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

Sebastian Gayler & Eckart Priesack

December 1, 2005

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

For more information please contact:

Dr. Sebastian Gayler
Institute of Soil Ecology
GSF – National Research Center for Environment and Health
Ingolstädter Landstraße 1
D – 85758 Oberschleißheim
E-mail: gayler@gsf.de
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.
Contents

1 Model overview ..................................................... 5

2 Technical realization ............................................. 7

3 Process description ................................................ 8

3.1 Morphology and canopy structure ............................... 8

3.1.1 Plant area ...................................................... 9

3.1.2 Calculation of competition coefficients ...................... 9

3.1.3 Plant height growth .......................................... 10

3.1.4 Stem diameter ............................................... 11

3.1.5 Leaf area and leaf area distribution ......................... 12

3.1.6 Specific leaf weight ......................................... 13

3.1.7 Root system ............................................... 14

3.2 Phenological development ........................................ 17

3.2.1 Influence of air temperature ................................ 18

3.2.2 Influence of light ........................................ 18

3.2.3 Influence of atmospheric ozone concentration .......... 19

3.3 Growth and allocation to biochemical pools ................... 20

3.3.1 Maintenance .................................................. 20

3.3.2 Growth and allocation of assimilates to plant organs .... 22

3.3.3 Defensive compounds ....................................... 27

3.3.4 Reserves pool .............................................. 28

3.3.5 Growth capacities ........................................... 29

3.4 Photosynthesis .................................................... 31

3.4.1 Light distribution ........................................... 31

3.4.2 Radiation absorption and CO₂ assimilation ............. 34

3.4.3 Photosynthetic capacity of leaves and responses to external and internal factors ........................................... 35

3.5 Transpiration and water uptake ................................ 40

3.5.1 Root resistance .............................................. 40

3.5.2 Soil resistance ............................................. 40

3.5.3 Influence of climatic conditions ......................... 41
3.6 Nitrogen uptake ......................................................... 43
  3.6.1 Nitrogen demand .............................................. 43
  3.6.2 Potential nitrogen uptake .................................... 43
  3.6.3 Actual nitrogen uptake ....................................... 44
  3.6.4 Nitrogen distribution in the plant ......................... 45
  3.6.5 Nitrogen distribution in leaves ............................. 46
3.7 Biomass loss and senescence ...................................... 48
  3.7.1 Relative death rate of leaves ............................... 48
  3.7.2 Relative death rate of fine roots ......................... 49
  3.7.3 Fruit fall .................................................. 49
  3.7.4 Biomass loss of woody plant organs ....................... 49
  3.7.5 Biomass loss caused by pathogens ......................... 50
  3.7.6 Biomass loss caused by ozone ............................. 50
3.8 Ozone uptake ........................................................ 51

References ............................................................. 53

A List of variables .................................................... 55

List of Variables ...................................................... 55
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).

\[\begin{array}{cccccc}
\triangle & \triangle & \triangle & \triangle & \triangle
\\
\triangle & \triangle & \triangle & j = 1 & \triangle & \triangle
\\
\triangle & \triangle & j = 4 & \triangle & j = 2 & \triangle
\\
\triangle & \triangle & \triangle & j = 3 & \triangle & \triangle
\\
\triangle & \triangle & \triangle & \triangle & \triangle & \triangle
\end{array}\]

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.
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 $HD$ [\text{\textendash}] , where $HD$ depends on development stage and competitive situation of the plant (3.1.3). The base area of this cylinder, $A_{plant}$ [\text{m}^2] (3.1.1), defines the influence zone of the plant individual and is used to calculated 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.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure4}
\caption{Geometry and symbols used for calculating plant morphology. $H$ [\text{m}] is the actual height of the plant, $z_R$ [\text{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. $h$ [\text{m}] is the height over the ground and $z$ [\text{m}] the depth in the soil. The distance $x$ [\text{m}] from the center of the plant is used for the calculation of competition coefficients, $A_{plant}$ [\text{m}^2] is the basal area of the cylinder and describes the zone that is influenced by the plant individual.}
\end{figure}
An example for the competitive situation in a mixed canopy (two species with individuals differing in size) shows figure 5.

3.1.1 Plant area

The base area $A_{Plant}$ [m$^2$] 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.

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

where $\varrho_{Canopy}$ [plants \cdot 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 $\xi = \xi$ (see figure 6) is given by equation 4.

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

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

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

(3)

and

$$\xi = \frac{r_i^2 + d^2 - r_j^2}{2 \cdot d}$$

(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 $HD_{\text{max}} [-]$. If $HD_{\text{max}}$ has been reached, further growth will continue at $HD = HD_{\text{max}}$. If there is no competition for light ($C_L = 0$), plants are assumed to pursue diameter growth until their minimum height-to-diameter $HD_{\text{min}} [-]$ has been reached. A single plant without light competition grows at height-to-diameter ratio $HD = HD_{\text{min}}$. For annual plants, $HD_{\text{max}}$ depends on actual height of the plant. For trees, $HD_{\text{max}}$ 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 $H_j \text{[m]}$ of
3 PROCESS DESCRIPTION

the next neighbours:

\[ C_L = \frac{\sum_{j=1}^{4} C_{i,j} \cdot LAI_j \cdot \min \{1, H_i/H_j\}}{\sum_{j=1}^{4} LAI_j} \]  \hspace{1cm} (5)

Case 1 (only diameter growth):

\[ \frac{dH}{dt} = 0 \quad \text{if} \quad HD > HD_{max} \quad \text{or} \quad C_L = 0 \land HD > HD_{min} \]  \hspace{1cm} (6)

Case 2 (only height growth):

\[ \frac{dH}{dt} = \frac{4 \cdot \frac{dW_S}{dt}}{\pi \cdot \rho_S \cdot d_S^2} \quad \text{if} \quad HD < HD_{min} \quad \text{or} \quad C_L > 0 \land HD < HD_{max} \]  \hspace{1cm} (7)

Case 3 (height/diameter is constant):

\[ \frac{dH}{dt} = \frac{4 \cdot \frac{dW_S}{dt}}{3\pi \cdot \rho_S \cdot d_S^2} \quad \text{if} \quad C_L = 0 \land HD = HD_{min} \text{ or } C_L > 0 \land HD = HD_{max} \]  \hspace{1cm} (8)

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

\[ HD = \frac{H}{d_S} \]  \hspace{1cm} (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 \( \rho_S \) [kg \cdot m\(^{-3}\)]:

\[ d_S = \sqrt{\frac{4 \cdot W_S}{\pi \cdot H \cdot \rho_S}} \]  \hspace{1cm} (10)

where \( H \) [m] is the actual plant height.
3.1.5 Leaf area and leaf area distribution

Total (living) plant leaf area $A_L$ [m$^2$] is calculated from actual leaf weight $W_L$ [kg], assuming a mean specific leaf weight, $\lambda_{\text{Lw}}$ [kg · m$^{-2}$ (leaf)]:

$$A_L = W_L/\lambda_{\text{Lw}}$$  \hfill (11)

For calculating the leaf area index $LAI$ [m$^2$(leaf) · m$^{-2}$(soil)], total plant leaf area is divided by the area, which can be potentially covered by the plant:

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

where $A_{\text{Plant}}$ [m$^2$] is the base of the cylinder representing the shape of the plant and $\varrho_{\text{Canopy}}$ [m$^{-2}$] is the number of plant individuals per square meter.

The cumulative leaf area $A_{L,\text{cum}}$ [m$^2$] over height $h$ [m] is assumed to follow a species specific leaf area distribution function:

$$A_{L,\text{cum}}(h) = \alpha_L + \frac{\beta_L}{1 + e^{-4(h/H-p_L)}}$$  \hfill (13)

with

$$\beta_L = A_L \cdot \frac{(e^{-4(1-p_L)} + 1) \cdot (e^{4p_L} + 1)}{e^{-4(1-p_L)} - e^{4p_L}}$$

$$\alpha_L = \frac{-\beta_L}{e^{-4(1-p_L)} + 1}$$

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 $LAI_{\text{cum}}$ [m$^2$(leaf) · m$^{-2}$(soil)] above $h$ (equation 14) and leaf area density $a_L$ [m$^2$(leaf) · m$^{-1}$] at height $h$ (equation 15) are derived from $A_{L,\text{cum}}(h)$:

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

$$a_L(h) = \frac{d}{dh}A_{L,\text{cum}}(h)$$  \hfill (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, $\lambda_{Lw}^* [\text{kg} \cdot \text{m}^{-2} (\text{leaf})]$, is estimated from actual leaf area index $LAI$, [m$^2$(leaf) $\cdot$ m$^{-2}$(soil)] and the mean nitrogen concentration in leaves, $\nu_{L,act} [\text{kg(N)} \cdot \text{kg}]$.

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

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

(16)

where $\alpha_N$ 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 $LAI \geq LAI_{crit}$. $\lambda_{Lw}^*$ is used to calculated 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:

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

(17)

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

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

(18)

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

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

(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, $\theta_{act}$ [m$^3 \cdot$ m$^{-3}$], in the lowest rooted soil layer $l_{zR}$ (see figure 4):

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

where $r_{zR}$ [m $\cdot$ d$^{-1}$] is the maximal root extension rate and $f_T$ [-] and $f_\theta$ [-] 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 $\lambda_{lR}$ [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.

$$\frac{d l_R(l)}{dt} = l_{R}^+(l) - l_{R}^-(l)$$ (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 \neq l_{zR}} [w(l) \cdot \min\{f_\theta(l), f_N(l)\} \cdot C_{RLD}(l)\]}$$ (22)
\[ l_R(l) = \lambda_R \cdot W_R \cdot \lambda_{IR} \cdot \frac{l_R(l) \cdot \max \{1 - f_0(l), 1 - f_N(l)\}}{\sum_{l=1}^{L_R} [l_R(l) \cdot \max \{1 - f_0(l), 1 - f_N(l)\}]} \] (23)

\[ C_{RLD}(l) = \left( 1 - \frac{l_{R,l}(l) + \sum_{z=1}^{4} C_{z} \cdot I_{R,z}}{K_{IR} \cdot A_{plant} \cdot (z_l - z_{l-1})} \right) \] (24)

and

\[ w(l) = \frac{\alpha_R}{\beta_R} \cdot \int_{z_{l-1}}^{z_l} \left( \frac{z}{\beta_R} \right)^{\alpha_{R}-1} \cdot e^{-\left(\frac{z}{\beta_R}\right)^{\alpha_R}} \, dz \]

with

\[ \alpha_R = 1 + 2 \cdot p_R \]

\[ \beta_R = \begin{cases} \frac{z_R}{2} & \text{if } p_R = 0 \\ \frac{p_R \cdot z_R}{\beta^{(\alpha_{R}-1) \alpha_R}} & \text{else} \end{cases} \] (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 \( l \), \( a_R(l) \) [m\(^2\)], is calculated from root length in layer \( l \), \( l_R(l) \), root density, \( \rho_R \) [kg · m\(^{-3}\)], and specific root length, \( \lambda_R \) [kg · m\(^{-1}\)], \( l_R(l) \):

\[ a_R(l) = \sqrt{\frac{4\pi}{\rho_R \cdot \lambda_{IR} \cdot I_R(l)}} \] (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 \( T_{rt,max} \).

