

Chapter 1

Detailed description of the original LintulCC

Phenology

LINTULCC2 keeps track of the total number of leaves on the main stem, and determines the dates of anthesis and maturity. The total number of leaves is calculated as a function of the plastochron and a parameter indicating the duration of the period during which leaf primordia are being initiated. The plastochron is assumed to be half the phyllochron (PHY), which is calculated at emergence as a function of the rate of change of the photoperiod (RCPHOE) (Mulholland et al. 1997).

$$PHY = \frac{1}{0.0117 + 0.024 * RCPHOE} \quad (1.1)$$

The parameter constants 0.0117 and 0.024 were taken from Minares spring wheat cultivar. Thermal time is required until flag leaf emergence (TTFLE, °Cd) is calculated by:

$$TTFLE = \max (LNUFLE * PHY, MSLPN * PHY) \quad (1.2)$$

Where LFLUFLE is leaf number at main stem when flag leaf appearance while MSLPN is total/possible leaf number of main stem. Anthesis occurs one phyllochron after the emergence of the flag leaf, and maturity occurs after a fixed cumulated thermal time after anthesis (900 dC°), or whenever the green leaf area is zero due to senescence.

$$TTANTH = \max (900, TTFLE + PHY) \quad (1.3)$$

Crop height

$$CROPHT = \max (0.05 + 1 / (1.0 + \exp (-10.79 * (TSUM/TTANTH - 0.684))), 0.05) \quad (1.4)$$

Where TSUM and TTANTH are sum of thermal time at current time and at anthesis (°Cd)

TOTASS (upscaling over canopy and time with Gaussian integration)

In LintulCC, the daily radiation, temperature were disaggregated to hourly using the sine function of time. The photosynthesis thus can be varied at “hourly” by this routine. This “hourly photosynthesis” then was summed-up to get the total daily assimilation rate. The equations for scaling up could be found at Equation 1.5.

The approach has been described in van Laar and Goudriaan’s “Textbook 1994” and see also the re-description in Nguyen et al., (2020) in terms of upscaling from leaf to canopy for photosynthesis and stomatal conductance. To scale up from leaf stomatal conductance to canopy and for computation efficiency, we approximate the integrals

$$\int_0^{LAI} f(l) dl \quad (1.5)$$

By Gaussian quadrature $LAI \sum_{j=1}^5 w_j * f(LAI * x_j)$ where x_j are the nodes and w_j the weights of the 5-point gaussian quadrature (Goudriaan and van Laar, 1994). LAI is the leaf area index and f is a function dependent on leaf area for instance gsH_2O . The above mentioned bulk stomatal conductance to CO_2 ($gs_{i,t}$ - $mol\ m^{-2}\ s^{-1}$) of sunlit and shaded leaf to stomatal conductance was converted to stomatal conductance to H_2O ($m\ s^{-1}$) based on the molar density of air.

$$gsH_2O_{sun} = 1.56 * gs_{sun} / 41.66 \quad (1.6)$$

$$gsH_2O_{shade} = 1.56 * gs_{shade} / 41.66 \quad (1.7)$$

Leaf stomatal conductance to H_2O ($m\ s^{-1}$) was calculated based on fraction of sunlit leaf area FSLLA

$$gsH_2O_{leaf} = gsH_2O_{sun} * FSLLA + gsH_2O_{shade} (1 - FSLLA) \quad (1.8)$$

The daily canopy conductance DailyGSCropH₂O ($m\ s^{-1}$) was calculated in Eq. (1.9)

$$DailyGSCropH_2O = LAI * \sum_{j=1}^5 w_j gsH_2O_{leaf} \quad (1.9)$$

Daily canopy resistance ($s\ m^{-1}$) was the reciprocal of daily canopy conductance

$$Dr_s = 1 / DailyGSCropH_2O \quad (1.10)$$

The ASSIM function (photosynthesis and stomatal conductance models)

