AgroC

- A model for the simulation of carbon fluxes in agricultural ecosystems -

Documentation
Version 1.0

12 June 2019

Introduction

AgroC is a coupling between the SOILCO2/RothC model developed by Herbst et al. (2008) and the SUCROS model for crop growth (Spitters et al., 1989). The SOILCO2/RothC model simulates water, heat, and CO_2 flux in a soil column as well as the source term of heterotrophic respiration over soil depth and time, which is given by the turnover of depth-specific carbon pools (Coleman and Jenkinson, 2008; Šimůnek and Suarez, 1993; Šimůnek et al., 1996). The carbon turnover rate modifiers in turn are calculated according to the one-dimensional profiles of soil water content and temperature. This coupling concept was validated in several laboratory and field studies (Bauer et al., 2008, 2012; Herbst et al., 2008; Palosuo et al., 2012; Weihermüller et al., 2009). The extension of this coupled model with SUCROS was expected to allow for an improved simulation of the soil autotrophic respiration source term, since the temporal development of root growth and the related growth and maintenance respiration is simulated by SUCROS in a mechanistic way. Further, this allows to close the one-dimensional carbon balance and to estimate NEE, since carbon assimilation as well as organ-specific growth and maintenance respiration can be estimated.

The coupled SOILCO2/RothC model allows for the use of any user-specified length and time unit, whereas the SUCROS module uses fixed units. For the AgroC model we preserved the flexibility in terms of length ([L]) and time units ([T]), but we kept the fixed mass and area unit (kg, ha) of the original SUCROS code. The mass unit of the AgroC output carbon fluxes is mol CO_2.For a documentation related to all processes related to the original SoilCO2 model the user is referred to to Simunek et al. (1996). For plant growth as implemented in SUCROS the reader is referred to the WAVE manual (Vancloster et al., 1995) The following topics are documented here since modifications were performed or process sub-modules were added:

1. Hourly time step
2. Water fluxes

3. Carbon fluxes
4. Maintenance and growth respiration
5. Root exudation and root decay
6. Grassland
7. Root water uptake according to Couvreur
8. Photosynthesis according to the big leaf approach (Farquhar)
9. Solar induced fluorescence SIF
10. CO_2 diffusion coefficients

1. Hourly Time Step

The SOILCO2/RothC model can handle any time step, however the original SUCROS explicitly runs at a daily time step. Since particularly NEE exposes distinct diurnal variations, the SUCROS code was adopted to handle hourly time steps, except for the calculation of development stage DVS (-), for which the original parameterization, based on the effective temperature sum, was retained. In the original SUCROS approach the daily total gross assimilation is obtained by three point Gauss integration of the instantaneous assimilation rates per unit leaf area over the daylight period. This could be omitted for the hour model, for which the hourly gross assimilation is computed from the hourly average inputs of global radiation and mean temperature, based on the same approach that was originally used for the instantaneous assimilation rate. Major changes were, however, required for the estimation of the photosynthetic active radiation (PAR) flux at the top of the canopy. In the original code the instantaneous PAR (W $[L]^{-2}$) is estimated in dependence of *sinB* (-), the sine of solar inclination, and *dsinBE* (-), the daily integral of *sinB* including a correction of lower atmospheric transmittance at lower solar elevation. In the original day model the integral daily value *dsinBE* is approximated and *sinB* is estimated for the day of the year in dependence of the geographic position. For the hourly time steps, the integral of the sine of solar inclination *dsinB* is now calculated according to:

$$dsinB = sinB * 3600 \quad (1)$$

where 3600 is the number of seconds in one hour, instantaneous *sinB* (= $\sin(\delta)\sin(\varphi) + \cos(\delta)\cos(\omega)\cos(\varphi)$) is the sine of solar elevation, δ (°) is the sun declination angle, φ (°) is the geographic latitude and ω (°) is the hour angle. The value of *dsinBE* is then estimated as:

$$dsinBE = \sin(\arcsin(sinB) + 0.4\, sinB) * 3600 \quad (2)$$

where 0.4 is the regression coefficient between transmission and solar angle (Supit et al., 1994).