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

with

\[
\begin{align*}
T_{mm} & = T_{soil}(l_R) - T_{rt,min} \\
T_{om} & = T_{rt,opt} - T_{rt,min} \\
T_{xm} & = T_{rt,max} - T_{rt,min}
\end{align*}
\]

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, \( \theta_{act}(l) \) [m\(^3\)·m\(^{-3}\)], decreases below the quarter of the available field capacity:

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

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

\[
f_{N}(l) = \begin{cases} 0.01 & \text{if } c_N(l) < 1.11 \text{ mg·kg}^{-1} \\
1 - 1.17 \cdot e^{-0.15 \cdot c_N(l)} & \text{if } c_N(l) \geq 1.11 \text{ mg·kg}^{-1} \end{cases}
\] (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>
<thead>
<tr>
<th>Table 1: Definition of development stages for herbs and trees</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Herbs</strong></td>
</tr>
<tr>
<td>$0 \leq t_B &lt; D_1$</td>
</tr>
<tr>
<td>$D_1 \leq t_B &lt; D_2$</td>
</tr>
<tr>
<td>$D_2 \leq t_B &lt; D_3$</td>
</tr>
<tr>
<td>$D_3 \leq t_B &lt; D_4$</td>
</tr>
<tr>
<td>$D_4 \leq t_B &lt; D_5$</td>
</tr>
<tr>
<td>$D_5 \leq t_B &lt; D_6$</td>
</tr>
</tbody>
</table>

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

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

where

$$\Delta D = D_{i+1} - D_i, \quad i = 0, \ldots, 5$$  (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].

\[
 f_{T,dev} = \begin{cases} 
 0 & \text{if } T_m < T_{dev,min} \lor T_m > T_{dev,max} \\
 \frac{2\left(T_{mm} T_{om}\right)\alpha - T_{2om}}{T_{mm}} & \text{if } T_{dev,min} \leq T_m \leq T_{dev,max}
\end{cases}
\]  

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.

\[
 f_{ph} = \begin{cases} 
 1 & \text{for } \text{"day-neutral" plants} \\
 \frac{1 - e^{-\omega \left(p_h - p_{h,opt} + \frac{4}{3}\right)}}{1 - e^{-4}} & \text{for } \text{"long day" plants} \\
 \frac{1 - e^{-\omega \left(p_h - p_{h,opt} + \frac{4}{3}\right)}}{1 - e^{-4}} & \text{for } \text{"short day" plants}
\end{cases}
\]

where $\omega$ 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 $c_{O_3,\text{crit}}$ [ppb] contribute to the acceleration of senescence.

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

where

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

$D_{4,0}$ is the number of development days before leaf fall without the effect of ozone, $\alpha_{O_3}$ 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 \( \Delta t \) [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

\[
A_{av} = (P_{act} + R \cdot \tau_R) \cdot \Delta t - D_M + A_{old}
\]  

(37)

where \( D_M \) [kg(glucose)] is the amount of assimilates required for maintenance processes and \( \tau_R \) [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.
The amount of glucose $m_{tu,k}$ [kg (glucose) $\cdot$ 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]:

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

(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. $MW_p = 120$ [g $\cdot$ mol$^{-1}$] and $MW_l = 900$ [g $\cdot$ 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, $m_{ion}$ [kg (glucose) $\cdot$ d$^{-1}$], are estimated in a similar way:

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

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

Gross photosynthesis, $P_{act} \text{ [kg(CO}_2 \cdot \text{d}^{-1}]$, is assumed to be a measure for the estimation of the component of maintenance respiration, $m_{met} \text{ [kg(glucose) \cdot d}^{-1}]$, that is due to metabolic activity:

$$m_{met} = \mu_{met} \cdot P_{act}$$

(40)

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

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

(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, $\varphi_C$ (equation 49), and nitrogen, $\varphi_N$ (equation 50). The potential growth of total biomass, $G_{pot} \text{ [kg(glucose)]}$, is calculated by means of equations 42 and 43. The actual usage of assimilates for synthesizing structural biomass, $G_W \text{ [kg(glucose)]}$, is calculated by equation 48, the actual usage for the synthesis of defensive compounds, $G_S \text{ [kg(glucose)]}$ by means of equation 67). $G_{pot}$ depends on the actual biological time, $t_B$ (equation 30) of the plant:

**Herbs:**

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

(42)

**Trees:**

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

(43)
3 PROCESS DESCRIPTION

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

\(G_{pot}\) is divided into demand for growth of structural biomass \(D_W\) [kg(glucose)] and demand for defence \(D_S\) [kg(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

\[ \sigma = \sigma_0 + \sigma_I \quad (46) \]

\(\sigma\) [-] is the potential defence investment, which consists of a permanent part \(\sigma_0\) and an induced part \(\sigma_I\). \(\sigma_I\) 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. \(\sigma_I\) 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, \( \varphi_C \) [-], and nitrogen, \( \varphi_N \) [-]:

\[
G_W = D_W \cdot \varphi_C \cdot \varphi_N
\]

(48)

where

\[
\varphi_C = \min \left\{ 1, \frac{A_{av}}{D_W} \right\}
\]

(49)

and

\[
\varphi_N = \min \left\{ 1, \frac{N_{av}}{N_{dem,grw}} \right\}
\]

(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.

\[
G_{W_k} = G_W \cdot \frac{f_k \cdot w_{C,k} w_{N,k}}{\sum_k f_k \cdot w_{C,k} w_{N,k}}
\]

(51)

where

\[
w_{C,k} = \begin{cases} 
\gamma_C^{1-\varphi_C} & \text{if } k = L, S, B \\
\gamma_C^{\varphi_C-1} & \text{if } k = R, FR, GR \\
1 & \text{if } k = F
\end{cases}
\]

(52)
\[ w_{N,k} = \begin{cases} \gamma_N^{1-\varphi_N} & \text{if } k = \text{R, FR} \\ \gamma_N^{\varphi_N-1} & \text{if } k = \text{S, B, GR} \\ 1 & \text{if } k = \text{L, F} \end{cases} \] \quad (53)

\( \gamma_C \) and \( \gamma_N \) 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):

\[ f_R = \begin{cases} \frac{f_{RL} f_{LS}}{f_{RL} f_{LS} + f_{LS} + 1} & \text{if } D_1 \leq t_B < D_2 \\ \frac{g_{FR}(K_{FR}-W_{FR})}{r_{max} W_{FR}} & \text{if } D_2 \leq t_B < D_3 \\ \frac{g_{FR}(K_{FR}-W_{FR}) f_{AH}}{g_{FR} W_{FR}^2} & \text{if } D_3 \leq t_B < D_4 \\ 0 & \text{if } D_4 \leq t_B < D_5 \end{cases} \] \quad (54)

\[ f_L = \begin{cases} \frac{f_{LS}}{f_{RL} f_{LS} + f_{LS} + 1} & \text{if } D_1 \leq t_B < D_2 \\ \frac{g_{FL}(K_{FL}-W_{FL})}{r_{max} W_{FL}} & \text{if } D_2 \leq t_B < D_3 \\ \frac{g_{FL}(K_{FL}-W_{FL}) f_{AH}}{g_{FL} W_{FL}^2} & \text{if } D_3 \leq t_B < D_4 \\ 0 & \text{if } D_4 \leq t_B < D_5 \end{cases} \] \quad (55)

\[ f_S = \begin{cases} \frac{1}{f_{RL} f_{LS} + f_{LS} + 1} & \text{if } D_1 \leq t_B < D_2 \\ 1 - f_R - f_L & \text{if } D_2 \leq t_B < D_3 \\ \frac{r_{max} W f_{AH}}{g_{FR} W_{FR}^2} - f_R - f_L & \text{if } D_3 \leq t_B < D_4 \\ 0 & \text{if } D_4 \leq t_B < D_5 \end{cases} \] \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):

\[ f_{FR} = \begin{cases} \frac{g_{FR}(K_{FR}-W_{FR})}{r_{max} W_{FR}} & \text{if } D_1 \leq t_B < D_6 \\ 0 & \text{else} \end{cases} \] \quad (58)
\[ f_{GR} = f_{Wood} \cdot f_{ugwd} \] (59)

\[ f_S = f_{Wood} \cdot (1 - f_{ugwd}) \cdot (1 - f_{frf}) \] (60)

\[ f_B = f_{Wood} \cdot (1 - f_{ugwd}) \cdot f_{frf} \] (61)

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

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

where

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

- \( f_{RL} \) allometric root to leaf ratio \([d^{-1}]\)
- \( f_{LS} \) allometric leaf to stem ratio \([d^{-1}]\)
- \( q_R \) root flush rate \([\text{kg(glucose)} \cdot \text{kg}^{-1} \cdot \text{d}^{-1}]\)
- \( q_{FR} \) fine root flush rate \([\text{kg(glucose)} \cdot \text{kg}^{-1} \cdot \text{d}^{-1}]\)
- \( q_L \) leaf flush rate \([\text{kg(glucose)} \cdot \text{kg}^{-1} \cdot \text{d}^{-1}]\)
- \( q_F \) fruit flush rate \([\text{kg(glucose)} \cdot \text{kg}^{-1} \cdot \text{d}^{-1}]\)
- \( K_R \) growth capacity of roots \([\text{kg}]\) (equation 75)
- \( K_{FR} \) growth capacity of fine roots \([\text{kg}]\) (equation 75)
- \( K_L \) growth capacity of leaves \([\text{kg}]\) (equation 72)
- \( K_F \) growth capacity of fruits \([\text{kg}]\) (equation 76)
- \( W \) actual structural biomass of the plant \([\text{kg}]\)
- \( W_R \) actual structural biomass of roots \([\text{kg}]\)
- \( W_{FR} \) actual structural biomass of fine roots \([\text{kg}]\)
- \( W_L \) actual structural biomass of leaves \([\text{kg}]\)
- \( W_F \) actual structural biomass of fruits \([\text{kg}]\)
- \( r_{max} \) maximal growth rate of the plant \([\text{kg(glucose)} \cdot \text{kg}^{-1} \cdot \text{d}^{-1}]\)
3 PROCESS DESCRIPTION