This function describes very in detail the calculation of sunlit and shaded leaves radiation, diffusive and reflected radiation from PAR. The photosynthesis for C3 crops was based on the Farquhar approach (Farquhar et al., 1982) which is the biochemical kinetics of Rubisco to CO_2 and O_2 concentrations. The stomatal conductance model was based on the coupled photosynthesis-stomatal conductance approach (Leuning, 1995). A detailed description in terms of equations and upscaling could be found in Rodriguez et al., (2000) and in Nguyen et al., (2020).

$$AMAX_{l,t} = \frac{VCMAX_{l,t} (Ci_{l,t} - \Gamma^*)}{Ci_{l,t} + KMC \left(1 + \frac{O_2}{KMO}\right)} f_{wat} \quad (1.11)$$

$$EFF_{l,t} = \frac{J}{2.1 \cdot 4.5 (Ci_{l,t} + 2\Gamma^*)} \quad (1.12)$$

$$FGR_{l,t} = AMAX_{l,t} \left(1 - e^{-I_{l,t} \frac{EFF_{l,t}}{AMAX_{l,t}}} \right) \quad (1.13)$$

$$Ci_{l,t} = Ca - \left(FGR_{l,t} \frac{1}{gs_{l,t}} \right) \quad (1.14)$$

$$gs_{l,t} = a_1 + \frac{b_1 FGR_{l,t}}{(Ci_{l,t} - \Gamma^*) \left(1 + \frac{DS_{l,t}}{D_0} \right)} f_{wat} \quad (1.15)$$

AMAX is light saturated leaf photosynthesis ($\mu\text{M CO}_2 \text{ m}^{-2} \text{ s}^{-1}$); VCMAX is maximum carboxylation rate of Rubisco enzyme ($\mu\text{M m}^{-2} \text{ s}^{-1}$); C_i is intercellular CO_2 concentration ($\mu\text{M mol}^{-1}$); C_a is atmospheric CO_2 concentration ($\mu\text{M mol}^{-1}$); KMC is Michaelis-Menten constant for CO_2 ($\mu\text{M mol}^{-1}$); KMO is Michaelis-Menten constant for O_2 ($\mu\text{M mol}^{-1}$); O_2 is atmospheric oxygen concentration ($\mu\text{M mol}^{-1}$); Γ^* is CO_2 compensation point ($\mu\text{M mol}^{-1}$); EFF is quantum yield ($\mu\text{M CO}_2 \text{ MJ}^{-1}$); J is conversion energy from radiation to mole photon (mole photons MJ^{-1}); FGR is leaf photosynthesis rate ($\mu\text{M CO}_2 \text{ m}^{-2} \text{ s}^{-1}$); I is the total absorbed flux of radiation ($\text{MJ m}^{-2} \text{ s}^{-1}$); g_s is bulk stomatal conductance ($\text{mol m}^{-2} \text{ s}^{-1}$); a_1 is residual stomatal conductance ($\text{mol m}^{-2} \text{ s}^{-1}$) when $FGR = 0$; b_1 is fitting parameter (-); DS is the vapor pressure deficit at the leaf surface (Pa); D_0 is empirical coefficient reflecting the sensitivity of the stomata to VPD (Pa); l is sub-indices indicates canopy layer (sunlit and shaded leaf) (-); t is sub-indices indicates time of the day (-); f_{wat} is water stress factor for stomatal conductance and maximum carboxylation rate (-);

GLA function (leaf growth)

This function simulates leaf growth. The leaf growth was divided into an exponential growth phase and linear growth phase. In LINTULCC2 leaf growth is calculated in two steps, (1) the potential leaf expansion is calculated as a function of mean air temperature (sink limitation), (2) the actual leaf growth is calculated as a function of the potential leaf growth and sink and source interactions. The sink term for leaf expansion is calculated exponentially with temperature sum, until a value of LAI=1 or if the end of leaf primordia initiation the period is reached. Afterward, the sink term for leaf expansion is linear with temperature until a maximum LAI ($LAI_{max} = 8$) or if anthesis is reached. The sink: source balance is calculated as a function of the calculated value of SLA for the new growth (SLAn). Then, if the calculated SLAn is higher than $0.03 \text{ m}^2 \text{ g}^{-1}$ the leaf area expansion is assumed to be source limited and then the leaf expansion reset to match the maximum possible SLA. If the SLA is lower than a minimum value of $0.017 \text{ m}^2 \text{ g}^{-1}$, the crop is assumed to be sink limited, the leaf expansion reset to match the the minimum possible value of SLA, and the excess of assimilates reallocated towards the root system.

