \sum_k W_k \cdot (\nu_{k,opt} - \nu_{k,act}) \quad (124)$$

where the ξ_{W_k} [kg(glucose)·kg⁻¹] are factors considering the conversion of glucose into structural biomass of organ k , G_{W_k} [kg(glucose)] are the amount of assimilates allocated to organ k (equation 51), and W_k [kg] is the actual weight of organ k . $\nu_{act,k}$ and $\nu_{opt,k}$ [kg(N)·kg⁻¹] are the actual and optimal nitrogen concentration in organ k .

3.6.2 Potential nitrogen uptake

In order to fulfill these demands, the single soil layers ($l = 1 \dots L$) can be depleted according to the *nitrogen uptake capacity of roots* and the *nitrogen supply of the respective soil layers*. Potential maximal uptake from a soil disc l under plant i , $N_{upt,max}$ [kg(N)] depends on: i) root surfaces, $A_{root,i}$ [m²], of all plants present in this disc; ii) the maximal

nitrogen uptake rates per unit root surface, $\zeta_{N,i}$ [$\text{kg(N)} \cdot \text{m}^{-2} \cdot \text{d}^{-1}$] and iii) availability factors, $f_{N,i}(l)$ [-], that consider the reduction of $\zeta_{N,i}$ depending on potential soil nitrogen supply in layer l :

$$N_{upt,max}(l) = \left(A_{root,i}(l) \cdot \zeta_{N,i} \cdot f_{N,i} + \sum_{j=1}^4 A_{root,j}(l) \cdot C_{j,i} \cdot \zeta_{N,j} \cdot f_{N,j} \right) \cdot \Delta t \quad (125)$$

with

$$f_{N,i}(l) = 1 - e^{-\eta_i \cdot c_N(l)} \quad (126)$$

where η_i are factors dependent on the plant species and $c_N(l)$ is the concentration of mineral N [$\text{kg(N)} \cdot \text{kg(soil)}$] in soil disc l .

The potential nitrogen uptake, $N_{upt,pot}(l)$ [kg(N)], is calculated taking into account soil moisture conditions using a factor $f_\theta(l)$ [-], that decreases root function in dry soil or, due to anaerobiosis, if soil is too wet.

$$N_{upt,pot}(l) = \begin{cases} N_{upt,max}(l) \cdot f_\theta(l) & \text{if } N_{upt,max}(l) \cdot f_\theta(l) < N_{soil,av}(l) \\ N_{soil,av} & \text{else} \end{cases} \quad (127)$$

where

$$N_{soil,av}(l) = (c_N(l) - c_{N,min}) \cdot \rho_{soil}(l) \cdot A_{plant,i} \cdot \Delta z(l) \quad (128)$$

is the amount of available mineral nitrogen in soil disc l and

$$f_\theta(l) = \begin{cases} \frac{\theta_{act}(l) - \theta_{pwp}(l)}{\theta_{fc}(l) - \theta_{pwp}(l)} & \text{if } \theta_{min}(l) \leq \theta_{act}(l) \leq \theta_{fc}(l) \\ \frac{\theta_{sat}(l) - \theta_{act}(l)}{\theta_{sat}(l) - \theta_{fc}(l)} & \text{if } \theta_{sat}(l) \geq \theta_{act}(l) > \theta_{fc}(l) \end{cases} \quad (129)$$

3.6.3 Actual nitrogen uptake

If the total demand, N_{dem} , of plant i is greater than its total potential uptake, actual and potential nitrogen uptake from soil disc l are identical. If less nitrogen is demanded

by the plant than could be absorbed by its roots, potential uptake from soil disc l will be reduced in each layer by the same factor:

$$N_{upt}(l) = \begin{cases} N_{upt,pot}(l) \cdot C_N(l) & \text{if } N_{dem} \geq \sum_{l=1}^L N_{upt,pot}(l) \cdot C_N(l) \\ N_{upt,pot}(l) \cdot C_N(l) \cdot \frac{N_{dem}}{\sum_{l=1}^L N_{upt,pot}(l) \cdot C_N(l)} & \text{else} \end{cases} \quad (130)$$

where

$$C_N(l) = \frac{A_{root,i}(l) \cdot \zeta_{N,i}}{A_{root,i}(l) \cdot \zeta_{N,i} + \sum_{j=1}^4 A_{root,j}(l) \cdot \zeta_{N,j} \cdot C_{j,i}} \quad (131)$$

are nitrogen competition factors for each soil layer. The total nitrogen uptake of plant i is

$$N_{upt,i} = \sum_{l=1}^L N_{upt}(l) \quad (132)$$

3.6.4 Nitrogen distribution in the plant

The distribution of nitrogen between plant organs k is governed by the actual sink strength of the single organs. Changes in nitrogen content N_k [kg] of organ k result from the increment of new nitrogen, $N_{inc,k}$ [kg], the translocation of mobile nitrogen, $N_{mob,k}$ [kg], and nitrogen losses due to senescence:

$$\Delta N_k = N_{inc,k} - N_{trans,k} - \lambda_k \cdot W_k \cdot \nu_{min,k} \quad (133)$$

where W_k [kg] is actual structural biomass, λ_k [d⁻¹] is the actual death rate and $\nu_{min,k}$ [kg kg⁻¹] is the minimal nitrogen concentration of organ k .