$W_{V2}$ 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]:

$$N_{av} = N_{upt, pot} + N_{mob}$$

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 $\lambda_k$ [d$^{-1}$]:

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

where the $\xi_{W_k}$ [kg(glucose)-kg$^{-1}$] are factors considering the conversion of glucose into structural biomass of organ $k$. $\lambda_k$ is a function of actual stress intensity $I$ [-] (0 < $I$ ≤ 1) and the effectiveness of plant defence. The effectiveness 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 $\varphi_N$, 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

\[
G_S = \begin{cases} 
  D_S \cdot \varphi_N & \text{if } A_{av} \geq G_W + D_S \\
  (A_{av} - G_W) \cdot \varphi_N & \text{if } A_{av} < G_W + D_S
\end{cases}
\]  

(67)

where \( G_W = \sum_k G_{W_k} \)  

(68)

and \( \delta \) [-] 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 \( \tau_S \) [d\(^{-1}\)] and the actual loss of living biomass.

\[
\Delta S = \frac{1}{\xi_S} \cdot G_S - \tau_S \cdot S \cdot \Delta t - \sum \lambda_k \cdot s_k \cdot W_k \cdot \Delta t
\]  

(69)

where \( \xi_S \) [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:

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

(70)

with

\[
\chi = \frac{D_M + G_W + G_S}{A_{old} + P_{act} \cdot \Delta t}
\]
where $\xi_R$ [kg(glucose)-kg(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 $A_{old}$ [kg(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.

$$\Delta A_{old} = P_{act} \cdot \Delta t - D_M - G_W - G_S - \Delta R$$  \hspace{1cm} (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, $\lambda_{L,max}$ [kg·m$^{-2}$] and the potential area per single plant, $A_{Plant,max}$ [m$^2$]:

$$K_L = LAI_{max} \cdot \lambda_{Lw,max} \cdot A_{Plant,max}$$  \hspace{1cm} (72)

with

$$A_{Plant,max} = \min \left\{ \frac{\pi}{\theta_{plant}}, \left( \frac{H_{max}}{HD_{min}} \cdot r_{C/S} \right)^2 \cdot \frac{\pi}{4} \right\}$$  \hspace{1cm} (73)

where $\theta_{plant}$ [plants·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:

$$r_{C/S} = \sqrt{\frac{f_{LS} \cdot H_{max} \cdot q_S}{LAI_{max} \cdot \lambda_{Lw,max}}}$$  \hspace{1cm} (74)

where $q_S$ [kg·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:

$$K_S = \min \left\{ \frac{\pi \cdot H_{max}^3 \cdot q_S}{4 \cdot \text{HD}_{min}^2} ; \frac{K_L}{f_{LS}} \right\} \quad (77)$$
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 CO\textsubscript{2} assimilation (section 3.4.2)
3. integration of CO\textsubscript{2} 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, $\phi_{PAR}$ [W·m\textsuperscript{-2}], reaching the top of the canopy, accounts for 50\% of global radiation, $\phi_{g}$ [W·m\textsuperscript{-2}], at this site (input value).

$$\phi_{PAR} = 0.5 \cdot \phi_{g}$$  \hspace{1cm} (78)

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

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

$$\phi_{PAR,\text{dif}} = \phi_{PAR} \cdot f_{\text{dif}}$$ \hspace{1cm} (80)

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

$$f_{\text{dif}} = \begin{cases} 
0.23 & \text{if } \tau_A < 0.75 \\
1.33 - 1.46 \cdot \tau_A & \text{if } \tau_A \leq 0.75 \land \tau_A > 0.35 \\
1.0 - 2.3(\tau_A - 0.07)^2 & \text{if } \tau_A \leq 0.35 \land \tau_A > 0.07 \\
1 & \text{if } \tau_A \leq 0.07
\end{cases}$$ \hspace{1cm} (81)
where \( \tau_A \) is derived from the ratio of global radiation \( \phi_g \) at the top of the canopy and the actual value of extra-terrestrial radiation, \( \phi_e \) [W·m\(^{-2}\)].

\[
\tau_A(t) = \frac{\int_{t-	au}^{t+\Delta t} \phi_g(t')dt'}{\int_{t-	au}^{t+\Delta t} \phi_e(t')dt'}
\]

(82)

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

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

(83)

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

\[
\sin \beta(t, d) = \sin \lambda \cdot \sin \delta_s(d) + \cos \lambda \cdot \cos \delta_s(d) \cdot \cos 2\pi (t - 0.5)
\]

(84)

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

(85)

If daily input values of global radiation, \( \phi_G \) [W·m\(^{-2}\)] are used instead of actual values \( \phi_g \), the distribution of actual global radiation over the day is calculated from the course of solar height:

\[
\phi_g(t) = \phi_G \cdot \frac{\sin \beta(t) \cdot (1 + \sin \beta(t))}{\int_0^{\beta(t)} \sin \beta(t) \cdot (1 + \sin \beta(t)) dt}
\]

(86)

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

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

(87)

where \( \varrho \) [-] is the reflexion coefficient of the canopy, \( k \) [-] the extinction coefficient of \( \phi_{PAR} \) 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 $\phi_{\text{dif}}$ [W·m$^{-2}$], the total direct flux $\phi_{\text{dir, tot}}$ [W·m$^{-2}$] and the direct component of the direct flux (total direct flux minus scattered light) $\phi_{\text{dir, dir}}$ [W·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:

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

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

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

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

$$
k_{\text{dir, tot}} = \frac{0.5 \cdot k_{\text{dif}}}{0.8 \cdot \sin \beta} \tag{91}
$$

is the extinction coefficient for (total) direct radiation,

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

is the extinction coefficient for direct component of direct radiation,

$$
\varrho_{\text{dif}} = \frac{1 - \sqrt{1 - \sigma_s}}{1 + \sqrt{1 - \sigma_s}} \tag{93}
$$

is the reflexion coefficient for diffuse radiation and

$$
\varrho_{\text{dir}} = \frac{2 \cdot \varrho_{\text{dif}}}{1 + 2 \cdot \sin \beta} \tag{94}
$$

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 CO$_2$ 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, $LAI_{cum}$ $[m^2(leaf) \cdot m^{-2}(soil)]$:

$$\phi_{a,sh}(h) = -\frac{d\phi_{dif}}{dLAI_{cum}} \bigg|_h - \left( \frac{d\phi_{dir,tot}}{dLAI_{cum}} \bigg|_h - \frac{d\phi_{dir,dir}}{dLAI_{cum}} \bigg|_h \right)$$  \hspace{1cm} (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:

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

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

The dependency of CO$_2$ 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, $\varepsilon$ [$\frac{kg(CO_2)}{m^2\cdot h}$ / $\frac{1}{m^2\cdot s}$]) and the asymptote (gross assimilation rate at light saturation, $p_{max}$ [$kg(CO_2)\cdot m^{-2}\cdot h^{-1}$], (equation 101)). The CO$_2$ 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 $\beta'$ (equation 98).

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

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

$$f_{su}(h) = e^{-\left(k_{dir,dir} \cdot LAI_{cum} + \sum_{j=1}^{4} C_{i,j} \cdot k_{dir,dir,j} \cdot LAI_{cum,j} \right)}$$  \hspace{1cm} (99)
The actual gross photosynthesis rate of the plant, $P_{act}(t) \text{[kg(glucose)\cdot d}^{-1}]$ follows from integration of $p_{sh}$ and $p_{su}$ over plant height $h$:

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

(100)

The factor 24 considers the conversion of $h^{-1}$ to $d^{-1}$, the factor $30/44$ considers the conversion from CO$_2$ 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, $p_{max} \text{[kg(CO$_2$)\cdot m}^{-2}\cdot h^{-1}]$, can be affected by several factors: atmospheric CO$_2$-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).

$$p_{max} = p_{opt} \cdot \varphi_{CO_2} \cdot \min \{\varphi_v, \varphi_{H_2O}, \varphi_T, \varphi_{CH_2O}\} \cdot \varphi_{O_3} \cdot \varphi_{Path}$$

(101)

where $p_{opt} \text{[kg(CO$_2$)\cdot m}^{-2}\cdot h^{-1}]$ is the photosynthetic capacity under light saturation, ambient CO$_2$ conditions and optimal physiological conditions.

In the following, the single response factors are explained.