Leaf death due to the shading effect was simulated when LAI is reached to critical LAI (LAICR). Dead leaf due to aging is estimated after anthesis based on the thermal time from anthesis to maturity and daily effective temperature. Water stress also has increase dead leaves.

PART function (carbon partitioning)

The carbon partitioning was calculated for shoot and root. From shoot then allocated to leaf and stem and storage organs based on interpolated approach thermal times and given carbon partitioning coefficients.

PEN-MONTH (evaporative demand)

This function estimates the daily potential evapotranspiration (ETP) after considering the energy-balance of soil and crop surface based on the Penman-Monteith equation (Equation 3, in Allen et al., 1998). IMPORTANT: the variable name ET0 in the code from LINTULCC2 was misleading which is not the reference evapotranspiration in this case. Moreover, this original routine should be revised that potential evapotranspiration (or ET0) is under non-water stress condition (water stress index fwat = 1, see Appendix B in Nguyen et al., 2020).

Hourly aerodynamic resistance (r_a) was calculated as Equation 4 in the Chapter 2 in the FAO Irrigation and Drainage Paper No. 56, (Allen et al., 1998).

$$ETP = \frac{\Delta(R_n - G) + \rho_a c_p \frac{(e_s - e_a)}{r_a}}{\lambda \left(\Delta + \gamma \left(1 + \frac{Dr_s}{r_a} \right) \right)} \quad (1.16)$$

R_n is net radiation ($\text{MJ m}^{-2} \text{d}^{-1}$); G is soil heat flux ($\text{MJ m}^{-2} \text{d}^{-1}$); e_s is saturation vapor pressure at the air temperature (kPa); e_a is actual vapor pressure at the air temperature (kPa); ρ_a is mean air density at constant pressure (kg m^{-3}); c_p is the specific heat at constant pressure of the air ($1.013 \cdot 10^{-3} \text{ MJ kg}^{-1} \text{ }^\circ\text{C}^{-1}$); Δ is slope of the saturation vapor pressure-temperature relationship; Dr_s is canopy resistance (s m^{-1})

PHOTOP (rate change of photoperiod)

This function calculates the rate change of photoperiod around emerge time based on the approach from Mulholland et al., 1997 that later is used to calculate the phyllochrone. The parameter constants are rather specific for the spring wheat Minaret cultivar (See Rodriguez et al., 2001).

RSICO (grain growth)

The grain growth was simulated based on potential grain growing rate from anthesis to maturity (see in Asseng et al 2011). The routine also considers the effect of heat stress on grain filling from CERES-WHEAT.

WATERB, WATUP, and WFLOW (tipping bucket water balance model and RWU)

The model uses the availability of water from the soil reservoir (tipping bucket) within the root zone as a method of restricting soil evaporation and crop transpiration as soil moisture is depleted. Calculations of water availability and uptake involved:

- The calculation of plant available water within the soil profile, i.e. soil water content held between -1.5 (wilting point) and -0.03 MPa (field capacity), is calculated by dividing the soil profile into layers.
- The downward root front velocity and distribution of root length density with depth is calculated as in Monteith et al. (1989),
- A root length density-weighted plant available water is calculated to linearly reduce stomatal conductance and, the rate of leaf expansion and value of saturated photosynthesis rate when the available water is lower than a fraction of 0.4 and 0.6 of the maximum soil water holding capacity, respectively,
- The determination of the demand for water imposed by available energy from solar radiation, the overlying atmosphere, and the crop, i.e. canopy stomatal conductance for water vapor), using the combination equation of Penman-Monteith
- The actual soil water uptake is calculated as the minimum of the demand for water, and the uptake of water as a function of a maximum uptake rate per unit of root length (0.3 mm day⁻¹ per km of root length).