$$N_{inc,k} = \begin{cases} \frac{N_{upt} + N_{mob} - N_{dem,grw}}{N_{dem,opt}} \cdot W_k \cdot (\nu_{opt,k} - \nu_{act,k}) + \Delta W_k \cdot \nu_{opt,k} & \text{if } N_{upt} + N_{mob} > N_{dem,grw} \\ \Delta W_k \cdot \nu_{opt,k} & \text{else} \end{cases} \quad (134)$$

$$N_{trans,k} = \begin{cases} N_{mob,k} & \text{if } N_{dem} \geq N_{mob} + N_{upt} \\ N_{mob,k} \cdot \frac{N_{dem} - N_{upt}}{N_{mob}} & \text{if } N_{upt} \leq N_{dem} < N_{mob} + N_{upt} \\ 0 & \text{if } N_{dem} < N_{upt} \end{cases} \quad (135)$$

N_{mob} [kg(N)] denotes the amount of mobile nitrogen, which can be translocated in other parts of the plant. $N_{mob,k}$ [kg(N)] is the part of mobile nitrogen, which is located in organ k .

$$N_{mob,k} = W_k \cdot (\nu_{act,k} - \nu_{min,k}) \cdot \tau_N \cdot \Delta t \quad (136)$$

and

$$N_{mob} = \sum_k N_{mob,k} \quad (137)$$

The actual nitrogen concentration in organ k , $\nu_{act,k}$ [kg(N) · kg⁻¹], is calculated in equation 138:

$$\nu_{act,k} = \frac{N_k}{W_k} \quad (138)$$

3.6.5 Nitrogen distribution in leaves

In the PLATHO model it is assumed, that leaf nitrogen, N_L [kg(N)], is not distributed homogeneously in the leaf compartment, but is distributed over plant height in a way that optimises light use rate by leaves. As maximal photosynthesis rate per unit leaf area is strongly related to leaf nitrogen content (see equation 101), nitrogen will accumulated in the upper leaf layers.

$$\nu_L(h) = \begin{cases} \nu_{L,min} & \text{if } \nu_{L,act} < \frac{\nu_{L,opt} + \nu_{L,min}}{2} \wedge w_L(h) \leq W_{\lambda 1} \\ \nu_{L,min} + \frac{\nu_{L,opt} - \nu_{L,min}}{W_L - W_{\lambda 1}} \cdot (w_L(h) - W_{\lambda 1}) & \text{if } \nu_{L,act} < \frac{\nu_{L,opt} + \nu_{L,min}}{2} \wedge w_L(h) > W_{\lambda 1} \\ \nu_{L,min} + \frac{\nu_{L,opt} - \nu_{L,min}}{W_{\lambda 2}} \cdot w_L(h) & \text{if } \nu_{L,act} \geq \frac{\nu_{L,opt} + \nu_{L,min}}{2} \wedge w_L(h) \leq W_{\lambda 2} \\ \nu_{L,opt} & \text{if } \nu_{L,act} \geq \frac{\nu_{L,opt} + \nu_{L,min}}{2} \wedge w_L(h) > W_{\lambda 2} \end{cases} \quad (139)$$

with

$$W_{\lambda 1} = W_L \cdot \left[1 - \frac{2 \cdot (\nu_{L,act} - \nu_{L,min})}{\nu_{L,opt} - \nu_{L,min}} \right] \quad (140)$$

and

$$W_{\lambda_2} = 2 \cdot W_L \cdot \frac{\nu_{L,opt} - \nu_{L,act}}{\nu_{L,opt} - \nu_{L,min}} \quad (141)$$

$w_L(h)$ [kg] is the cumulative leaf weight at height h . It is calculated from leaf area density, $a_L(h)$ [$\text{m}^2 \cdot \text{m}^{-1}$] (equation 15), and specific leaf weight, $\lambda_L(h)$ [$\text{kg} \cdot \text{m}^{-2}$] (equation 18):

$$w_L(h) = \int_0^h a_L(h') \cdot \lambda_L(h') dh' \quad (142)$$

3.7 Biomass loss and senescence

The actual loss rate, λ_k [d^{-1}], of organ k is the sum of loss rates due to senescence and damages caused by stress.

$$\lambda_k = \lambda_{k,snc} + \lambda_{k,I,pot} - \varepsilon_k(s_k) \quad (143)$$

where $\lambda_{k,snc}$ [d^{-1}] is the actual loss rate of organ k due to senescence, $\lambda_{k,I,pot}$ [d^{-1}] is the potential loss rate of organ k due to stress in case of no defence (equation 151) and $\varepsilon(s_k)$ [d^{-1}] describes the reduction of $\lambda_{k,I,pot}$ due to the defence effectivity (equation 152).