2. Water Fluxes

In terms of water fluxes, the coupling between SOILCO2 and SUCROS mainly covers two processes: rainfall interception and root water uptake. The interception loss is estimated according to the concept of an overflowing bucket (Rutter et al., 1971). For the estimation of canopy interception storage capacity S_i ([L]) at hourly time steps, it was assumed that S_i is proportional to the total leaf area index LAI ([L^2 L^{-2}]) with $S_i = 0.2 \cdot LAI$. Water is removed from the interception storage by evaporation E_i ([L T^{-1}]):

$$E_i = \left(ET_{p,crop} - E_p\right)\frac{C_i}{S_i} \quad (3)$$

where C_i ([L]) represents the interception storage at a certain time step, $ET_{p,crop}$ ([L T^{-1}]) is the potential crop evapotranspiration, and E_p ([L T^{-1}]) is the potential soil evaporation. The amount of interception N_i ([L T^{-1}]) is then estimated according to:

$$N_i = \begin{cases} 0 & \text{for } N_0 = 0 \\ S_i - C_i & \text{for } S_i - C_i < N_0 \\ N_0 & \text{for } S_i - C_i > N_0 \end{cases} \quad (4)$$

where N_0 ([L T^{-1}]) represents the precipitation. Finally, the amount of precipitation entering the soil N_p ([L T^{-1}]) is calculated as the difference between N_0 and N_i.

In SUCROS $ET_{p,crop}$ is computed by scaling the potential grass reference evapotranspiration (Penman-Monteith approach; Allen et al., 1998) with the dimensionless crop conversion factor K_c. On the basis of Beer's law, $ET_{p,crop}$ is split into potential soil evaporation E_p ([L T^{-1}]) and potential transpiration T_p ([L T^{-1}]) in dependence of the *LAI*:

$$E_p = ET_{p,crop} \exp(-0.6 \cdot LAI) \quad (5)$$

$$T_p = ET_{p,crop} - E_p - E_i \quad (6)$$

The potential soil evaporation is passed to the water flux routine, where it prescribes the potential upward water flux for the upper boundary condition. Potential transpiration is distributed over the soil depth according to the relative root density distribution to provide the potential sink term of root water uptake over soil depth. The depth-specific actual root water uptake is computed by scaling the potential root water uptake with the reduction factor α (-) in dependence of soil pressure head h ([L]) following the approach of Feddes et al. (1978):

$$\alpha(h) = \begin{cases} \frac{h_0 - h}{h_0 - h_1} & h_0 \le h \le h_1 \\ 1 & \text{for} \quad h_1 \le h \le h_2 \\ 10^{\frac{h_2 - h}{h_3}} & h_2 \le h \le h_3 \end{cases} \quad (7)$$

where h_0, h_1, h_2, and h_3 ([L]) are prescribed threshold pressure heads (Vanclooster et al., 1995), which are plant dependent. Integrating the actual root water uptake over depth provides the actual transpiration T_a ([L T^{-1}]). The reduction of stomatal conductance due to water stress was assumed to correspond to the ratio between actual and potential transpiration T_a/T_p.

3. Carbon Fluxes

In this study the atmospheric convention is used. Downward carbon fluxes from the atmosphere to the ecosystem are defined as negative fluxes, and upward fluxes are positive. The water stress ratio (T_a/T_p) is subsequently used to scale down gross carbon assimilation and to account for the effect of limited soil water availability on crop activity in terms of the negatively defined gross primary productivity *GPP* (mol CO_2 $[L]^{-2}$ $[T]^{-1}$):

$$GPP = -\frac{G_{phot}}{Mol_{CH_2O}} \cdot \frac{T_a}{T_p} \tag{8}$$

where G_{phot} (kg CH_2O $[L]^{-2}$ $[T]^{-1}$) is the glucose equivalent of the total gross assimilation per time step (Spitters et al., 1989), and Mol_{CH_2O} is the molar mass of CH_2O (= 0.030 kg mol^{-1}). The net primary productivity *NPP* (mol CO_2 $[L]^{-2}$ $[T]^{-1}$) is defined as:

$$NPP = GPP + R_{gr} + R_m \tag{9}$$

where R_{gr} (mol CO_2 $[L]^{-2}$ $[T]^{-1}$) is the total growth respiration, and R_m (mol CO_2 $[L]^{-2}$ $[T]^{-1}$) is the maintenance respiration. Net ecosystem exchange *NEE* (mol CO_2 $[L]^{-2}$ $[T]^{-1}$) is finally computed as:

$$NEE = NPP + R_h \tag{10}$$

where R_h (mol CO_2 $[L]^{-2}$ $[T]^{-1}$) is the depth-integral of the heterotrophic CO_2 source term provided by the RothC module.