Chapter 2

Coupling root and shoot model with hourly photosynthesis, stomatal conductance, water balance, and Feddes RWU model

Feddes RWU model in HILLFLOW 1D

The Feddes RWU model (Feddes et al., 1978) was already built in the HILLFLOW 1D model (Bronstert and Plate, 1997). In the Feddes model, root water uptake from a soil layer is proportional to the normalized root density, NRLD (m^{-1}), in that layer and is multiplied by a stress function α that depends on the soil water pressure head, ψ_m (m), in that soil layer and the potential transpiration rate:

$$RWU_i = \alpha(\psi_{m,i}, T_{pot}) T_{pot} NRLD_i \Delta z_i \quad (5.1)$$

where NRLDi is calculated from the root length density, RLD (m m^{-3}) and discretized soil depth Δz_i (m) as: The normalized root length density at each soil layer (NRLDi) is calculated from the root length density, RLD (m m^{-3}) and discretized soil depth Δz_i (m) as:

$$NRLD_i = RLD_i / \sum_{i=1}^N RLD_i \Delta z_i \quad (5.2)$$

The root water uptake in HILLFLOW 1D model which is limited by soil water content in the root zone calculated by reduction of potential transpiration (T_{pot}). The semi-empirical reduction function $\alpha(\Psi_{m,i})$ is derived from soil pressure head (Feddes et al., 1978). The $\alpha(\psi_{m,i})$ also depends on T_{pot} because ψ_3 (soil pressure head where optimum condition for transpiration) is calculated via piecewise linear function of T_{pot} (Wesseling and Brandyk, 1985). The root water uptake was calculated based on relative root length density which is output from the SLIMROOT root growth model.

$$\alpha(\psi_{m,i}) = \begin{cases} 0 & \psi_{m,i} \geq \psi_1, \psi_{m,i} \leq \psi_4 \\ (\psi_{m,i} - \psi_1)/(\psi_2 - \psi_1) & \psi_2 \leq \psi_{m,i} \leq \psi_1 \\ 1 & \psi_3 \leq \psi_{m,i} \leq \psi_2 \\ (\psi_{m,i} - \psi_4)/(\psi_3 - \psi_4) & \psi_4 \leq \psi_{m,i} \leq \psi_3 \end{cases} \quad (5.3)$$

$$\psi_3 = \begin{cases} \psi_{3h} & T_{pot} > T_{3h} \\ \psi_{3h} + \frac{(\psi_{3l} - \psi_{3h})(T_{3h} - T_{pot})}{(T_{3h} - T_{3l})} & T_{3l} < T_{pot} < T_{3h} \\ \psi_{3l} & T_{pot} < T_{3l} \end{cases} \quad (5.4)$$

$\alpha(\Psi_{m,i})$ transpiration reduction as function of soil pressure head (-); Ψ_1 is soil water pressure head at anaerobic limit (m); Ψ_4 is soil pressure head at wilting point (m); Ψ_2 and Ψ_3 are upper and lower limits of pressure head for optimal transpiration (m), respectively; T_{pot} is potential transpiration (m h^{-1}); Ψ_{3h} is lower limit of pressure head range for optimal transpiration for high transpiration rate, T_{pot3h} (m); T_{3h} is high potential transpiration rate (m h^{-1}); Ψ_{3l} is lower limit of pressure head range for low transpiration rate, T_{pot3l} (m); T_{3l} is low potential transpiration rate (m h^{-1}).