3.7.1 Relative death rate of leaves

Senescence of leaves occurs due to aging or if leaves shade each other. In the model, the relative death rate of leaf biomass, $\lambda_{L,snc}$ [d^{-1}], is set to be the larger one of both factors:

$$\lambda_{L,snc} = \max \{ \lambda_{age} + \lambda_{shade} \} \quad (144)$$

In the model senescence due to aging starts if biological time, t_B [-], reaches the critical value D_4 (see section 3.2). Death rate depends on air temperature (high temperatures accelerate senescence) and nitrogen concentration in leaves, $\nu_{L,act}$ [$\text{kg}(\text{N}) \cdot \text{kg}^{-1}$].

$$\lambda_{age} = \begin{cases} \lambda_{L,0} \cdot f_T \cdot \frac{\nu_{L,opt}}{\nu_{L,act}} & \text{if } t_B < D_4 \\ W_{L,3} \cdot \left(\frac{t_B}{D_5 - D_4} \right) \cdot f_T \cdot \frac{\nu_{L,opt}}{\nu_{L,act}} & \text{if } D_4 \leq t_B < D_5 \end{cases} \quad (145)$$

$\lambda_{L,0}$ [d^{-1}] is the leaf loss rate, $W_{L,3}$ [kg] the leaf dry weight at the end of stage 3, f_T a temperature response factor (input), $\nu_{L,opt}$ [$\text{kg}(\text{N}) \cdot \text{kg}^{-1}$] the optimal nitrogen concentration in leaves.

Senescence caused by shading occurs, if the leaf area index, LAI [$\text{m}^2(\text{leaf}) \cdot \text{m}^{-2}(\text{soil})$], reaches a critical value LAI_{crit} [$\text{m}^2(\text{leaf}) \cdot \text{m}^{-2}(\text{soil})$], which depends on actual nitrogen concentration in leaves. In case of high leaf nitrogen concentrations, leaves can survive under lower light conditions.

$$\lambda_{shade} = \begin{cases} \lambda_{L,0} \cdot \left(\frac{LAI}{LAI_{crit}} \right)^2 \cdot f_T & \text{if } LAI > LAI_{crit} \\ \lambda_{L,0} \cdot f_T & \text{else} \end{cases} \quad (146)$$

where

$$LAI_{crit} = LAI_{crit,0} \cdot \frac{\nu_{L,act}}{\nu_{L,opt}} \quad (147)$$

$LAI_{crit,0}$ [$\text{m}^2(\text{leaf}) \cdot \text{m}^{-2}(\text{soil})$] is the critical leaf area index in case of optimal leaf nitrogen concentration.

3.7.2 Relative death rate of fine roots

The death rate of root biomass is related to the relative turnover rate, $\lambda_{R,0}$ [d^{-1}] and on nitrogen concentration of roots, $\nu_{R,act}$ [$\text{kg} \cdot \text{kg}^{-1}$].

$$\lambda_{R,snc} = \lambda_{R,0} \cdot \frac{\nu_{R,opt}}{\nu_{R,act}} \quad (148)$$

3.7.3 Fruit fall

Fruit fall of trees occurs if biological time, t_B [-], reaches D_5 (see section 3.2). The loss rate, λ_F [d^{-1}], is assumed to be proportional to the actual development rate, r_{dev} [d^{-1}].

$$\lambda_{F,snc} = \begin{cases} 0 & \text{if } t_B < D_5 \\ \min \left\{ 1, \frac{W_{F,4} \cdot r_{dev}}{W_F} \right\} & \text{if } t_B \geq D_5 \end{cases} \quad (149)$$

where W_F [kg] is the actual fruit weight and $W_{F,4}$ [kg] is the fruit weight at the end of stage 4.

3.7.4 Biomass loss of woody plant organs

In case of trees, a permanent biomass loss rate of woody plant organs ($k = S, B, GR$) is assumed due to the die off of the bark.

$$\lambda_{k,snc} = \lambda_{k,0} \cdot f_T \quad (150)$$

3.7.5 Biomass loss caused by pathogens

The potential biomass loss rate of an organ k , $\lambda_{k,I,pot}$ [d^{-1}], caused by pathogen diseases is a function of stress intensity I [-] ($0 < I \leq 1$). In the PLATHO model, only stress induced biomass loss of leaves and fine roots are considered. In case of pathogen diseases, I [-] is a forcing function (input) that describes the fraction of leaves or fine roots that is infected with the pathogen ¹. The intensity and form of potential biomass loss rate $\lambda_{k,I,pot}$ [d^{-1}] on a pathogen disease is described by two input parameters n_I , and ν_I .

$$\lambda_{k,I,pot}(I) = n_I \cdot I^{\nu_I} \quad (151)$$

Due to the effectivity of defensive compounds in leaves or fine roots, the potential biomass loss rate is reduced. This stress reduction is a function of concentration of defensive compounds, s_k [$kg \cdot kg^{-1}$], in the infected plant organ k . This function is also described by help of two input parameters m_ε and μ_ε .