4. Maintenance and Growth Respiration

In a first step, the total maintenance respiration demand at 25°C $R_{m,r}$ (kg CH_2O $[L]^{-2}$ $[T]^{-1}$) is computed as a glucose equivalent according to:

$$R_{m,r} = \sum_{o=1}^{4} f_{m,o}\, W_o\, f_t \tag{11}$$

where $f_{m,o}$ (kg CH_2O kg^{-1} DM $[T]^{-1}$) is the maintenance coefficient with index o looping over the four plant organs leaves, stems, roots, and storage organs with values of 0.03, 0.015, 0.015, and 0.01, respectively (Spitters et al., 1989). W_o (kg DM $[L]^{-2}$) is the respective organ dry weight and f_t (-) is a time conversion factor accounting for the either hourly or daily time step. In the next step, $R_{m,r}$ is corrected for temperature to estimate total maintenance respiration $R_{m,c}$ (kg CH_2O $[L]^{-2}$ $[T]^{-1}$) as described by Spitters et al. (1989). In a last step, the CO_2 equivalent maintenance respiration R_m (mol CO_2 $[L]^{-2}$ $[T]^{-1}$) is computed as the quotient of $R_{m,c}$ and Mol_{CH_2O}.

Total growth respiration rate R_{gtot} (kg CH_2O $[L]^{-2}$ $[T]^{-1}$), again as the glucose equivalent, is estimated as:

$$R_{gtot} = \left(G_{phot} \cdot \frac{T_a}{T_p} - R_{m,c}\right) - \Delta W \cdot C_{cont} \cdot \frac{Mol_{CH_2O}}{Mol_C} \tag{12}$$

where ΔW is the overall dry matter growth rate (kg DM $[L]^{-2}$ $[T]^{-1}$), C_{cont} (g C g^{-1} DM) is the conversion factor between carbon and biomass dry matter weight, and Mol_C is the molar mass of C (= 0.012 kg mol^{-1}). Growth respiration for each plant organ $R_{gr,o}$ (mol CO_2 $[L]^{-2}$ $[T]^{-1}$) is computed from R_{gtot} according to:

$$R_{gr,o} = \frac{R_{gtot} \cdot f_o}{Mol_{CH_2O}} \tag{13}$$

where index *o* loops over the plant organs, and f_o (-) is the organ-specific partitioning factor also used to compute the organ-specific growth rate. Total growth respiration R_{gr} (mol CO_2 $[L]^{-2}$ $[T]^{-1}$) is finally computed as the sum of all $R_{gr,o}$. The sum of maintenance and growth respiration of the roots represents the autotrophic source term of soil CO_2 and was distributed over profile depth according to the time-variable relative root density distribution over depth.

5. Root Exudation and Root Decay

In SUCROS the daily or hourly glucose assimilation rate G_{phot} (kg CH_2O $[L]^{-2}$ $[T]^{-1}$) is partitioned in dependence of the DVS into the fraction for the shoot and for the root system to build up biomass. According to the labelling experiments performed by Swinnen et al. (1995) for winter wheat, 18.2% of the net assimilation are transferred to the roots, 7.1% are used to build up root biomass, and 5.3% are released as young photosynthetate rhizodeposition. In relation to the amount transferred to the roots this translates into relative fractions of 0.39 and 0.29 for root biomass and exudates, respectively,. The relative root exudation fraction f_{exu} (-) thus equals 0.43 (= 0.29 / (0.39 + 0.29)) for winter wheat. In AgroC the root exudation rate Rt_{exu} (kg C $[L]^{-2}$ $[T]^{-1}$) is computed according to the above-mentioned constant partitioning factor from the dry matter root growth rate (kg DM $[L]^{-2}$ $[T]^{-1}$):

$$Rt_{exu} = \Delta W \cdot f_{rt} \cdot f_{exu} \cdot 0.467 \qquad (14)$$

where f_{rt} is the dimensionless partitioning coefficient for roots, and 0.467 kg C kg^{-1} DM is the root-specific dry matter carbon content (Goudriaan et al., 1997). This way, the root exudation shows diurnal variations in the simulations due to the assimilation rate as suggested by, e.g., Hopkins et al. (2013) and Kuzyakov (2006). Please note that the description of root exudation

as documented above was implemented this way for all plant types when switched on (rootExudation=t). The relative root exudation fraction f_{exu} can be specified for each plant type in 'plants.in' at line 25.