The photosynthesis and stomatal conductance subroutines, Feddes RWU and HILLFLOW 1D water balance model, and evaporative demand (ETP) were run or specified with hourly time steps, while phenology, leaf growth, root growth, and biomass partitioning were updated daily. For a certain hourly time step $\Delta t_i = t_i - t_{i-1}$, different modules were solved in the following sequence. First, LINTULCC2 was used with a water stress factor $fwat = 1$ to calculate the leaf and canopy resistance, and the potential transpiration rate. T_{pot} was then used in HILLFLOW 1D to calculate the soil water pressure head changes, water content changes, the actual transpiration, and $fwat$ during the time step. LINTULCC2 was then run again using the $fwat$. The leaf conductance and assimilation rate were calculated. For the next time step, the same loop was run and hourly assimilation was accumulated to a daily value. Daily assimilation rates were used in modules that run with a daily time step. For instance, modules of LINTLCC2 that calculate assimilate partitioning which is used to calculate shoot (LAI) development and passed to SLIMROOT to simulate root development (see Nguyen et al., 2020).

Chapter 3

Plant hydraulic conductance

Analogue Ohm law equation:

$$T = K_{plant}(\psi_{sr} - \psi_{leaf}) \quad (3.1)$$

Where ψ_{sr} is soil to root water potential (MPa); ψ_{leaf} is leaf water potential (MPa), and K_{plant} is plant hydraulic conductance ($\text{mm d}^{-1} \text{MPa}^{-1}$), and T is transpiration rate (mm d^{-1})

Units of water potential and plant hydraulic

Plants take up water from the soil through their roots and transport it to the leaves where it is transpired through the stomata. The driver for this transport is the difference in water potential (a measure of energy stage of water between the atmosphere and the soil). The energy of the plant (or soil) water or water potential can be either stated as total water pressure (Ψ [MPa], energy per volume) or as the hydraulic head (H [m], energy per weight). The first term is often used to express Psi in crop physiologists, while the latter must be used for Psi in the hydrological community. These two units can be converted to each other for instance 1 m is equivalent to 1 MPa. For the plant physiologist, knowing water potential (MPa) and water flux (mm d^{-1}), the K_{plant} will be $\text{mm d}^{-1} \text{MPa}^{-1}$. For the hydrologist, the unit of K_{plant} will be $\text{mm d}^{-1} \text{m}^{-1}$ or $1000 * \text{d}^{-1}$.

Calculation of K_{plant}

In the PlantSystemConductance.java subroutine, the K_{plant} is estimated based on the known root system conductance per unit root length per surface area ($K_{rs, normalized}$, $\text{d}^{-1} \text{cm}^{-1} \text{cm}^2$) (Cai et al., 2017; Cai et al., 2018). We followed the approach of Cai et al., (2017) to estimate the root hydraulic conductance ($K_{rs, doy}$) and compensatory root water uptake (K_{comp}) based on the total length of the root system below a unit surface area, $TRLD_{doy}$ (m m^{-2}), at a given day of year (DOY) (Eq. 3.2), which is the output from SLIMROOT:

$$TRLD_{doy} = \sum_i^N RLD_{i, doy} \Delta z_i \quad (3.2)$$

Assuming the same conductance for all root segments, the root system conductance scales with the TRLD:

$$K_{rs, doy} = K_{rs, normalized} TRLD_{doy} \quad (3.3)$$

where $K_{rs, normalized}$ ($\text{d}^{-1} \text{cm}^{-1} \text{cm}^2$) is the root system conductance per unit root length per surface area. The K_{comp} is also crop specific parameter. The K_{comp} could be smaller or equal to K_{rs} . A fraction was given to calculate the K_{comp} from K_{rs} , namely, `cCompensatoryConductanceFactor`).

To upscale from K_{rs} to K_{plant} , we derived K_{plant} (d^{-1}) from the root hydraulic conductance ($K_{rs,doy}$) assuming that K_{plant} is a constant fraction β of $K_{rs,doy}$ (d^{-1}):

$$K_{plant} = \beta K_{rs,doy} \tag{3.4}$$

Chapter 4

Coupling root and shoot model with hourly photosynthesis, stomatal conductance, water balance, and Couvreur RWU model