$$\varepsilon_k(s_k) = m_\varepsilon \cdot s_k^{\mu_\varepsilon} \quad (152)$$

3.7.6 Biomass loss caused by ozone

In case of ozone stress (only leaf damage is considered), intensity of stress, I [-], is calculated as a cumulative effect of leaf internal ozone $c_{O_3,L}$ [$\mu g \cdot kg^{-1}$] concentrations exceeding a critical value $c_{O_3,L,crit}$ [$\mu g \cdot kg^{-1}$]:

$$I_{O_3} = \frac{\int_0^t F(t') dt'}{\int_0^t c_{O_3,L}(t') dt'} \quad (153)$$

where

$$F(t') = \begin{cases} 0 & \text{if } c_{O_3,L}(t') \leq c_{O_3,L,crit} \\ c_{O_3,L}(t') - c_{O_3,L,crit} & \text{if } c_{O_3,L}(t') > c_{O_3,L,crit} \end{cases} \quad (154)$$

Leaf damage caused by ozone is also calculated by means of equation 151. A reduction of the damage is only considered in an indirect way, as leaf internal ozone is degraded by defensive compounds in leaves (see equation 155).

¹a dynamic model of intensity of pathogen diseases including a feedback mechanism of plant reaction to pathogens is not yet integrated in the PLATHO model

3.8 Ozone uptake

In order to take into account the relation between ozone exposition and plant reaction, a simple ozone uptake model is integrated in PLATHO. The calculation of leaf internal ozone concentration follows Trapp et al. (1994), who proposes a model for the uptake of xenobiotics into plants. The uptake rate is assumed to be proportional to leaf area, A_L [m^2], conductivity of leaves for ozone, g_{O_3} [m s^{-1}], and to the concentration gradient between atmosphere, c_{O_3} [$\mu\text{g m}^{-3}$], and leaf material, $c_{O_3,L}$ [$\mu\text{g kg}^{-1}$]. In PLATHO, a second order reaction kinetic is assumed for the degradation of leaf internal ozone by defensive compounds in leaves, s_L [$\text{kg}\cdot\text{kg}^{-1}$]. λ_{O_3} [$\text{d}^{-1}\cdot(\text{kg}\cdot\text{kg}^{-1})^{-1}$] considers that two molecules of ascorbate are required per molecule ozone (Van der Vliet et al. 1995).

$$\frac{dc_{O_3,L}}{dt} = \frac{A_L \cdot g_{O_3} \cdot \left(c_{O_3} - \frac{c_{O_3,L}}{K_{LA}}\right)}{W_L} - \lambda_{O_3} \cdot c_{O_3,L} \cdot s_L \quad (155)$$

K_{LA} [$(\mu\text{g}\cdot\text{kg}^{-1})/(\mu\text{g}\cdot\text{m}^{-3})$] is the equilibrium distribution coefficient between the gaseous phase and the cell wall. As ozone is taken up almost solely via stomata (Kerstiens and Lendzian 1989), conductivity for ozone can be estimated from conductivity for water vapour, g_{H_2O} [$\text{m}\cdot\text{d}^{-1}$]. g_{H_2O} depends on actual aperture of the stomata and is estimated from actual transpiration rate, q_w [$\text{kg}\cdot\text{d}^{-1}$] and the difference of water concentration in stomatal cavities and atmosphere.

$$g_{O_3} = g_{H_2O} \cdot \sqrt{\frac{18}{48}} \quad (156)$$

with

$$g_{H_2O} = \frac{q_w}{A_L \cdot (PA - h \cdot PA)} \quad (157)$$

and

$$PA = 611 \cdot \frac{10^{\frac{7.5 \cdot T}{T+237}}}{461 \cdot (T + 273)} \quad (158)$$

where PA [kg m^{-3}] is the saturation concentration of water vapour, h [%/100] the actual relative air humidity and T [$^{\circ}\text{C}$] the actual air temperature. The equilibrium distribution

coefficient between atmosphere and leaves, K_{LA} [$(\mu\text{g} \cdot \text{kg}^{-1}) \cdot (\mu\text{g} \cdot \text{m}^{-3})$], depends also from temperature:

$$K_{LA}(T) = K_{LA}(T = 20) \cdot e^{-\frac{\Delta H \cdot (T-20)}{R \cdot 293 \cdot (T+273)}} = 1.54 \cdot 10^4 \cdot e^{-6.7 \cdot \frac{T-20}{T+273}} \quad (159)$$

where T is actual air temperature [$^{\circ}\text{C}$] and $K_{LA}(T = 20) = 15.4$ (Plöchel et al. 2000). ΔH is the enthalpy of dissolution ($16319 \text{ J} \cdot \text{mol}^{-1}$) and R the universal gas constant ($8.314 \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$).