Swinnen et al. (1995) also determined that 3.1% of the net assimilation ends up as dead roots. In relation to 18.2% transferred to the roots, this equals a relative fraction of 0.17. In order to account for the process of root death (rootDeath=t), the root death factor f_{dea} (-) was introduced. The basic assumption is that during the crop juvenile stages the root death rate is lower than at flowering:

$$f_{dea} = \begin{cases} 0 & DVS < 0.2 \\ \frac{f_{deamax}(DVS-0.2)}{0.5-0.2} & \text{for} \quad 0.2 \leq DVS \leq 0.5 \\ f_{deamax} & DVS > 0.5 \end{cases} \tag{15}$$

where f_{dea} is the death fraction in relation to the total amount of roots, and f_{deamax} (-) is the maximum value of the root death fraction (specified in line 26 of 'plants.in'). For the winter wheat model runs a f_{deamax} of 0.43 was used, which approximately reproduced the cumulative fraction of dead roots of 0.17 of net assimilation determined by Swinnen et al. (1995). Please note that root death is only implemented for winter wheat, summer wheat, barley and grassland. The rate of root death in terms of carbon release Rt_{dea} (kg C $[L]^{-2}$ $[T]^{-1}$) is computed as:

$$Rt_{dea} = \Delta W \cdot f_{rt} \cdot f_{dea} \cdot 0.467 \tag{16}$$

The root dry matter growth rate is reduced according to the loss of root exudates and dead roots. The total amount of root exudates and dead roots is, analogous to root respiration, distributed over depth according to the relative root density profile. The carbon equivalent of

root exudates is transferred to the depth-specific decomposable plant material pool (DPM) of the RothC subroutine, in order to reflect the rapid decomposition of these labile substances by rhizosphere microorganisms, whereas the dead root carbon is split into the DPM pool and the resistant plant material pool (RPM) according to the original partitioning for incoming plant material of 0.59 and 0.41 (Coleman and Jenkinson, 2008), respectively.

For winter wheat and barley harvest residues can be considered in the simulation. At harvest the existing root biomass and 25% of the stem biomass is added to the DPM and RPM pool up to a user-specified soil depth, i.e., ploughing depth. Figure 1 shows a schematic representation of the carbon cycling in AgroC.