Couvreur RWU model in HILLFLOW1D

We implemented the Couvreur RWU model (Couvreur et al., 2014a; Couvreur et al., 2012) into HILLFLOW. Both models, T_{plant} is calculated from the sum of the simulated RWU in the different soil layers and used to calculate the water stress factor (f_{wat}) (see the photosynthesis model Chapter 1, Equation 1.15). The normalized root length density at each soil layer ($NRLD_i$) is calculated from the root length density, RLD ($m\ m^{-3}$) and discretized soil depth Δz_i (m) as:

$$NRLD_i = RLD_i / \sum_{i=1}^N RLD_i \Delta z_i \quad (5.1)$$

In the Couvreur model, the root water uptake in a given soil layer is related to the water potentials in the root system and root water uptake in other soil layers so that compensatory uptake is considered in this model. Root water uptake in a certain layer is obtained from:

$$RWU_i = T_{plant} NRLD_i \Delta z_i + K_{comp} (\psi_i - \psi_{sr}) NRLD_i \Delta z_i \quad (5.2)$$

where ψ_i (m) is the total hydraulic head (or hydraulic head which is the sum of the pressure head and gravitation potential heads) in layer i , ψ_{sr} (m) is the average hydraulic head in the root zone and K_{comp} (d^{-1}) is the root system conductance for compensatory uptake. The first term of Equation 5.2 represents the uptake from that soil layer when the hydraulic head is uniform in the root zone and the second term represents the increase or decrease of uptake from the soil layer due to a respectively higher and lower hydraulic head in layer i than the average hydraulic head. The average root zone hydraulic head is calculated as the weighted average of the hydraulic heads in the different soil layers as:

$$\psi_{sr} = \sum_{i=1}^N \psi_i NRLD_i \Delta z_i \quad (5.3)$$

The plant transpiration rate is the minimum of the potential transpiration rate and the transpiration rate, $T_{threshold}$ ($mm\ h^{-1}$), when the hydraulic head in the leaves reaches a threshold value, $\psi_{threshold}$ (m) that triggers stomatal closure:

$$T_{plant} = \max(0, \min(T_{pot}, T_{threshold})) \quad (5.4)$$

$T_{threshold}$ is calculated from difference between the root zone hydraulic head and the threshold hydraulic head in the leaves $\psi_{threshold}$ that is multiplied by the plant hydraulic conductance, K_{plant} as:

$$T_{threshold} = K_{plant}(\psi_{sr} - \psi_{threshold}) \quad (5.5)$$

The photosynthesis and stomatal conductance subroutines, Couvreur RWU and HILLFLOW 1D water balance model, and evaporative demand (ETP) were run or specified with hourly time steps, while phenology, leaf growth, root growth, and biomass partitioning were updated daily. For a certain hourly time step $\Delta t_i = t_i - t_{i-1}$, different modules were solved in the following sequence. First, LINTULCC2 was used with a water stress factor $fwat = 1$ to calculate the leaf and canopy resistance, and the potential transpiration rate. T_{pot} was then used in HILLFLOW 1D to calculate the soil water pressure head changes, water content changes, the actual transpiration, and $fwat$ during the time step. LINTULCC2 was then run again using the $fwat$. The leaf conductance and assimilation rate were calculated. For the next time step, the same loop was run and hourly assimilation was accumulated to a daily value. Daily assimilation rates were used in modules that run with a daily time step. For instance, modules of LINTLCC2 that calculate assimilate partitioning which is used to calculate shoot (LAI) development and passed to SLIMROOT to simulate root development (see Nguyen et al., 2020).

Chapter 5

Inclusion ozone flux model and ozone stress functions

Coupled photosynthesis and stomatal conductance model

$$C_i = C_a - \left(\frac{FGR_{l,t}}{g_{s_{l,t}}} \right) \quad (2.1)$$

The CO₂ diffuses from atmospheric to the leaf stomata follows the Fick's law:

Stomatal conductance was simulated based on the Leuning approach (1995) with consideration of the effect of leaf to air vapor pressure deficit ($1 + DS/D_0$), intercellular CO₂ concentration (C_i), Γ^* is CO₂ compensation point in the absence of day respiration (see also Chapter 1).