**CO$_2$ effect:**

The response of photosynthetic capacity with respect to concentration of atmospheric CO$_2$ is estimated by equation 102:

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

(102)

with

$$c_i = c_{CO_2} \cdot R_{c_i/c_a}$$

(103)

and

$$c_{i,amb} = c_{CO_2,amb} \cdot R_{c_i/c_a}$$

(104)
\( \varphi_{CO_2} \) 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]

\( \Gamma_0 \) CO\(_2\) compensation point [ppm]

\( R_{ci/ca} \) internal/external CO\(_2\) ratio [-]

\textbf{Nitrogen:}

\[
\varphi_N(h) = \begin{cases} 
  1 & : \nu_{act,L}(h) > \nu_{opt,L} \\
  \frac{\psi_N(h)^{(k+1)}}{\psi_N(h)^{1+k}} & : \nu_{min,L} \leq \nu_{act,L}(h) \leq \nu_{opt,L} \\
  0 & : \nu_{act,L}(h) < \nu_{min,L}
\end{cases}
\]

where

\[
\psi_N(h) = \frac{\nu_{act,L}(h) - \nu_{min,L}}{\nu_{opt,L} - \nu_{min,L}}
\]

\( \varphi_N(h) \) 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 \( \frac{kg(N)}{kg} \)

\( \gamma \) parameter [-]

\( k \) parameter [-]

\textbf{Temperature:}

\[
\varphi_T = \begin{cases} 
  0 & \text{if } T < T_{ps,min} \lor T > T_{ps,max} \\
  \frac{2(T_{ps,act}-T_{ps,min})^p(T_{ps,act}-T_{ps,min})^p-(T-T_{ps,min})^{2p}}{(T_{ps,act}-T_{ps,min})^{2p}} & \text{if } T_{ps,min} \leq T \leq T_{ps,max}
\end{cases}
\]

\( \varphi_T \) temperature response function
where

\[ p = \frac{\ln 2}{\ln \left( \frac{T_{ps,\text{max}} - T_{ps,\text{min}}}{T_{ps,\text{opt}} - T_{ps,\text{min}}} \right)} \]  \hspace{1cm} (108)

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

**Water relation:**

\[ \varphi_{H_2O} = \frac{T_{act}}{T_{pot}} \]  \hspace{1cm} (109)

\[ \varphi_{H_2O} \quad \text{stomatal aperture response factor [-]} \]
\[ T_{act} \quad \text{actual transpiration rate [cm}^3\text{]} \]
\[ T_{pot} \quad \text{potential transpiration rate [cm}^3\text{]} \]

**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.

\[ \varphi_{CH_2O} = \max \left\{ 0 ; 1 - \left( \frac{A_{av}}{(W_L + W_S) \gamma} \right) \right\} \]  \hspace{1cm} (110)

\[ l_C = 0.2 + \alpha \cdot \varphi_{\nu} \]  \hspace{1cm} (111)
3 PROCESS DESCRIPTION

\( \varphi_{CH_2O} \) 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 [-]

\( \varphi_{N} \) nitrogen response factor [-]

\( \gamma \) form parameter [-]

\( \alpha \) (= 0.1) parameter [-]

Ozone:

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

\[
\varphi_{O_3} = \max \left\{ 0 ; 1 - \beta_{O_3} \cdot I_{O_3} \right\}
\]

\( \varphi_{O_3} \) ozone response factor [-]

\( I_{O_3} \) leaf internal ozone concentration [\( \mu g \cdot m^{-3} \)] (equation 153)

\( \beta_{O_3} \) ozone sensitivity parameter [-]

Leaf pathogens:

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

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

\( \varphi_{Path} \) response factor [-]

\( I_{P,L} \) fraction of infested leaf area [m\(^2\)(infested leaf area) \cdot m\(^2\)(total leaf area)]

\( I_{P,L,\text{crit}} \) critical fraction of infested leaf area [m\(^2\)(infested leaf area) \cdot m\(^2\)(total leaf area)]
\beta_{Path} \quad \text{parameter [-]}
\alpha_{Path} \quad \text{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

Legitimation 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, \( \zeta_W \) [cm\(^3\) \cdot m\(^{-2}\) \cdot d\(^{-1}\)]. The fractions of root surface of the four next neighbours \((j = 1 \ldots 4)\), 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 \( i \), \( q_{W,\text{max}}(l) \) [cm\(^3\)], is:

\[
q_{W,\text{max}}(l) = \left( A_{\text{root},i}(l) \cdot \zeta_W \cdot C_{j,i} \right) \cdot \Delta t
\]

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, \( \theta_{\text{act}}(l) \) [cm\(^3\) \cdot cm\(^{-3}\)], in soil layer \( l \). If \( \theta_{\text{act}}(l) \) is greater than permanent wilting point \( \theta_{\text{pwp}}(l) \) [cm\(^3\) \cdot cm\(^{-3}\)] and lower than field capacity \( \theta_{\text{fc}}(l) \) [cm\(^3\) \cdot 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 \( \theta_{\text{sat}}(l) \) [cm\(^3\) \cdot 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, \( W_{\text{av}} \) [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 \( i \), \( q_{W,pot}(l) \) [cm\(^3\)], is:

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

where

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

and

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

\( A_{plant,i} \) [m\(^2\)] 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 \( f_\theta(l) \):

\[
f_\Psi(l) = \begin{cases} 
0 & \text{if } \Psi_{act}(l) \geq \Psi_{pwp}(l) \\
\frac{\Psi_{act}(l) - \Psi_{pwp}(l)}{\Psi_{fc}(l) - \Psi_{pwp}(l)} & \text{if } \Psi_{fc}(l) < \Psi_{act}(l) < \Psi_{pwp}(l) \\
1 & \text{if } \Psi_{sat}(l) \leq \Psi_{act}(l) \leq \Psi_{fc}(l)
\end{cases} 
\]  
(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, \( T_{pot} \) [cm\(^3\)]. In this case, water uptake from
each disc is reduced by the same factor.

\[
q_{W,act}(l) = \begin{cases} 
q_{W,pot}(l) & \text{if } T_{pot} > \sum_l q_{W,pot}(l) \\
q_{W,pot}(l) \cdot \frac{T_{pot}}{\sum_l q_{W,pot}(l)} & \text{if } T_{pot} \leq \sum_l q_{W,pot}(l)
\end{cases} 
\]  
(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, $T_{i, act}$ [cm$^3$], 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:

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

(120)

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

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

(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:

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

where

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

and

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

where the $\xi_k W_k$ [kg(glucose)-kg$^{-1}$] are factors considering the conversion of glucose into structural biomass of organ $k$, $G_W$ [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 ($l = 1 \ldots L$) 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, $A_{root,i}$ [m$^2$], of all plants present in this disc; ii) the maximal
nitrogen uptake rates per unit root surface, \(\zeta_{N,i} \text{ [kg(N) m}^{-2} \text{ d}^{-1}]\) and iii) availability factors, \(f_{N,i}(l) \text{ [-]}\), that consider the reduction of \(\zeta_{N,i}\) depending on potential soil nitrogen supply in layer \(l\):

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

(125)

with

\[
f_{N,i}(l) = 1 - e^{-\eta_i c_{N}(l)}
\]

(126)

where \(\eta_i\) are factors dependent on the plant species and \(c_{N}(l)\) is the concentration of mineral N [kg(N) · kg(soil)] in soil disc \(l\).

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

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

(127)

where

\[
N_{\text{soil, av}}(l) = (c_{N}(l) - c_{N, min}) \cdot \theta_{\text{soil}}(l) \cdot A_{\text{plant},i} \cdot \Delta z(l)
\]

(128)

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

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

(129)

### 3.6.3 Actual nitrogen uptake

If the total demand, \(N_{\text{dem}}\) 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:

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

where

\[
C_N(l) = \frac{A_{\text{root},i}(l) \cdot \zeta_{N,i}}{A_{\text{root},i}(l) \cdot \zeta_{N,i} + \sum_{j=1}^{4} A_{\text{root},j}(l) \cdot \zeta_{N,j} \cdot C_{j,i}}
\]

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

\[
N_{\text{upt},i} = \sum_{l=1}^{L} N_{\text{upt}}(l)
\]

### 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, \( N_{\text{inc,k}} \) [kg], the translocation of mobile nitrogen, \( N_{\text{mob,k}} \) [kg], and nitrogen losses due to senescence:

\[
\Delta N_k = N_{\text{inc,k}} - N_{\text{trans,k}} - \lambda_k \cdot W_k \cdot \nu_{\text{min},k}
\]

where \( W_k \) [kg] is actual structural biomass, \( \lambda_k \) [d\(^{-1}\)] is the actual death rate and \( \nu_{\text{min},k} \) [kg kg\(^{-1}\)] is the minimal nitrogen concentration of organ \( k \).

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

\[
N_{\text{trans,k}} = \begin{cases} 
N_{\text{mob,k}} & \text{if } N_{\text{dem}} \geq N_{\text{mob}} + N_{\text{upt}} \\
N_{\text{mob,k}} \cdot \frac{N_{\text{dem}} - N_{\text{upt}}}{N_{\text{mob}}} & \text{if } N_{\text{upt}} \leq N_{\text{dem}} < N_{\text{mob}} + N_{\text{upt}} \\
0 & \text{if } N_{\text{dem}} < N_{\text{upt}}
\end{cases}
\]
$N_{\text{mob}}$ [kg(N)] denotes the amount of mobile nitrogen, which can be translocated in other parts of the plant. $N_{\text{mob},k}$ [kg(N)] is the part of mobile nitrogen, which is located in organ $k$.

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

(136)

and

$$N_{\text{mob}} = \sum_k N_{\text{mob},k}$$

(137)

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

$$\nu_{\text{act},k} = \frac{N_k}{W_k}$$

(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.

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

(139)

with

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

(140)
and

\[
W_{x_2} = 2 \cdot W_L \cdot \frac{\nu_{L,\text{opt}} - \nu_{L,\text{act}}}{\nu_{L,\text{opt}} - \nu_{L,\text{min}}}
\]  

(141)

\(w_L(h) \text{ [kg]}\) 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):

\[
w_L(h) = \int_0^h a_L(h') \cdot \lambda_L(h') \, dh'
\]  

(142)
3.7 Biomass loss and senescence

The actual loss rate, $\lambda_k$ [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 effectiveness (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, $\nu_{L, act}$ [kg(N) · kg$^{-1}$].

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

$\lambda_{L,0}$ [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), $\nu_{L, opt}$ [kg(N) · kg$^{-1}$] the optimal nitrogen concentration in leaves.