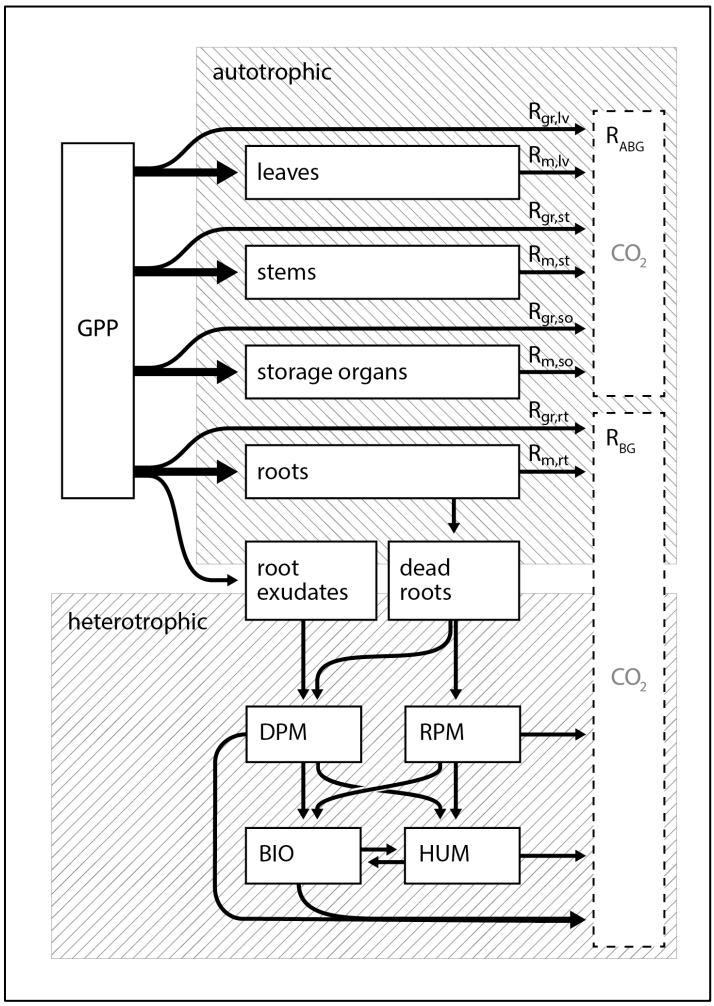

*Fig. 1:*Carbon fluxes and partitioning in AgroC. Gross primary production (GPP) is partitioned to the different plant organs, leaves (subscript lv), stems (st), storage organs (so), and roots (rt), whereat CO_2 is lost due to growth (R_{gr}) and maintenance respiration (R_m). The sum of these autotrophic CO_2 source terms by the shoot organs account for the above-ground respiration (R_{ABG}). Carbon or CO_2,

respectively, is added to the soil profile by the autotrophic root respiration, root exudates, and dead roots. The latter two are transferred to the decomposable and resistant plant material pool (DPM, RPM) of the RothC model and decomposed. The heterotrophic CO_2 source term consists of the microbial decomposition of those and further soil organic matter pools (humified organic matter (HUM), microbial biomass (BIO)). The root respiration and the heterotrophic components are part of the below-ground respiration (R_{BG}).

6. Grassland

The original SUCROS code is not capable of simulating managed grassland, characterized by multiple mowing events over the season. Mowing initiates the transfer of glucose from the roots and the stubble to the remaining leaves, which allows for a faster compensation of defoliation. The routines implemented in AgroC for the simulation of the above-mentioned processes follow to some extent the sink/source approach suggested by Schapendonk et al. (1998) for the grassland productivity model LINGRA.

At prescribed mowing dates the current green leaf area index LAI_g is set to a fixed post-mowing leaf area index LAI_{post} of 0.35. The ratio between the pre-mowing LAI and post-mowing LAI_{post} is used to compute the respective loss of dry matter biomass:

$$f_{lai} = \frac{LAI_g}{LAI_{post}} \tag{17}$$

$$w_{post,i} = \frac{w_{pre,i}}{f_{lai}} \tag{18}$$

where f_{lai} (-) is the pre-/post-mowing LAI ratio, w_{pre} (kg DM $[L]^{-2}$) is the biomass prior to mowing, and w_{post} (kg DM $[L]^{-2}$) is the respective biomass after mowing. Index i loops over leaves, stems, and storage organs/inflorescence. At each mowing event DVS is also reset to a prescribed value of $DVS_{reset} = 0.5$. In order to simulate the transfer of glucose after defoliation, we implemented a glucose storage, which is filled between a DVS_{lo} of 0.6 and a DVS_{hi} of 1.0. The rate of glucose storage increase λ_{s+} (kg CH_2O $[L]^{-2}$ $[T]^{-1}$) is computed as a fraction f_{stor} (-) of global net glucose production:

$$\lambda_{s+} = \left(G_{phot} \cdot \frac{T_a}{T_p} - R_{m,c}\right) \cdot f_{stor} \tag{19}$$

The part of global net glucose production (= $G_{phot} \cdot T_a/T_p - R_{m,c}$) available for biomass growth and respiration is reduced accordingly by λ_{s+}. The storage fraction is computed in dependence of DVS:

$$f_{stor} = \begin{cases} 0 & DVS \leq DVS_{lo} \\ \frac{f_{stormax}(DVS - DVS_{lo})}{(DVS_{hi} - DVS_{lo})} & \text{for} \quad DVS_{lo} < DVS < DVS_{hi} \\ f_{stormax} & DVS \geq DVS_{hi} \end{cases} \tag{20}$$

where $f_{stormax}$ (-) is the user-specified maximum storage fraction. Thus, the glucose storage $S_{stor,t}$ (kg CH_2O $[L]^{-2}$) increases by λ_{s+} until a user-defined maximum value of $S_{stormax}$ (kg CH_2O $[L]^{-2}$) is reached and $S_{stor,t}$ remains constant. After mowing the glucose storage is emptied, assuming an exponential decay over time. The release of dry matter transfer rate λ_{s-} ($[T^{-1}]$) from $S_{stor,t}$ to the shoot is estimated as:

$$\lambda_{s-} = \frac{\log(100)}{t_{stor}} \tag{21}$$

where t_{stor} ([T]) is the user-specified time required to reach a value of 1% of the storage at the time of the mowing event. According to Gonzales et al. (1989) and Prud'homme et al. (1992) the mobilization of carbohydrates in ryegrass is highest during the first 6 days after defoliation and levelled out in a second phase, 6 to 29 days after cutting. As a default value, t_{stor} could be set to 15 days, equivalent to a λ_{s-} rate of 0.31 d^{-1}.