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A List of variables

Symbol	Meaning	Unit	Equation
A_{av}	pool of assimilates	kg(glucose)	37
A_L	total leaf area	m ²	11
$A_{L,cum}(h)$	cumulative leaf area over h	m ²	13
A_{Plant}	soil area covered by plant	m ²	1
A_{old}	assimilate surplus from prior time step	kg(glucose)	71
$a_L(h)$	leaf area density	m ² /m	15
$a_R(l)$	root surface in soil layer l	m ²	26
$C_{i,j}$	competition coefficient between individuals i and j	–	2
C_L	light competition factor	–	5
$C_N(l)$	nitrogen competition factor in soil layer l	–	131
$C_{RLD}(l)$	root length density stress factor in soil layer l	–	24
$C_W(l)$	water competition factor in soil layer l	–	121
c_{CO_2}	actual atmospheric CO ₂ concentration	ppm	input
c_i	leaf internal CO ₂ concentration	ppm	103
$c_{i,amb}$	leaf internal CO ₂ concentration at ambient CO ₂ conditions	ppm	104
$c_N(l)$	concentration of mineral nitrogen in soil layer l	kg(N) · kg ⁻¹	extern
$c_{N,min}$	minimal concentration of mineral nitrogen in soil layer l	kg(N) · kg ⁻¹	input
c_{O_3}	atmospheric O ₃ concentration	ppb	input
$c_{O_3,L}$	leaf internal O ₃ concentration	ppb	155
$c_{O_3,crit}$	critical leaf internal O ₃ concentration	ppb	input
D_i	phenological development days until stage i	–	input
D_4	phenological development days until stage 4	–	35
$D_{4,0}$	phenological development days until stage 4, without the effect of ozone	–	input

Symbol	Meaning	Unit	Equation
D_M	assimilates required for maintenance	–	41
D_S	demand for defensive compounds	kg (glucose)	45
D_W	demand for growth of structural biomass	kg (glucose)	44
d	day number	–	
d_{act}	actual day number	–	
d_S	stem diameter	m	10
f_{brf}	allometric branch fraction	–	input
f_{cbh}	fraction of carbohydrates in structural dry matter	$\frac{\text{kg (carbohydrates)}}{\text{kg (dry matter)}}$	input
f_{dif}	fraction of diffuse radiation at the top of the canopy k	–	81
f_{FL}	allometric fruit to leaves ratio (trees)	d^{-1}	input
f_k	partitioning coefficients to organ k	–	54 – 63
f_{lig}	fraction of lignins in structural dry matter	$\frac{\text{kg (lignins)}}{\text{kg (dry matter)}}$	input
f_{lip}	fraction of lipids in structural dry matter	$\frac{\text{kg (lipids)}}{\text{kg (dry matter)}}$	input
f_{LS}	allometric leaf to stem ratio	d^{-1}	input
f_{min}	fraction of minerals in structural dry matter	$\frac{\text{kg (minerals)}}{\text{kg (dry matter)}}$	input
f_{oac}	fraction of organic acids in structural dry matter	$\frac{\text{kg (organic acids)}}{\text{kg (dry matter)}}$	input
f_N	nitrogen response factor	–	29, 126
f_{O_3}	ozone response factor	–	36
f_{ph}	photoperiod response factor	–	34
f_{prt}	fraction of proteins in structural dry matter	$\frac{\text{kg (proteins)}}{\text{kg (dry matter)}}$	input
f_{RL}	allometric (fine) root to leaf ratio	d^{-1}	input
$f_{su}(h)$	fraction of sunlit leaves at height h	[–]	99
f_T	temperature response factor	–	27
$f_{T,dev}$	temperature response factor of phenological development	–	33

Symbol	Meaning	Unit	Equation
f_{ugwd}	allometric underground wood fraction	–	input
f_{θ}	soil moisture response factor	–	28, 129
f_{Ψ}	water potential response factor	–	118
G_{pot}	potential growth of total biomass	kg (glucose)	42,43
G_S	actual assimilate consumption for synthesis of defensive compounds	kg (glucose)	67
G_W	actual assimilate consumption for growth of structural biomass	kg (glucose)	48
G_{W_k}	actual assimilate consumption for structural growth of organ k	kg (glucose)	51
g_{O_3}	conductivity of leaves for ozone k	$m \cdot d^{-1}$	156
H	plant height	m	6–8
HD	height to diameter ratio	–	9
HD_{min}	minimal height to diameter ratio	–	input
HD_{max}	maximal height to diameter ratio	–	input
h	height	m	
I	intensity of plant stress	0–1	input
$I_{P,L}$	intensity of plant stress caused by leaf pathogens	0–1	input
$I_{P,L,crit}$	critical intensity of plant stress caused by leaf pathogens	0–1	input
$I_{P,R}$	intensity of plant stress caused by root pathogens	0–1	input
$I_{P,R,crit}$	critical intensity of plant stress caused by root pathogens	0–1	input
K_k	maximal weight of organ k	kg	72, 75, 76
k	index for plant organ. $k = R$ (roots), S (stem), L (leaves), F (fruits/tubers) in case of herbs, or $k = FR$ (fine roots), GR (gross roots), S (stem), B (branches), L (leaves), F (fruits) in case of trees	–	–