Senescence caused by shading occurs, if the leaf area index, $LAI$ [m$^2$(leaf) · m$^{-2}$(soil)], reaches a critical value $LAI_{crit}$ [m$^2$(leaf) · m$^{-2}$(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

\[ LAI_{crit} = LAI_{crit,0} \cdot \frac{\nu_{L,act}}{\nu_{L,opt}} \]  

(147)

\( LAI_{crit,0} \) [m\(^2\) (leaf) \cdot m\(^{-2}\) (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, \( \nu_{R,act} \) [kg \cdot kg\(^{-1}\)].

\[ \lambda_{R,snc} = \lambda_{R,0} \cdot \frac{\nu_{R,opt}}{\nu_{R,act}} \]  

(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, \( \lambda_F \) [d\(^{-1}\)], is assumed to be proportional to the actual development rate, \( r_{dev} \) [d\(^{-1}\)].

\[ \lambda_{F,snc} = \begin{cases} 0 & \text{if } t_B < D_5 \\ \min \{1, \frac{W_{F,4} \cdot r_{dev}}{W_F} \} & \text{if } t_B \geq D_5 \end{cases} \]  

(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.

\[ \lambda_{k,snc} = \lambda_{k,0} \cdot f_T \]  

(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 $\nu_I$.

$$\lambda_{k,I,pot}(I) = n_I \cdot I^{\nu_I}$$ (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 · kg$^{-1}$], in the infected plant organ $k$. This function is also described by help of two input parameters $m_z$ and $\mu_z$.

$$\varepsilon_k(s_k) = m_z \cdot s_k^{\mu_z}$$ (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 $c_{O_3,L}$ [μg · kg$^{-1}$] concentrations exceeding a critical value $c_{O_3,L,crit}$ [μg · kg$^{-1}$]:

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

where

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

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

---

$^1$a 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, $c_{O_3}$ [$\mu$g m$^{-3}$], and leaf material, $c_{O_3,L}$ [$\mu$g kg$^{-1}$]. In PLATHO, a second order reaction kinetic is assumed for the degradation of leaf internal ozone by defensive compounds in leaves, $s_L$ [kg kg$^{-1}$]. $\lambda_{O_3}$ [d$^{-1}$(kg·kg$^{-1}$)$^{-1}$] considers that two molecules of ascorbate are required per molecule ozone (Van der Vliet et al. 1995).

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

$K_{LA} [(\mu$g·kg$^{-1})/(\mu$g·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, $g_{H_2O}$ [m·d$^{-1}$]. $g_{H_2O}$ depends on actual aperture of the stomata and is estimated from actual transpiration rate, $q_w$ [kg·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

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

and

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

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

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

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

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


Kropff MJ, Laar HHv, eds. () Modelling Crop-Weed Interactions. CAB International, Wallingford, UK


Ritchie JT, Godwin DC, Otter-Nacke S (1987) CERES-WHEAT. A simulation model of wheat growth and development. Texas A&M University Press, College Station, TX


# List of variables

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Meaning</th>
<th>Unit</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_{av}$</td>
<td>pool of assimilates</td>
<td>kg(glucose)</td>
<td>37</td>
</tr>
<tr>
<td>$A_L$</td>
<td>total leaf area</td>
<td>m$^2$</td>
<td>11</td>
</tr>
<tr>
<td>$A_{L,cum}(h)$</td>
<td>cumulative leaf area over $h$</td>
<td>m$^2$</td>
<td>13</td>
</tr>
<tr>
<td>$A_{Plant}$</td>
<td>soil area covered by plant</td>
<td>m$^2$</td>
<td>1</td>
</tr>
<tr>
<td>$A_{old}$</td>
<td>assimilate surplus from prior time step</td>
<td>kg(glucose)</td>
<td>71</td>
</tr>
<tr>
<td>$a_L(h)$</td>
<td>leaf area density</td>
<td>m$^2$/m</td>
<td>15</td>
</tr>
<tr>
<td>$a_R(l)$</td>
<td>root surface in soil layer $l$</td>
<td>m$^2$</td>
<td>26</td>
</tr>
<tr>
<td>$C_{i,j}$</td>
<td>competition coefficient between individuals $i$</td>
<td>–</td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>and $j$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$C_L$</td>
<td>light competition factor</td>
<td>–</td>
<td>5</td>
</tr>
<tr>
<td>$C_{N(l)}$</td>
<td>nitrogen competition factor in soil layer $l$</td>
<td>–</td>
<td>131</td>
</tr>
<tr>
<td>$C_{RLD}(l)$</td>
<td>root length density stress factor in soil layer</td>
<td>–</td>
<td>24</td>
</tr>
<tr>
<td></td>
<td>$l$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$C_W(l)$</td>
<td>water competition factor in soil layer $l$</td>
<td>–</td>
<td>121</td>
</tr>
<tr>
<td>$c_{CO_2}$</td>
<td>actual atmospheric CO$_2$ concentration</td>
<td>ppm</td>
<td>input</td>
</tr>
<tr>
<td>$c_i$</td>
<td>leaf internal CO$_2$ concentration</td>
<td>ppm</td>
<td>103</td>
</tr>
<tr>
<td>$c_{i,amb}$</td>
<td>leaf internal CO$_2$ concentration at ambient</td>
<td>ppm</td>
<td>104</td>
</tr>
<tr>
<td></td>
<td>CO$_2$ conditions</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$c_{N(l)}$</td>
<td>concentration of mineral nitrogen in soil layer</td>
<td>kg(N) · kg$^{-1}$</td>
<td>extern</td>
</tr>
<tr>
<td></td>
<td>$l$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$c_{N,min}$</td>
<td>minimal concentration of mineral nitrogen in</td>
<td>kg(N) · kg$^{-1}$</td>
<td>input</td>
</tr>
<tr>
<td></td>
<td>soil layer $l$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$c_{O_3}$</td>
<td>atmospheric O$_3$ concentration</td>
<td>ppb</td>
<td>input</td>
</tr>
<tr>
<td>$c_{O_3,L}$</td>
<td>leaf internal O$_3$ concentration</td>
<td>ppb</td>
<td>155</td>
</tr>
<tr>
<td>$c_{O_3, crit}$</td>
<td>critical leaf internal O$_3$ concentration</td>
<td>ppb</td>
<td>input</td>
</tr>
<tr>
<td>$D_i$</td>
<td>phenological development days until stage $i$</td>
<td>–</td>
<td>input</td>
</tr>
<tr>
<td>$D_4$</td>
<td>phenological development days until stage 4</td>
<td>–</td>
<td>35</td>
</tr>
<tr>
<td>$D_{4,0}$</td>
<td>phenological development days until stage 4,</td>
<td>–</td>
<td>input</td>
</tr>
<tr>
<td></td>
<td>without the effect of ozone</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Symbol</td>
<td>Meaning</td>
<td>Unit</td>
<td>Equation</td>
</tr>
<tr>
<td>--------</td>
<td>---------</td>
<td>------</td>
<td>----------</td>
</tr>
<tr>
<td>$D_M$</td>
<td>assimilates required for maintenance</td>
<td>–</td>
<td>41</td>
</tr>
<tr>
<td>$D_S$</td>
<td>demand for defensive compounds</td>
<td>kg (glucose)</td>
<td>45</td>
</tr>
<tr>
<td>$D_W$</td>
<td>demand for growth of structural biomass</td>
<td>kg (glucose)</td>
<td>44</td>
</tr>
<tr>
<td>$d$</td>
<td>day number</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>$d_{act}$</td>
<td>actual day number</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>$d_S$</td>
<td>stem diameter</td>
<td>m</td>
<td>10</td>
</tr>
<tr>
<td>$f_{brf}$</td>
<td>allometric branch fraction</td>
<td>–</td>
<td>input</td>
</tr>
<tr>
<td>$f_{cbh}$</td>
<td>fraction of carbohydrates in structural dry matter</td>
<td>kg (carbohydrates) kg (dry matter)</td>
<td>input</td>
</tr>
<tr>
<td>$f_{dif}$</td>
<td>fraction of diffuse radiation at the top of the canopy</td>
<td>–</td>
<td>81</td>
</tr>
<tr>
<td>$f_{FL}$</td>
<td>allometric fruit to leaves ratio (trees)</td>
<td>d$^{-1}$</td>
<td>input</td>
</tr>
<tr>
<td>$f_k$</td>
<td>partitioning coefficients to organ $k$</td>
<td>–</td>
<td>54 – 63</td>
</tr>
<tr>
<td>$f_{lig}$</td>
<td>fraction of lignins in structural dry matter</td>
<td>kg (lignins) kg (dry matter)</td>
<td>input</td>
</tr>
<tr>
<td>$f_{lip}$</td>
<td>fraction of lipids in structural dry matter</td>
<td>kg (lipids) kg (dry matter)</td>
<td>input</td>
</tr>
<tr>
<td>$f_{LS}$</td>
<td>allometric leaf to stem ratio</td>
<td>–</td>
<td>input</td>
</tr>
<tr>
<td>$f_{min}$</td>
<td>fraction of minerals in structural dry matter</td>
<td>kg (minerals) kg (dry matter)</td>
<td>input</td>
</tr>
<tr>
<td>$f_{oac}$</td>
<td>fraction of organic acids in structural dry matter</td>
<td>kg (organic acids) kg (dry matter)</td>
<td>input</td>
</tr>
<tr>
<td>$f_N$</td>
<td>nitrogen response factor</td>
<td>–</td>
<td>29, 126</td>
</tr>
<tr>
<td>$f_{O_3}$</td>
<td>ozone response factor</td>
<td>–</td>
<td>36</td>
</tr>
<tr>
<td>$f_{ph}$</td>
<td>photoperiod response factor</td>
<td>–</td>
<td>34</td>
</tr>
<tr>
<td>$f_{prt}$</td>
<td>fraction of proteins in structural dry matter</td>
<td>kg (proteins) kg (dry matter)</td>
<td>input</td>
</tr>
<tr>
<td>$f_{RL}$</td>
<td>allometric (fine) root to leaf ratio</td>
<td>kg (dry matter) d$^{-1}$</td>
<td>input</td>
</tr>
<tr>
<td>$f_{su}(h)$</td>
<td>fraction of sunlit leaves at height $h$</td>
<td>[–]</td>
<td>99</td>
</tr>
<tr>
<td>$f_T$</td>
<td>temperature response factor</td>
<td>–</td>
<td>27</td>
</tr>
<tr>
<td>$f_{T,dev}$</td>
<td>temperature response factor of phenological development</td>
<td>–</td>
<td>33</td>
</tr>
<tr>
<td>Symbol</td>
<td>Meaning</td>
<td>Unit</td>
<td>Equation</td>
</tr>
<tr>
<td>---------</td>
<td>-------------------------------------------------------------------------</td>
<td>--------------------------</td>
<td>----------</td>
</tr>
<tr>
<td>$f_{ugwd}$</td>
<td>allometric underground wood fraction</td>
<td>–</td>
<td>input</td>
</tr>
<tr>
<td>$f_\theta$</td>
<td>soil moisture response factor</td>
<td>–</td>
<td>28, 129</td>
</tr>
<tr>
<td>$f_\Psi$</td>
<td>water potential response factor</td>
<td>–</td>
<td>118</td>
</tr>
<tr>
<td>$G_{pot}$</td>
<td>potential growth of total biomass</td>
<td>kg (glucose)</td>
<td>42, 43</td>
</tr>
<tr>
<td>$G_S$</td>
<td>actual assimilate consumption for synthesis of defensive compounds</td>
<td>kg (glucose)</td>
<td>67</td>
</tr>
<tr>
<td>$G_W$</td>
<td>actual assimilate consumption for growth of structural biomass</td>
<td>kg (glucose)</td>
<td>48</td>
</tr>
<tr>
<td>$G_{W_k}$</td>
<td>actual assimilate consumption for structural growth of organ $k$</td>
<td>kg (glucose)</td>
<td>51</td>
</tr>
<tr>
<td>$g_{O_3}$</td>
<td>conductivity of leaves for ozone $k$</td>
<td>m d$^{-1}$</td>
<td>156</td>
</tr>
<tr>
<td>$H$</td>
<td>plant height</td>
<td>m</td>
<td>6–8</td>
</tr>
<tr>
<td>$HD$</td>
<td>height to diameter ratio</td>
<td>–</td>
<td>9</td>
</tr>
<tr>
<td>$HD_{min}$</td>
<td>minimal height to diameter ratio</td>
<td>–</td>
<td>input</td>
</tr>
<tr>
<td>$HD_{max}$</td>
<td>maximal height to diameter ratio</td>
<td>–</td>
<td>input</td>
</tr>
<tr>
<td>$h$</td>
<td>height</td>
<td>m</td>
<td></td>
</tr>
<tr>
<td>$I$</td>
<td>intensity of plant stress</td>
<td>0–1</td>
<td>input</td>
</tr>
<tr>
<td>$I_{P,L}$</td>
<td>intensity of plant stress caused by leaf pathogens</td>
<td>0–1</td>
<td>input</td>
</tr>
<tr>
<td>$I_{P,L,crit}$</td>
<td>critical intensity of plant stress caused by leaf pathogens</td>
<td>0–1</td>
<td>input</td>
</tr>
<tr>
<td>$I_{P,R}$</td>
<td>intensity of plant stress caused by root pathogens</td>
<td>0–1</td>
<td>input</td>
</tr>
<tr>
<td>$I_{P,R,crit}$</td>
<td>critical intensity of plant stress caused by root pathogens</td>
<td>0–1</td>
<td>input</td>
</tr>
<tr>
<td>$K_k$</td>
<td>maximal weight of organ $k$</td>
<td>kg</td>
<td>72, 75, 76</td>
</tr>
<tr>
<td>$k$</td>
<td>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</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>Symbol</td>
<td>Meaning</td>
<td>Unit</td>
<td>Equation</td>
</tr>
<tr>
<td>------------</td>
<td>-------------------------------------------------------------------------</td>
<td>----------</td>
<td>----------</td>
</tr>
<tr>
<td>$k_{dif}$</td>
<td>light extinction coefficient for diffuse radiation</td>
<td>–</td>
<td>input</td>
</tr>
<tr>
<td>$k_{dir,dir}$</td>
<td>light extinction coefficient for direct component of direct radiation</td>
<td>–</td>
<td>92</td>
</tr>
<tr>
<td>$k_{dir,tot}$</td>
<td>light extinction coefficient for total direct radiation</td>
<td>–</td>
<td>91</td>
</tr>
<tr>
<td>$k_{ion}$</td>
<td>average ion leakage rate</td>
<td>d$^{-1}$</td>
<td>input</td>
</tr>
<tr>
<td>$k_{lip}$</td>
<td>turnover rate of lipids</td>
<td>d$^{-1}$</td>
<td>input</td>
</tr>
<tr>
<td>$k_{prt}$</td>
<td>turnover rate of proteins</td>
<td>d$^{-1}$</td>
<td>input</td>
</tr>
<tr>
<td>LAI</td>
<td>leaf area index</td>
<td>m$^2$(leaf)</td>
<td>12</td>
</tr>
<tr>
<td>LAI$_{cum}(h)$</td>
<td>cumulative leaf area index over $h$</td>
<td>m$^2$(soil)</td>
<td>14</td>
</tr>
<tr>
<td>LAI$_{crit}(h)$</td>
<td>critical leaf area</td>
<td>m$^2$(leaf)</td>
<td>input</td>
</tr>
<tr>
<td>LAI$_{max}$</td>
<td>maximal leaf area index</td>
<td>m$^2$(soil)</td>
<td>input</td>
</tr>
<tr>
<td>$l_c$</td>
<td>critical value of soluble carbohydrates in leaves with respect to photosynthesis</td>
<td>–</td>
<td>111</td>
</tr>
<tr>
<td>$l_R(l)$</td>
<td>root length density in soil layer $l$</td>
<td>m</td>
<td>21</td>
</tr>
<tr>
<td>$m_{tu,k}$</td>
<td>rate of assimilate consumption to resynthesise proteins and lipids in organ $k$</td>
<td>kg (glucose)$\cdot$d$^{-1}$</td>
<td>38</td>
</tr>
<tr>
<td>$m_{ion,k}$</td>
<td>rate of assimilate consumption to maintain ionic concentrations in organ $k$</td>
<td>kg (glucose)$\cdot$d$^{-1}$</td>
<td>39</td>
</tr>
<tr>
<td>$m_{met}$</td>
<td>rate of assimilate consumption due to metabolic activities</td>
<td>kg (glucose)$\cdot$d$^{-1}$</td>
<td>40</td>
</tr>
<tr>
<td>$m_c$</td>
<td>parameter for efficiency of plant defense</td>
<td>–</td>
<td>input</td>
</tr>
<tr>
<td>$N_{av}$</td>
<td>available plant internal nitrogen</td>
<td>kg (N)</td>
<td>65</td>
</tr>
<tr>
<td>$N_{dem}$</td>
<td>total nitrogen demand of the plant</td>
<td>kg (N)</td>
<td>122</td>
</tr>
<tr>
<td>$N_{dem,grw}$</td>
<td>nitrogen demand for growth</td>
<td>kg (N)</td>
<td>123</td>
</tr>
<tr>
<td>$N_{dem,opt}$</td>
<td>difference between optimal and actual nitrogen level in the plant</td>
<td>kg (N)</td>
<td>123</td>
</tr>
<tr>
<td>$N_k$</td>
<td>nitrogen content in organ $k$</td>
<td>kg (N)</td>
<td>133</td>
</tr>
<tr>
<td>$N_{mob}$</td>
<td>potential plant internal nitrogen mobilisation</td>
<td>kg (N)</td>
<td>137</td>
</tr>
<tr>
<td>$N_{mob,k}$</td>
<td>potential nitrogen mobilisation in organ $k$</td>
<td>kg (N)</td>
<td>136</td>
</tr>
<tr>
<td>$N_{inc,k}$</td>
<td>increment of nitrogen content in organ $k$</td>
<td>kg (N)</td>
<td>134</td>
</tr>
</tbody>
</table>
A LIST OF VARIABLES