The additional dry matter growth rate ΔW_{stor} (kg DM $[L]^{-2}$ $[T]^{-1}$) resulting from the declining $S_{stor,t}$ is added to the dry matter growth rate of the shoot $\Delta W_{sh,}$ (kg DM $[L]^{-2}$ $[T]^{-1}$), which is the outcome of the photosynthetic activity of the plant. The additional shoot growth rate ΔW_{stor} is computed as:

$$\Delta W_{stor} = \frac{S_{stor,t}\ \lambda_{s-}}{f_{sh}\,(1.46\,f_{lv} + 1.51\,f_{st})} \tag{22}$$

where f_{sh}, f_{lv}, and f_{st} are the dimensionless partitioning factors for shoot, leaves, and stems, respectively. The assimilate requirement coefficients 1.46 and 1.51 have a unit of kg CH_2O kg^{-1} DM (Spitters et al., 1989). Correspondingly, $S_{stor,t}$ is reduced down to a limiting value of zero according to:

$$S_{stor,t+1} = S_{stor,t}\,(1 - \lambda_{s-}) \tag{23}$$

As suggested by Schapendonk et al. (1998) a mechanism was implemented by which the specific leaf area (ha leaf kg^{-1} DM) varies over the season as a function of DVS. Further, as suggested by Barrett et al. (2004) a mechanism to distinguish between vegetative and reproductive development of grass was appended. Those two stages of development differ in the productivity of the grass crop and in several major physiological processes, which alter the response of the plant to environmental drivers (e.g., Anslow and Green, 1967; Leafe et al., 1974; Parsons, 1988; Robson et al., 1988).

7. Root water uptake according to Couvreur

Alternatively to the Feddes approach, root water uptake can be simulated according to the approach of Couvreur et al. (2012) by setting waterstress=3 in the 'plants.in' input file. The weighted average total head in the root zone H_s (L) is computed as:

$$H_s = \sum_{j=1}^{n} RRD_j * H_j \tag{24}$$

where *RRD* is the relative root length density at node *j* [-] and *H* is the corresponding total hydraulic head (equal to *h*+*z*) and the entire soil profile is discretized into *n* nodes. The hydraulic head at the collar of the plant H_{col} is estimated at every time step as

$$H_{col} = -\frac{|T_p|}{K_{rs}} + H_s \tag{25}$$

where K_{rs} [cm^3 cm^{-3} T^{-1}] is the root system conductance and T_p [L T^{-1}] is potential transpiration. A threshold at the root collar H_{xmin} [L] is introduced (usually set to -16000 cm) and for $H_{col}<H_{xmin}$ the value of H_{col} is set equal to H_{xmin} and the actual transpiration T_a [L T^{-1}] is computed as:

$$T_a = K_{rs} * Max(0, H_s - H_{col}) \quad for\ H_{col} < H_{xmin} \tag{26}$$

For $H_{col} \geq H_{xmin}$ T_a is equal to T_p. Finally, the root water uptake in terms of the sink term *S* [T^{-1}] at node *j* is defined as:

$$S_j = \frac{RRD_j * \left(T_a + K_{comp} * (H_j - H_s)\right)}{dz_j} \tag{27}$$

where K_{comp} is the compensatory root conductance [T^{-1}] and *dz* [L] is the layer thickness related to node *j*.

8. Photosynthesis according to the big leaf approach (Farquhar)

The big leaf approach of Farquhar et al. (1980) as extended by Collatz et al. (1992) for C4 plants can be used alternatively to estimate photosynthesis (set farquhar=t in 'plants.in'). The atmospheric pressure P_{atm} [Pa], the ambient CO_2 partial pressure c_s [Pa], the oxygen partial

pressure o_i [Pa], the CO_2 partial pressure at compensation point Γ_* [Pa], the maxiumum rate of carboylation V_{cmax} [μmol CO_2 m^{-2} s^{-1}] and the leaf internal CO_2 partial pressure c_i [Pa] are required to estimate photosynthesis. Further, quantum efficiency α was set to 0.06 μmol CO_2 μmol photons^{-1} for C3 plants and it was assumed to be 0.04 μmol CO_2 μmol photons^{-1} for C4 plants. (Note: For the units the area ('m^2') in this section always refers to the leaf area.)