Symbol	Meaning	Unit	Equation
k_{dif}	light extinction coefficient for diffuse radiation	–	input
$k_{dir,dir}$	light extinction coefficient for direct component of direct radiation	–	92
$k_{dir,tot}$	light extinction coefficient for total direct radiation	–	91
k_{ion}	average ion leakage rate	d^{-1}	input
k_{lip}	turnover rate of lipids	d^{-1}	input
k_{prt}	turnover rate of proteins	d^{-1}	input
LAI	leaf area index	$\frac{m^2(\text{leaf})}{m^2(\text{soil})}$	12
$LAI_{cum}(h)$	cumulative leaf area index over h	$\frac{m^2(\text{leaf})}{m^2(\text{soil})}$	14
$LAI_{crit}(h)$	critical leaf area	$\frac{m^2(\text{leaf})}{m^2(\text{soil})}$	input
LAI_{max}	maximal leaf area index	$\frac{m^2(\text{leaf})}{m^2(\text{soil})}$	input
l_c	critical value of soluble carbohydrates in leaves with respect to photosynthesis	–	111
$l_R(l)$	root length density in soil layer l	m	21
$m_{tu,k}$	rate of assimilate consumption to resynthesise proteins and lipids in organ k	$kg(\text{glucose}) \cdot d^{-1}$	38
$m_{ion,k}$	rate of assimilate consumption to maintain ionic concentrations in organ k	$kg(\text{glucose}) \cdot d^{-1}$	39
m_{met}	rate of assimilate consumption due to metabolic activities	$kg(\text{glucose}) \cdot d^{-1}$	40
m_ε	parameter for efficiency of plant defense	–	input
N_{av}	available plant internal nitrogen	kg (N)	65
N_{dem}	total nitrogen demand of the plant	kg (N)	122
$N_{dem,grw}$	nitrogen demand for growth	kg (N)	123
$N_{dem,opt}$	difference between optimal and actual nitrogen level in the plant	kg (N)	123
N_k	nitrogen content in organ k	kg (N)	133
N_{mob}	potential plant internal nitrogen mobilisation	kg (N)	137
$N_{mob,k}$	potential nitrogen mobilisation in organ k	kg (N)	136
$N_{inc,k}$	increment of nitrogen content in organ k	kg (N)	134

Symbol	Meaning	Unit	Equation
$N_{soil,av}$	available mineral nitrogen in soil disc l	kg (N)	128
$N_{trans,k}$	translocation of mobile nitrogen of organ k	kg (N)	135
$N_{upt}(l)$	actual nitrogen uptake from soil	kg (N)	130
N_{upt}	actual nitrogen uptake	kg (N)	132
$N_{upt,max}$	maximal nitrogen uptake from soil	kg (N)	125
$N_{upt,pot}$	potential nitrogen uptake from soil	kg (N)	127
n	index for leaf layer	–	–
n_I	parameter for potential damage in case of stress	–	input
$ph(d)$	photoperiod of day d	m	extern
ph_{opt}	optimal photoperiod for development	h	input
p_L	relative maximum of leaf area density	(0-1)	input
p_R	relative maximum of root length density	(0-1)	input
P_{act}	actual gross assimilation rate	kg(CO ₂)·d ⁻¹	100
p_{max}	actual maximal assimilation rate	kg(CO ₂)·m ⁻² ·h ⁻¹	101
p_{opt}	maximal assimilation rate under optimal conditions	kg(CO ₂)·m ⁻² ·h ⁻¹	input
p_{sh}	assimilation rate of shaded leaves	kg(CO ₂)·m ⁻² ·h ⁻¹	97
p_{su}	assimilation rate of sunlit leaves	kg(CO ₂)·m ⁻² ·h ⁻¹	98
$q_{W,act}(l)$	actual water uptake rate from soil disc l	cm ³	119
$q_{W,max}(l)$	maximal water uptake rate from soil disc l	cm ³	114
$q_{W,pot}(l)$	potential water uptake rate from soil disc l	cm ³	115
R	pool of reserves	kg(starch)	70
R_{c_i/c_a}	leaf internal/external CO ₂ ratio	–	input
$r_{C/S}$	crown to stem diameter ratio	–	input, 74
r_{dev}	actual development rate	d ⁻¹	32
r_{max}	maximal plant growth rate	d ⁻¹	input