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Meaning</th>
<th>Unit</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N_{soil,av}$</td>
<td>available mineral nitrogen in soil disc $l$</td>
<td>kg (N)</td>
<td>128</td>
</tr>
<tr>
<td>$N_{trans,k}$</td>
<td>translocation of mobile nitrogen of organ $k$</td>
<td>kg (N)</td>
<td>135</td>
</tr>
<tr>
<td>$N_{upt}(l)$</td>
<td>actual nitrogen uptake from soil</td>
<td>kg (N)</td>
<td>130</td>
</tr>
<tr>
<td>$N_{upt}$</td>
<td>actual nitrogen uptake</td>
<td>kg (N)</td>
<td>132</td>
</tr>
<tr>
<td>$N_{upt,max}$</td>
<td>maximal nitrogen uptake from soil</td>
<td>kg (N)</td>
<td>125</td>
</tr>
<tr>
<td>$N_{upt,pt}$</td>
<td>potential nitrogen uptake from soil</td>
<td>kg (N)</td>
<td>127</td>
</tr>
<tr>
<td>$n$</td>
<td>index for leaf layer</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>$n_I$</td>
<td>parameter for potential damage in case of stress</td>
<td>–</td>
<td>input</td>
</tr>
<tr>
<td>$ph(d)$</td>
<td>photoperiod of day $d$</td>
<td>m</td>
<td>extern</td>
</tr>
<tr>
<td>$p_{hopt}$</td>
<td>optimal photoperiod for development</td>
<td>h</td>
<td>input</td>
</tr>
<tr>
<td>$p_L$</td>
<td>relative maximum of leaf area density</td>
<td>(0-1)</td>
<td>input</td>
</tr>
<tr>
<td>$p_R$</td>
<td>relative maximum of root length density</td>
<td>(0-1)</td>
<td>input</td>
</tr>
<tr>
<td>$P_{act}$</td>
<td>actual gross assimilation rate</td>
<td>kg($CO_2$)·d$^{-1}$</td>
<td>100</td>
</tr>
<tr>
<td>$p_{max}$</td>
<td>actual maximal assimilation rate</td>
<td>kg($CO_2$)·m$^{-2}$·h$^{-1}$</td>
<td>101</td>
</tr>
<tr>
<td>$p_{opt}$</td>
<td>maximal assimilation rate under optimal conditions</td>
<td>kg($CO_2$)·m$^{-2}$·h$^{-1}$</td>
<td>input</td>
</tr>
<tr>
<td>$p_{sh}$</td>
<td>assimilation rate of shaded leaves</td>
<td>kg($CO_2$)·m$^{-2}$·h$^{-1}$</td>
<td>97</td>
</tr>
<tr>
<td>$p_{su}$</td>
<td>assimilation rate of sunlit leaves</td>
<td>kg($CO_2$)·m$^{-2}$·h$^{-1}$</td>
<td>98</td>
</tr>
<tr>
<td>$q_{W,act}(l)$</td>
<td>actual water uptake rate from soil disc $l$</td>
<td>cm$^3$</td>
<td>119</td>
</tr>
<tr>
<td>$q_{W,max}(l)$</td>
<td>maximal water uptake rate from soil disc $l$</td>
<td>cm$^3$</td>
<td>114</td>
</tr>
<tr>
<td>$q_{W,pt}(l)$</td>
<td>potential water uptake rate from soil disc $l$</td>
<td>cm$^3$</td>
<td>115</td>
</tr>
<tr>
<td>$R$</td>
<td>pool of reserves</td>
<td>kg(starch)</td>
<td>70</td>
</tr>
<tr>
<td>$R_{ci/c_e}$</td>
<td>leaf internal/external CO$_2$ ratio</td>
<td>–</td>
<td>input</td>
</tr>
<tr>
<td>$r_{C/S}$</td>
<td>crown to stem diameter ratio</td>
<td>–</td>
<td>input, 74</td>
</tr>
<tr>
<td>$r_{dev}$</td>
<td>actual development rate</td>
<td>d$^{-1}$</td>
<td>32</td>
</tr>
<tr>
<td>$r_{max}$</td>
<td>maximal plant growth rate</td>
<td>d$^{-1}$</td>
<td>input</td>
</tr>
</tbody>
</table>
## A LIST OF VARIABLES