Ambient CO_2 partial pressure c_s [Pa] is computed from the constant atmospheric CO_2 concentration and P_{atm} (both provided in the selector.in). O_2 partial pressure is calculated as $o_i=0.209*P_{atm}$.

In order to estimate the compensation point CO_2 partial pressure a Michaelis-Menten type approach is applied. The Michaelis-Menten constants K_c [Pa] and K_o [Pa], for CO_2 and O_2 respectively, are given as:

$$K_c = K_{c25}(a_{kc})^{\frac{t_a-25}{10}} \quad (28)$$

$$K_o = K_{o25}(a_{ko})^{\frac{t_a-25}{10}} \quad (29)$$

where K_{c25}=30 Pa and K_{o25}=30000 Pa at 25°C and a_{Kc}=2.1 and a_{Ko}=1.2, representing the relative change in K_{c25} and K_{o25} for a 10°C change of ambient temperature t_a. The compensation point CO_2 partial pressure [Pa] is subsequently estimated as:

$$\Gamma_* = 0.5 * \frac{K_c}{K_o} * 0.21 * o_i \quad (30)$$

In order to estimate V_{cmax}, first the temperature sensitivity factor $f(t_a)$ has to be estimated according to:

$$f(t_a) = \left[1 + exp\left(\frac{-220000+710*(t_a+t_f)}{0.001*R_{gas}*(t_a+t_f)}\right)\right]^{-1} \quad (31)$$

where t_f [K] is the freezing temperature of water and R_{gas} [J K^{-1} $kmol^{-1}$] represents the universal gas constant. This also accounts for the thermal breakdown of carbon assimilation due to freezing. In the next step V_{cmax} [µmol CO_2 m^{-2} s^{-1}] is computed from $V_{cmacx25}$ [µmol CO_2 m^{-2} s^{-1}] (plant specific input parameter) scaled by $f(t_a)$ [-], root water uptake stress α_{avg} [-] ($=T_a/T_p$) and relative day length $f(DYL)$ [-]:

$$V_{cmax} = V_{cmax25} * (2.4)^{\frac{t_a-25}{10}} * f(t_a) * \propto_{avg} * f(DYL) \quad (32)$$

As implemented in SCOPE, the leaf internal CO_2 partial pressure c_i [Pa] was estimated as:

$$\begin{aligned} c_i &= Maximum\left(\Gamma_*, c_s * \left(1 - 1.6/\left(m * R_h * \alpha_{avg}\right)\right)\right) \quad for\ C3\ plants \\ c_i &= Maximum\left(0.99 * P_{atm}, c_s * \left(1 - 1.6/\left(m * R_h * \alpha_{avg}\right)\right)\right) \quad for\ C4\ plants \end{aligned} \quad (33)$$

where m [-] is the Ball-Berry slope parameter (Collatz et al., 1991; plant specific input parameter) and R_h [-] is the relative humidity (last column in 'atmosph.in').

Photosynthesis A [µmol CO_2 m^{-2} s^{-1}] of C3 plants is finally estimated as:

$$A = Minimum\left(\frac{V_{cmax}*(c_i-\Gamma_*)}{c_i+K_c*(1+o_i/K_o)}, \frac{(c_i-\Gamma_*)*4.6*APAR*\alpha}{c_i+2*\Gamma_*}, V_{cmax} * 0.5\right) \quad (34)$$

whereas the photosynthesis of a C4 plants is finally estimated as

$$A = Minimum\left(V_{cmax}, 4.6 * APAR * \alpha, 4000 * V_{cmax} * \frac{c_i}{P_{atm}}\right) \quad (35)$$

The single terms of the minimum functions represent the RuBP carboxylase limited rate of carboxylation, the light-limited rate and the export limited rate of carboxylation (from left to right).