Symbol	Meaning	Unit	Equation
$r_{FR/L}$	potential fine root to leaf ratio	–	input
r_R	relative reserves growth rate	d^{-1}	input
r_{zR}	maximal root extension rate	$\frac{\text{m}}{\text{d}}$	input
S	pool of defensive compounds	kg	69
s_k	concentration of defensive compounds in organ k	$\text{kg}\cdot\text{kg}^{-1}$	
T	actual air Temperature	$^{\circ}\text{C}$	input
T_m	daily mean air temperature	$^{\circ}\text{C}$	input
T_{act}	actual transpiration	cm^3	120
T_{pot}	actual transpiration	cm^3	extern
$T_{dev,max}$	maximal temperature for phenological development	$^{\circ}\text{C}$	input
$T_{dev,min}$	minimal temperature for phenological development	$^{\circ}\text{C}$	input
$T_{dev,opt}$	optimal temperature for phenological development	$^{\circ}\text{C}$	input
$T_{ps,max}$	maximal temperature for photosynthesis	$^{\circ}\text{C}$	input
$T_{ps,min}$	minimal temperature for photosynthesis	$^{\circ}\text{C}$	input
$T_{ps,opt}$	optimal temperature for photosynthesis	$^{\circ}\text{C}$	input
$T_{rt,max}$	maximal temperature for root extension	$^{\circ}\text{C}$	input
$T_{rt,min}$	minimal temperature for root extension	$^{\circ}\text{C}$	input
$T_{rt,opt}$	optimal temperature for root extension	$^{\circ}\text{C}$	input
$T_{soil}(l)$	soil temperature in layer l	$^{\circ}\text{C}$	extern
t	time	days	
t_B	biological time	–	30
W	(= $\sum W_k$) total structural plant biomass	kg	–
$W_{av}(l)$	available water in soil disc l	cm^3	117
$W_{F,4}$	fruit biomass at the end of stage 4	kg	–
W_k	dry weight of organ k	kg	66

Symbol	Meaning	Unit	Equation
W_{seed}	seed weight in units of glucose	kg (glucose)	input
W_{V2}	vegetative structural biomass at the end of stage 2	kg	intern
$w_L(h)$	cumulative leaf weight under height h	kg	142
z	soil depth	m	intern
z_l	depth of soil layer l	m	input
z_R	rooting depth	m	20
$z_{R,max}$	maximal rooting depth	m	input
α_{O_3}	ozone sensitivity parameter of development	$\text{kg} \cdot \mu\text{g}^{-1} \cdot \text{d}^{-1}$	input
β_{O_3}	ozone sensitivity parameter of photosynthesis	$\text{kg} \cdot \mu\text{g}^{-1}$	input
β	solar height	degree	84
Γ_0	CO ₂ compensation point	ppm	input
γ_C	parameter for regulation of allocation in case of plant internal C shortage	–	input
γ_N	parameter for regulation of allocation in case of plant internal N shortage	–	input
$\delta_z(l)$	thickness of soil layer l	m	input
δ	parameter for defensive compounds formation	–	input
δ_s	declination of the sun	degree	85
ε	light use efficiency	$\frac{\text{kg}}{\text{m}^2 \cdot \text{h}} / \frac{\text{J}}{\text{m}^2 \cdot \text{s}}$	input
η	parameter considering the effect of soil nitrogen availability on nitrogen uptake rate per unit root surface	$\text{kg}^3 \text{kg}(\text{N})^{-1}$	input
ζ_N	maximal nitrogen uptake rate	$\frac{\text{kg}(\text{N})}{\text{m}^2 \cdot \text{d}}$	input
ζ_W	maximal water uptake rate	$\frac{\text{cm}^3}{\text{m}^2 \cdot \text{d}}$	input
$\theta_{act}(l)$	actual water content in layer l	$\frac{\text{cm}^3}{\text{cm}^3}$	extern
$\theta_{fc}(l)$	water content in layer l at field capacity	$\frac{\text{cm}^3}{\text{cm}^3}$	extern
$\theta_{pwp}(l)$	water content in layer at permanent wilting point l	$\frac{\text{cm}^3}{\text{cm}^3}$	extern