$$g_{s_{l,t}} = g_0 + \frac{a_1 FGR_{l,t}}{(C_i - \Gamma^*) \left(1 + \frac{DS}{D_0}\right)} \quad (2.2)$$

Following the approach from Farquhar et al. (1980) and von Caemmerer (2000), the light saturated photosynthesis rate ($AMAX_{l,t}$) is given as follows:

$$AMAX_{l,t} = \frac{V_{cmax} (C_i - \Gamma^*)}{C_i + K_{MC} \left(1 + \frac{O_2}{K_{MO}}\right)} \min(f_{03t}, f_{LS}) \quad (2.3)$$

Where C_i and O_2 are the intercellular CO₂ and O₂ concentration, respectively; V_{cmax} is the maximum catalytic activity of Rubisco at leaf temperature; Γ^* is CO₂ compensation point at the absence of leaf respiration; K_{MC} and K_{MO} are Michaelis-Menten kinetics for CO₂ and O₂ (see also Chapter 1).

$$EFF_{l,t} = \frac{J}{2.1 \cdot 4.5 (C_i + 2\Gamma^*)} \quad (2.4)$$

Where C_i is the intercellular CO₂ concentration. J is conversion energy from radiation to mole photon (mole photons MJ⁻¹). The leaf photosynthesis rate ($FGR_{l,t}$) is the function of both $AMAX_{l,t}$ and $EFF_{l,t}$ where $EFF_{l,t}$ is quantum yield [$\mu\text{M CO}_2 \text{ MJ}^{-1}$].

$$FGR_{l,t} = AMAX_{l,t} \left(1 - e^{-I_{l,t} \frac{EFF_{l,t}}{AMAX_{l,t}}} \right) \quad (2.5)$$

Ozone flux calculation

Ozone concentration might be different at top and within the crop canopy and vegetation height (Emberson et al., 2018). In our model, we estimated ozone flux from the top of canopy (sunlit leaves). The ozone conductance $gsO3_t$ [$m\ s^{-1}$] of the sunlit leaves was calculated from sunlit leaves' stomatal conductance for CO_2 [$mol\ m^{-2}\ s^{-1}$] using Equation C1 based on diffusive ratio between CO_2 and O_3 (DIFFO = 0.93) (Ewert and Porter, 2000).

$$gsO3_t = gs_t * DIFFO * 1000/41000 \quad (2.6)$$

Leaf surface resistance ($rO3_t - s\ m^{-1}$) to ozone was calculated based on the cuticle ($G_{cuticle} - m\ s^{-1}$) and stomatal conductance $gsO3_t$ through Equation 2.8 where the $G_{cuticle}$ was assumed the same for sunlit leaf as $1/2500$ [$m\ s^{-1}$] (Mills et al., 2017).

$$rO3_t = 1/(G_{cuticle} + gsO3_t) \quad (2.8)$$

The ozone concentration at the canopy height was converted from ppb to $nmol\ m^{-3}$ using multiplication with 41.56. Ozone flux to the leaf stomata ($OZIF_t - nmol\ m^{-2}\ leaf\ area\ s^{-1}$) was the function of hourly ozone concentration ($OZIH_t$) and the resistance of leaf surface to ozone ($rO3_t$) and boundary layer resistance ($r_b - s\ m^{-1}$).

$$OZIF_t = OZIH_t * gsO3_t * \frac{rO3_t}{r_b + rO3_t} \quad (2.9)$$

The r_b depends on wind speed ($u - m\ s^{-1}$) at given measured height and leaf width ($L - m$). Since the leaf width will be changed during growing season, for the sake of simplification, r_b was assumed constant at 7 [$s\ m^{-1}$].