9. Solar induced fluorescence SIF

SIF was basically estimated following the concept of Lee et al. (2015). The maximum possible electron transport rate J_o [µmol CO_2 m^{-2} s^{-1}] was computed according to

$$J_o = 4.6 * APAR * \alpha \quad (36)$$

where the photosynthetic active radiation APAR [W m^{-2} = J m^{-2} s^{-1}] is scaled with 4.6 µmol photons $Joule^{-1}$ to convert to photosynthetic photon flux and with quantum efficiency α (=0.06 µmol CO_2 µmol $photons^{-1}$ for C3 and =0.04 for C4 plants) to convert to CO_2 flux. The actual electron transport rate J_e of C3 plants is given by

$$J_e = A * \frac{c_i + 2*\Gamma_*}{c_i - \Gamma_*} \quad (37)$$

where A [µmol CO_2 m^{-2} s^{-1}] is the actual photosynthesis rate, c_i [Pa] represents the leaf internal CO_2 partial pressure and Γ_* [Pa] is the CO_2 partial pressure at compensation point. For C4 plants J_e is equal to A. The photochemical quantum yield ϕ_p [-] is estimated from

$$\phi_p = \phi_{po} * \frac{J_e}{J_o} \quad (38)$$

where ϕ_{po} [-] is the efficiency of photochemical trapping in the dark adapted state. According to Björkman and Demmig (1987) the typical value of ϕ_{po} for a healthy plant is 0.8. The rate coefficient of chlorophyll fluorescence k_f is set to 0.05 s^{-1}, whereas the dark adapted rate coefficient k_d [s^{-1}] is estimated in dependence of ambient temperature t_a [°C]:

$$k_d = Maximum(0.03 * t_a + 0.0773, 0.087) \quad (39)$$

The light adapted rate coefficient k_n [s^{-1}] was estimated as

$$k_n = (6.2473 * x - 0.5944) * x \quad (40)$$

where x is equal to $1\text{-}\phi_p/\phi_{po}$. Fluorescence yield ϕ_f [-] is subsequently computed as

$$\phi_f = \frac{k_f}{k_f + k_d + k_n} * (1 - \phi_p) \quad (41)$$

Leaf level sun induced fluorescence F [µmol photons m^{-2} s^{-1}] is

$$F = \phi_f * APAR * 4.6 \quad (42)$$

Following Lee et al. (2015) leaf-level fluorescence can be converted to spectrometer-measured fluorescence at 755 nm F_{755nm} using the conversion factor k which accounts for the integration over all wavelengths in the fluorescence emission spectrum, observing angle and unit conversion from µmol photons m^{-2} s^{-1} to W m^{-2}:

$$F_{755nm} = \frac{F}{k} \quad (43)$$

An empirical step-wise linear relation between k and V_{cmax25} [µmol CO_2 m^{-2} s^{-1}] is finally used to compute the conversion factor (Lee et al., 2015):

$$\begin{aligned} k &= 0.047716 * V_{cmax25} + 7.70092 \quad for \;\; V_{cmax25} \leq 70 \\ k &= 0.032686 * V_{cmax25} + 8.75302 \quad for \;\; V_{cmax25} > 70 \end{aligned} \tag{44}$$

10. CO_2 diffusion coefficients

The diffusion coefficient of CO_2 in the porous system D_a [L^2 T^{-1}] is computed from the temperature dependent CO_2 diffusion coefficient in free air D_{as} [L^2 T^{-1}] and the air-filled porosity θ_a [cm^3 cm^{-3}]. Alternatively to the originally implemented Millington-Quirk approach (iGasdiff=1), the approach of Kristensen et al. (2010) accounting for diffusion in macropores can be applied (set iGasdiff=5):

$$\begin{aligned} D_a &= D_{as} * H * \theta_a && for\ \theta_a < \varepsilon^* \\ D_a &= D_{as} * \left(H * \varepsilon^* + (\theta_a - \varepsilon^*)^{X_m} \left(\frac{\theta_a - \varepsilon^*}{\theta_s - \varepsilon^*} \right) \right) && for\ \theta_a > \varepsilon^* \end{aligned} \tag{45}$$

where H is the macropore tortuosity factor [L L^{-1}], X_m is the matrix tortuosity factor [L L^{-1}], θ_s [cm^3 cm^{-3}] is the water content at saturation (assumed to be equal to porosity) and $\varepsilon*$ is the macropore porosity [cm^3 cm^{-3}]. In relation to Millington-Quirk, this allows for higher diffusion coefficients near water saturation. Three parameters are required as input for each material: ε∗, H and X_m.

Further, diffusion coefficients can be estimated according to Moldrup et al. (2000a, iGasdiff=2) for repacked soils, according to Moldrup et al. (2000b, iGasdiff=3) and according to a double-linear approach (iGasdiff=4).

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