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Meaning</th>
<th>Unit</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>$r_{FR/L}$</td>
<td>potential fine root to leaf ratio</td>
<td>–</td>
<td>input</td>
</tr>
<tr>
<td>$r_R$</td>
<td>relative reserves growth rate</td>
<td>d(^{-1})</td>
<td>input</td>
</tr>
<tr>
<td>$r_{zR}$</td>
<td>maximal root extension rate</td>
<td>m/d</td>
<td>input</td>
</tr>
<tr>
<td>$S$</td>
<td>pool of defensive compounds</td>
<td>kg</td>
<td>69</td>
</tr>
<tr>
<td>$s_k$</td>
<td>concentration of defensive compounds in organ $k$</td>
<td>kg·kg(^{-1})</td>
<td></td>
</tr>
<tr>
<td>$T$</td>
<td>actual air Temperature</td>
<td>°C</td>
<td>input</td>
</tr>
<tr>
<td>$T_m$</td>
<td>daily mean air temperature</td>
<td>°C</td>
<td>input</td>
</tr>
<tr>
<td>$T_{act}$</td>
<td>actual transpiration</td>
<td>cm(^3)</td>
<td>120</td>
</tr>
<tr>
<td>$T_{pot}$</td>
<td>actual transpiration</td>
<td>cm(^3)</td>
<td>extern</td>
</tr>
<tr>
<td>$T_{dev,max}$</td>
<td>maximal temperature for phenological development</td>
<td>°C</td>
<td>input</td>
</tr>
<tr>
<td>$T_{dev,min}$</td>
<td>minimal temperature for phenological development</td>
<td>°C</td>
<td>input</td>
</tr>
<tr>
<td>$T_{dev,opt}$</td>
<td>optimal temperature for phenological development</td>
<td>°C</td>
<td>input</td>
</tr>
<tr>
<td>$T_{ps,max}$</td>
<td>maximal temperature for photosynthesis</td>
<td>°C</td>
<td>input</td>
</tr>
<tr>
<td>$T_{ps,min}$</td>
<td>minimal temperature for photosynthesis</td>
<td>°C</td>
<td>input</td>
</tr>
<tr>
<td>$T_{ps,opt}$</td>
<td>optimal temperature for photosynthesis</td>
<td>°C</td>
<td>input</td>
</tr>
<tr>
<td>$T_{rt,max}$</td>
<td>maximal temperature for root extension</td>
<td>°C</td>
<td>input</td>
</tr>
<tr>
<td>$T_{rt,min}$</td>
<td>minimal temperature for root extension</td>
<td>°C</td>
<td>input</td>
</tr>
<tr>
<td>$T_{rt,opt}$</td>
<td>optimal temperature for root extension</td>
<td>°C</td>
<td>input</td>
</tr>
<tr>
<td>$T_{soil(l)}$</td>
<td>soil temperature in layer $l$</td>
<td>°C</td>
<td>extern</td>
</tr>
<tr>
<td>$t$</td>
<td>time</td>
<td>days</td>
<td></td>
</tr>
<tr>
<td>$t_B$</td>
<td>biological time</td>
<td>–</td>
<td>30</td>
</tr>
<tr>
<td>$W$</td>
<td>(= $\sum W_k$) total structural plant biomass</td>
<td>kg</td>
<td>–</td>
</tr>
<tr>
<td>$W_{av(l)}$</td>
<td>available water in soil disc $l$</td>
<td>cm(^3)</td>
<td>117</td>
</tr>
<tr>
<td>$W_{F,4}$</td>
<td>fruit biomass at the end of stage 4</td>
<td>kg</td>
<td>–</td>
</tr>
<tr>
<td>$W_k$</td>
<td>dry weight of organ $k$</td>
<td>kg</td>
<td>66</td>
</tr>
<tr>
<td>Symbol</td>
<td>Meaning</td>
<td>Unit</td>
<td>Equation</td>
</tr>
<tr>
<td>----------</td>
<td>------------------------------------------------------------------------</td>
<td>---------------------------</td>
<td>----------</td>
</tr>
<tr>
<td>$W_{seed}$</td>
<td>seed weight in units of glucose</td>
<td>kg (glucose)</td>
<td>input</td>
</tr>
<tr>
<td>$W_{V2}$</td>
<td>vegetative structural biomass at the end of stage 2</td>
<td>kg</td>
<td>intern</td>
</tr>
<tr>
<td>$w_L(h)$</td>
<td>cumulative leaf weight under height $h$</td>
<td>kg</td>
<td>142</td>
</tr>
<tr>
<td>$z$</td>
<td>soil depth</td>
<td>m</td>
<td>intern</td>
</tr>
<tr>
<td>$z_l$</td>
<td>depth of soil layer $l$</td>
<td>m</td>
<td>input</td>
</tr>
<tr>
<td>$z_R$</td>
<td>rooting depth</td>
<td>m</td>
<td>20</td>
</tr>
<tr>
<td>$z_{R,\text{max}}$</td>
<td>maximal rooting depth</td>
<td>m</td>
<td>input</td>
</tr>
<tr>
<td>$\alpha_{O_3}$</td>
<td>ozone sensitivity parameter of development</td>
<td>kg $\cdot \mu g^{-1} \cdot d^{-1}$</td>
<td>input</td>
</tr>
<tr>
<td>$\beta_{O_3}$</td>
<td>ozone sensitivity parameter of photosynthesis</td>
<td>kg $\cdot \mu g^{-1}$</td>
<td>input</td>
</tr>
<tr>
<td>$\beta$</td>
<td>solar height</td>
<td>degree</td>
<td>84</td>
</tr>
<tr>
<td>$\Gamma_0$</td>
<td>CO$_2$ compensation point</td>
<td>ppm</td>
<td>input</td>
</tr>
<tr>
<td>$\gamma_C$</td>
<td>parameter for regulation of allocation in case of plant internal C shortage</td>
<td>–</td>
<td>input</td>
</tr>
<tr>
<td>$\gamma_N$</td>
<td>parameter for regulation of allocation in case of plant internal N shortage</td>
<td>–</td>
<td>input</td>
</tr>
<tr>
<td>$\delta_z(l)$</td>
<td>thickness of soil layer $l$</td>
<td>m</td>
<td>input</td>
</tr>
<tr>
<td>$\delta$</td>
<td>parameter for defensive compounds formation</td>
<td>–</td>
<td>input</td>
</tr>
<tr>
<td>$\delta_s$</td>
<td>declination of the sun</td>
<td>degree</td>
<td>85</td>
</tr>
<tr>
<td>$\varepsilon$</td>
<td>light use efficiency</td>
<td>$\frac{\text{kg}}{\text{m}^2 \cdot \text{h} / \text{J} / \text{m}^2 \cdot \text{s}}$</td>
<td>input</td>
</tr>
<tr>
<td>$\eta$</td>
<td>parameter considering the effect of soil nitrogen availability on nitrogen uptake rate per unit root surface</td>
<td>$\text{kg}^3 \cdot \text{kg(N)}^{-1}$</td>
<td>input</td>
</tr>
<tr>
<td>$\zeta_N$</td>
<td>maximal nitrogen uptake rate</td>
<td>$\frac{\text{kg(N)}}{\text{m}^2 \cdot \text{d}}$</td>
<td>input</td>
</tr>
<tr>
<td>$\zeta_W$</td>
<td>maximal water uptake rate</td>
<td>$\frac{\text{cm}^3}{\text{m}^2 \cdot \text{d}}$</td>
<td>input</td>
</tr>
<tr>
<td>$\theta_{act}(l)$</td>
<td>actual water content in layer $l$</td>
<td>$\frac{\text{cm}^3}{\text{cm}^2}$</td>
<td>extern</td>
</tr>
<tr>
<td>$\theta_{f_c}(l)$</td>
<td>water content in layer $l$ at field capacity</td>
<td>$\frac{\text{cm}^3}{\text{cm}^2}$</td>
<td>extern</td>
</tr>
<tr>
<td>$\theta_{pwp}(l)$</td>
<td>water content in layer at permanent wilting point $l$</td>
<td>$\frac{\text{cm}^3}{\text{cm}^2}$</td>
<td>extern</td>
</tr>
<tr>
<td>Symbol</td>
<td>Meaning</td>
<td>Unit</td>
<td>Equation</td>
</tr>
<tr>
<td>------------</td>
<td>-------------------------------------------------------------------------</td>
<td>-----------------------</td>
<td>----------</td>
</tr>
<tr>
<td>$\theta_{sat}(l)$</td>
<td>water content in layer $l$ at water saturation</td>
<td>$\frac{cm^3}{cm^3}$</td>
<td>extern</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>latitude of the location</td>
<td>degree</td>
<td>input</td>
</tr>
<tr>
<td>$\lambda_{age}$</td>
<td>loss rate of leaves due to aging</td>
<td>$d^{-1}$</td>
<td>145</td>
</tr>
<tr>
<td>$\lambda_k$</td>
<td>actual loss rate of organ $k$</td>
<td>$d^{-1}$</td>
<td>143</td>
</tr>
<tr>
<td>$\lambda_{k,snc}$</td>
<td>actual loss rate of organ $k$ due to senescence</td>
<td>$d^{-1}$</td>
<td>144,148–150</td>
</tr>
<tr>
<td>$\lambda_{k,I,pot}$</td>
<td>potential loss rate of organ $k$ due to stress</td>
<td>$d^{-1}$</td>
<td>151</td>
</tr>
<tr>
<td>$\lambda_{k,0}$</td>
<td>turnover rate of orgen $k$</td>
<td>$d^{-1}$</td>
<td>input</td>
</tr>
<tr>
<td>$\lambda_{IR}$</td>
<td>specific root length</td>
<td>$m\cdot kg^{-1}$</td>