Symbol	Meaning	Unit	Equation
$\theta_{sat}(l)$	water content in layer l at water saturation	$\frac{\text{cm}^3}{\text{cm}^3}$	extern
λ	latitude of the location	degree	input
λ_{age}	loss rate of leaves due to aging	d^{-1}	145
λ_k	actual loss rate of organ k	d^{-1}	143
$\lambda_{k,snc}$	actual loss rate of organ k due to senescence	d^{-1}	144,148–150
$\lambda_{k,I,pot}$	potential loss rate of organ k due to stress	d^{-1}	151
$\lambda_{k,0}$	turnover rate of organ k	d^{-1}	input
λ_{lR}	specific root length	$\text{m}\cdot\text{kg}^{-1}$	input
$\lambda_{Lw}(h)$	specific leaf weight of leaves at height h	$\text{kg}\cdot\text{m}^{-2}$	18
$\lambda_{Lw,max}$	maximal specific leaf weight	$\text{kg}\cdot\text{m}^{-2}$	input
λ_{Lw}^*	mean specific leaf weight	$\text{kg}\cdot\text{m}^{-2}$	19
$\lambda_{Lw,min}^*$	minimal mean specific leaf weight	$\text{kg}\cdot\text{m}^{-2}$	17
$\lambda_{O_3}^*$	leaf internal ozone degradation rate	$\text{d}^{-1}\cdot(\text{kg}\cdot\text{kg}^{-1})^{-1}$	input
λ_{shade}	loss rate of leaves due to shading	d^{-1}	145
μ_ε	parameter for efficiency of plant defense	–	input
μ_{met}	fraction of gross photosynthesis used for metabolic processes	–	input
ν_I	parameter for potential damage in case of stress	–	input
$\nu_{act,k}$	actual nitrogen concentration in organ k	$\text{kg}(\text{N})\cdot\text{kg}^{-1}$	138
$\nu_{act,L}(h)$	actual nitrogen concentration in leaves at height h	$\text{kg}(\text{N})\cdot\text{kg}^{-1}$	138
$\nu_{min,k}$	minimal nitrogen concentration in organ k	$\text{kg}(\text{N})\cdot\text{kg}^{-1}$	input
$\nu_{opt,k}$	optimal nitrogen concentration in organ k	$\text{kg}(\text{N})\cdot\text{kg}^{-1}$	input
ξ_{W_k}	growth efficiency of organ k	$\frac{\text{kg}(\text{glucose})}{\text{kg}}$	input
ξ_S	efficiency of synthesis of defensive compounds	$\frac{\text{kg}(\text{glucose})}{\text{kg}}$	input
ξ_R	efficiency of conversion of glucose to starch	$\frac{\text{kg}(\text{glucose})}{\text{kg}(\text{starch})}$	input
ρ_{dif}	leaf reflexion coefficient for diffuse radiation	–	93

Symbol	Meaning	Unit	Equation
ϱ_{dir}	leaf reflexion coefficient for direct radiation	–	94
ϱ_F	fruit filling rate	d^{-1}	input
ϱ_L	leaf flush rate	d^{-1}	input
ϱ_{plant}	canopy density	$\frac{\text{plants}}{\text{m}^2}$	input
ϱ_R	root density	$\text{kg}\cdot\text{m}^{-3}$	input
$\varrho_{soil}(l)$	soil density in soil layer	$\text{kg}\cdot\text{m}^{-3}$	input
$\varrho_{(F)R}$	(fine) root flush rate	d^{-1}	input
ϱ_S	stem density	$\text{kg}\cdot\text{m}^{-3}$	input
σ	potential defence investment	–	46
σ_s	leaf scattering coefficient	–	input
σ_0	potential permanent defence investment	–	input
σ_I	potential induced defence investment	–	47
τ_A	atmospheric transmissivity	–	82
τ_N	nitrogen mobilisation rate	d^{-1}	input
τ_R	reserves mobilisation rate	d^{-1}	input
τ_S	turnover rate of defensive compounds	d^{-1}	input
ϕ_{PAR}	photosynthetic active radiation	$\text{W}\cdot\text{m}^{-2}$	78
$\phi_{PAR,dif}$	diffuse component of photosynthetic active radiation	$\text{W}\cdot\text{m}^{-2}$	80
$\phi_{PAR,dir}$	direct component of photosynthetic active radiation	$\text{W}\cdot\text{m}^{-2}$	79
ϕ_e	extraterrestrial radiation	$\text{W}\cdot\text{m}^{-2}$	83
$\phi_{a,sh}$	radiation absorption by shaded leaves	$\text{W}\cdot\text{m}^{-2}(\text{leaf})$	95
$\phi_{a,su}$	radiation absorption by sunlit leaves	$\text{W}\cdot\text{m}^{-2}(\text{leaf})$	96
$\phi_{dif}(h)$	flux of diffuse photosynthetic active radiation at height h	$\text{W}\cdot\text{m}^{-2}$	88
$\phi_{dir,tot}(h)$	flux of total direct photosynthetic active radiation at height h	$\text{W}\cdot\text{m}^{-2}$	89

Symbol	Meaning	Unit	Equation
$\phi_{dir,dir}(h)$	flux of direct component of direct photosynthetic active radiation at height h	$\text{W}\cdot\text{m}^{-2}$	90
ϕ_g	global radiation	$\text{W}\cdot\text{m}^{-2}$	input
φ_C	plant internal C availability	–	49
φ_N	plant internal N availability	–	50
φ_{CO_2}	atmospheric CO_2 response factor of photosynthetic capacity	–	102
φ_ν	leaf nitrogen response factor of photosynthetic capacity	–	105
φ_T	temperature response factor of photosynthetic capacity	–	107
φ_{H_2O}	stomatal aperture response factor of photosynthetic capacity	–	109
φ_{CH_2O}	soluble sugars response factor of photosynthetic capacity	–	110
φ_{O_3}	ozone response factor of photosynthetic capacity	–	112
φ_{Path}	leaf pathogens response factor of photosynthetic capacity	–	113
ω	photoperiodism sensitivity parameter	–	input