Ozone stress functions

Following the approach by Ewert and Porter (2000), we distinguished between instantaneous and accumulative effects of ozone exposure. To consider the instantaneous effects on photosynthesis, we assumed that ozone becomes toxic if the ozone flux into the stomata is above a certain threshold. The instantaneous damage factor on photosynthesis (f_{O3t} , [-]) was calculated hourly for sunlit leaves. The f_{O3t} was set to 1 if ozone uptake is low and decreased linearly with increasing instantaneous ozone flux $OZIF_t$ based on two instantaneous ozone damage coefficients γ_1 [-] and γ_2 [$(nmol\ O_3\ m^{-2}\ s^{-1})^{-1}$] (Equation 2.11, 2.12 and 2.13). The γ_1 / γ_2 [$nmol\ O_3\ m^{-2}\ s^{-1}$] allows for low ozone concentrations to be detoxified without direct effects on the photosynthetic system.

$$f_{O3t} = 1 \quad \text{for } OZIF_t \leq \gamma_1/\gamma_2 \quad (2.10)$$

$$f_{O3t} = 1 + \gamma_1 - \gamma_1 * OZIF_t \quad \text{for } \gamma_1/\gamma_2 < OZIF_t \leq (1 + \gamma_1)/\gamma_2 \quad (2.11)$$

$$f_{O3t} = 0 \quad \text{for } OZIF_t \geq (1 + \gamma_1)/\gamma_2 \quad (2.12)$$

In our modelling work, we assumed that the onset of leaf senescence was characterized via a cumulative ozone flux threshold (C_{LAO3} , [mmol m^{-2}]). Above this C_{LAO3} , the rate of green leaf area loss increases linearly (brown leaf is increased while green leaf is decreased). The leaf area loss per soil area unit due to ozone ($DLAI_{O3}$, [-]) was estimated based on the daily rate of leaf area loss $dDLAI_{O3}/dt$ (Equation 2.14).

$$\frac{dDLAI_{O3}}{dt} = f_{LA} * \text{MaxO3Se} * LAI \quad (2.14)$$

Where LAI [-] is leaf area index. MaxO3Se [d^{-1}] is the maximum rate of the leaf area loss due to ozone. f_{LA} is a factor accounting for the effects of ozone on the rate of leaf area loss. f_{LA} increases linearly with the increase of the cumulative ozone flux (C_{O3}) towards the completion of leaf senescence with the coefficient (γ_4 , [$(\text{mmol m}^{-2})^{-1}$]):

$$f_{LA} = \max(\min(\gamma_4 * (C_{O3} - C_{LAO3}), 1), 0) \quad (2.15)$$

Where cumulative ozone flux (C_{O3} , [mmol m^{-2}]) was calculated as in Equation D4:

$$C_{O3} = \int_{t_1}^{t_2} OZIF_t * dt \quad (2.16)$$

Where t_1 and t_2 are the time start and end of ozone fumigation, respectively. The green leaf area ($GLAI$) was calculated by subtracting the leaf area loss due to ozone by equation 2.17:

$$\frac{dGLAI}{dt} = \frac{dLAI_{gl}}{dt} - \frac{dDLAI_{O3}}{dt} \quad (2.17)$$

Where $dLAI_{gl}/dt$ is daily green leaf area change rate after considering effects of shading, aging, and water stress on leaf growth after anthesis. Finally, in our model, we considered the effect of leaf senescence on photosynthesis via the factor (f_{LS} , [-]). This factor was based on a coefficient (γ_3 , [$(\text{mmol m}^{-2})^{-1}$]) which characterizes the slope of a linear relationship between photosynthesis and a cumulative ozone flux threshold (C_{LSO3} , [mmol m^{-2}]) (Equation 2.18).

$$f_{LS} = 1 - \max(\min(1, (\gamma_3 * (C_{O3} - C_{LSO3})), 0) \quad (2.18)$$

For parameterization of instantaneous and accumulative effects on photosynthesis, we employ the function $\min(f_{O3t}, f_{LS})$ which is used in Equation 2.3). The instantaneous effects might become significant in the case of acute and high ozone concentration exposure ($f_{O3t} < f_{LS}$). When wheat plants are exposed to low ozone for prolonged periods, ozone induced leaf senescence resulted in a considerable reduction of

photosynthetic capacity (Feng et al., 2011). The f_{LS} comes into operation ($f_{LS} < f_{O3t}$) when $C_{O3} > C_{LSO3}$.

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