<td>input</td>
</tr>
<tr>
<td>$\lambda_{Lw}(h)$</td>
<td>specific leaf weight of leaves at height $h$</td>
<td>$kg\cdot m^{-2}$</td>
<td>18</td>
</tr>
<tr>
<td>$\lambda_{Lw,max}$</td>
<td>maximal specific leaf weight</td>
<td>$kg\cdot m^{-2}$</td>
<td>input</td>
</tr>
<tr>
<td>$\lambda_{Lw}^*$</td>
<td>mean specific leaf weight</td>
<td>$kg\cdot m^{-2}$</td>
<td>19</td>
</tr>
<tr>
<td>$\lambda_{Lw,min}^*$</td>
<td>minimal mean specific leaf weight</td>
<td>$kg\cdot m^{-2}$</td>
<td>17</td>
</tr>
<tr>
<td>$\lambda_{O_3}^*$</td>
<td>leaf internal ozone degradation rate</td>
<td>$d^{-1}\cdot (kg\cdot kg^{-1})^{-1}$</td>
<td>input</td>
</tr>
<tr>
<td>$\lambda_{shade}$</td>
<td>loss rate of leaves due to shading</td>
<td>$d^{-1}$</td>
<td>145</td>
</tr>
<tr>
<td>$\mu_e$</td>
<td>parameter for efficiency of plant defense</td>
<td>–</td>
<td>input</td>
</tr>
<tr>
<td>$\mu_{met}$</td>
<td>fraction of gross photosynthesis used for metabolic processes</td>
<td>–</td>
<td>input</td>
</tr>
<tr>
<td>$\nu_I$</td>
<td>parameter for potential damage in case of stress</td>
<td>–</td>
<td>input</td>
</tr>
<tr>
<td>$\nu_{act,k}$</td>
<td>actual nitrogen concentration in organ $k$</td>
<td>$kg(N)\cdot kg^{-1}$</td>
<td>138</td>
</tr>
<tr>
<td>$\nu_{act,L}(h)$</td>
<td>actual nitrogen concentration in leaves at height $h$</td>
<td>$kg(N)\cdot kg^{-1}$</td>
<td>138</td>
</tr>
<tr>
<td>$\nu_{min,k}$</td>
<td>minimal nitrogen concentration in organ $k$</td>
<td>$kg(N)\cdot kg^{-1}$</td>
<td>input</td>
</tr>
<tr>
<td>$\nu_{opt,k}$</td>
<td>optimal nitrogen concentration in organ $k$</td>
<td>$kg(N)\cdot kg^{-1}$</td>
<td>input</td>
</tr>
<tr>
<td>$\xi_{W_k}$</td>
<td>growth efficiency of organ $k$</td>
<td>$\frac{kg}{kg\ (glucose)}$</td>
<td>input</td>
</tr>
<tr>
<td>$\xi_S$</td>
<td>efficiency of synthesis of defensive compounds</td>
<td>$\frac{kg\ (glucose)}{kg}$</td>
<td>input</td>
</tr>
<tr>
<td>$\xi_R$</td>
<td>efficiency of conversion of glucose to starch</td>
<td>$\frac{kg\ (glucose)}{kg\ (starch)}$</td>
<td>input</td>
</tr>
<tr>
<td>$\varrho_{dif}$</td>
<td>leaf refraction coefficient for diffuse radiation</td>
<td>–</td>
<td>93</td>
</tr>
<tr>
<td>Symbol</td>
<td>Meaning</td>
<td>Unit</td>
<td>Equation</td>
</tr>
<tr>
<td>--------------</td>
<td>--------------------------------------------------------</td>
<td>--------------</td>
<td>----------</td>
</tr>
<tr>
<td>$\varrho_{\text{dir}}$</td>
<td>leaf reflexion coefficient for direct radiation</td>
<td>–</td>
<td>94</td>
</tr>
<tr>
<td>$\varrho_F$</td>
<td>fruit filling rate</td>
<td>d$^{-1}$</td>
<td>input</td>
</tr>
<tr>
<td>$\varrho_L$</td>
<td>leaf flush rate</td>
<td>d$^{-1}$</td>
<td>input</td>
</tr>
<tr>
<td>$\varrho_{\text{plant}}$</td>
<td>canopy density</td>
<td>plants m$^{-2}$</td>
<td>input</td>
</tr>
<tr>
<td>$\varrho_R$</td>
<td>root density</td>
<td>kg m$^{-3}$</td>
<td>input</td>
</tr>
<tr>
<td>$\varrho_{\text{soil}}(l)$</td>
<td>soil density in soil layer</td>
<td>kg m$^{-3}$</td>
<td>input</td>
</tr>
<tr>
<td>$\varrho_{(F)R}$</td>
<td>(fine) root flush rate</td>
<td>d$^{-1}$</td>
<td>input</td>
</tr>
<tr>
<td>$\varrho_S$</td>
<td>stem density</td>
<td>kg m$^{-3}$</td>
<td>input</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>potential defence investment</td>
<td>–</td>
<td>46</td>
</tr>
<tr>
<td>$\sigma_s$</td>
<td>leaf scattering coefficient</td>
<td>–</td>
<td>input</td>
</tr>
<tr>
<td>$\sigma_0$</td>
<td>potential permanent defence investment</td>
<td>–</td>
<td>input</td>
</tr>
<tr>
<td>$\sigma_I$</td>
<td>potential induced defence investment</td>
<td>–</td>
<td>47</td>
</tr>
<tr>
<td>$\tau_A$</td>
<td>atmospheric transmissivity</td>
<td>–</td>
<td>82</td>
</tr>
<tr>
<td>$\tau_N$</td>
<td>nitrogen mobilisation rate</td>
<td>d$^{-1}$</td>
<td>input</td>
</tr>
<tr>
<td>$\tau_R$</td>
<td>reserves mobilisation rate</td>
<td>d$^{-1}$</td>
<td>input</td>
</tr>
<tr>
<td>$\tau_S$</td>
<td>turnover rate of defensive compounds</td>
<td>d$^{-1}$</td>
<td>input</td>
</tr>
<tr>
<td>$\phi_{\text{PAR}}$</td>
<td>photosynthetic active radiation</td>
<td>W m$^{-2}$</td>
<td>78</td>
</tr>
<tr>
<td>$\phi_{\text{PAR, dif}}$</td>
<td>diffuse component of photosynthetic active radiation</td>
<td>W m$^{-2}$</td>
<td>80</td>
</tr>
<tr>
<td>$\phi_{\text{PAR, dir}}$</td>
<td>direct component of photosynthetic active radiation</td>
<td>W m$^{-2}$</td>
<td>79</td>
</tr>
<tr>
<td>$\phi_e$</td>
<td>extraterrestrial radiation</td>
<td>W m$^{-2}$</td>
<td>83</td>
</tr>
<tr>
<td>$\phi_{a, sh}$</td>
<td>radiation absorption by shaded leaves</td>
<td>W m$^{-2}$ (leaf)</td>
<td>95</td>
</tr>
<tr>
<td>$\phi_{a, su}$</td>
<td>radiation absorption by sunlit leaves</td>
<td>W m$^{-2}$ (leaf)</td>
<td>96</td>
</tr>
<tr>
<td>$\phi_{\text{dif}}(h)$</td>
<td>flux of diffuse photosynthetic active radiation</td>
<td>W m$^{-2}$</td>
<td>88</td>
</tr>
<tr>
<td>$\phi_{\text{dir, tot}}(h)$</td>
<td>flux of total direct photosynthetic active radiation</td>
<td>W m$^{-2}$</td>
<td>89</td>
</tr>
<tr>
<td>Symbol</td>
<td>Meaning</td>
<td>Unit</td>
<td>Equation</td>
</tr>
<tr>
<td>--------------</td>
<td>-------------------------------------------------------------------------</td>
<td>------------</td>
<td>----------</td>
</tr>
<tr>
<td>$\phi_{\text{dir,dir}}(h)$</td>
<td>flux of direct component of direct photosynthetic active radiation at height $h$</td>
<td>$\text{W} \cdot \text{m}^{-2}$</td>
<td>90</td>
</tr>
<tr>
<td>$\phi_g$</td>
<td>global radiation</td>
<td>$\text{W} \cdot \text{m}^{-2}$</td>
<td>input</td>
</tr>
<tr>
<td>$\varphi_C$</td>
<td>plant internal C availability</td>
<td>–</td>
<td>49</td>
</tr>
<tr>
<td>$\varphi_N$</td>
<td>plant internal N availability</td>
<td>–</td>
<td>50</td>
</tr>
<tr>
<td>$\varphi_{\text{CO}_2}$</td>
<td>atmospheric CO$_2$ response factor of photosynthetic capacity</td>
<td>–</td>
<td>102</td>
</tr>
<tr>
<td>$\varphi_\nu$</td>
<td>leaf nitrogen response factor of photosynthetic capacity</td>
<td>–</td>
<td>105</td>
</tr>
<tr>
<td>$\varphi_T$</td>
<td>temperature response factor of photosynthetic capacity</td>
<td>–</td>
<td>107</td>
</tr>
<tr>
<td>$\varphi_{\text{H}_2\text{O}}$</td>
<td>stomatal aperture response factor of photosynthetic capacity</td>
<td>–</td>
<td>109</td>
</tr>
<tr>
<td>$\varphi_{\text{CH}_2\text{O}}$</td>
<td>soluble sugars response factor of photosynthetic capacity</td>
<td>–</td>
<td>110</td>
</tr>
<tr>
<td>$\varphi_{\text{O}_3}$</td>
<td>ozone response factor of photosynthetic capacity</td>
<td>–</td>
<td>112</td>
</tr>
<tr>
<td>$\varphi_{\text{Path}}$</td>
<td>leaf pathogens response factor of photosynthetic capacity</td>
<td>–</td>
<td>113</td>
</tr>
<tr>
<td>$\omega$</td>
<td>photoperiodism sensitivity parameter</td>
<td>–</td>
<td>input</td>
</tr>
</tbody>
</table>