Appendix A1 Documentation for algorithms

In this section, wereviewed and re-documented algorithms of heat and drought stress on biomass production and yield formation with detailed equations for each crop model we have reviewed.The models we reviewed have different levels of documentation support. A few models (e.g. AquaCrop, HYBRID-maize, STICS and SWAT) provide well-organized documentation on theoretical background and detailed algorithms, whereas most of them only have partial documentations on specific modules or narrative descriptions rather than explicit mathematical equations for the algorithms. Therefore we also reviewed model source codes (if publically accessible) as a complementary. It should also be mentioned that inconsistence between documentations and the implementation happened occasionally. In this case, we prioritized the actual source code over literatures and documentations. The algorithms documented here can serve as a quick reference for or a gateway to the heat and drought stress algorithms implemented in major crop models.

A1.1 Agro-IBIS

Major documentation

https://lter.limnology.wisc.edu/project/agro-ibis

Introduction

Agro-IBIS is an adaptation of IBIS to the agro-ecosystem by Kucharik and Brye (2003). For C3 species, Agro-IBIS uses a widely tested semi-mechanistic model for photosynthesis (Farquhar et al., 1980) and an empirical model for stomatal conductance (Ball et al., 1987).For C4 species, Agro-IBIS uses a coupled model of photosynthesis and stomatal conductance (Farquhar & Sharkey, 1982; Collatz et al., 1992).

C4 photosynthesis model

The following is the original version of C4 photosynthesis model.

The relationships between limiting steps and the rate of net photosynthesis (A_n) for the simplified model can be expressed as a combination of quantum limit (J_i), CO2 limit (J_c) and rubisco enzyme limit (J_e):

$$A_n \approx min\begin{Bmatrix} J_i, f(\alpha, Q_p) \\ J_c, f(p_i, K, T_l) \\ J_e, f(V_{max}, T_l) \end{Bmatrix} - R_d, f(T_l)$$

where the parameters' definition are given by:

Table 2. Parameters used in the simplified C_4 photosynthesis model

Name	Symbol	Equation	Value (Q_{10})
Initial slope of photosynthetic CO_2 response	k	6	$0{\cdot}7$ mol m^{-2} s^{-1} (2)
Maximum rubisco capacity	V_{max}	6	39 μmol m^{-2} s^{-1} (2)
Initial slope of photosynthetic light response	α	6	$0{\cdot}04$ mol m^{-1}
Leaf respiration	R_d	6	$0{\cdot}8$ μmol m^{-2} s^{-1} (2)
Stomatal slope factor	m	1	$3{\cdot}0$
Stomatal intercept factor	b	1	$0{\cdot}08$
Atmospheric pressure	P	1	10^5 Pa
Curvature parameter	θ	2B	$0{\cdot}83$
Curvature parameter	β	3B	$0{\cdot}93$

The quantum yield of C3 photosynthesis is dependent on temperature, O2 and CO2 partial pressures, which is not the case for C4 plants. But leaves of C4 plants may show variable photosynthetic responses depending upon the light intensity for growth, nitrogen nutrition or drought stress. These variations can generally be accommodated by adjusting the parametersV_{max} , k and $R_d$of Collatz's model.

The C4 leaf model is derived from the following equations that define the three unknowns, stomatal conductance (g), net photosynthesis (A_n) and the partial pressure of CO2 in the intercellular spaces of the leaf (p_i).

The stomatal conductance is given by:

$$g = m\frac{h_s A_n P}{p_s} + b$$

whereh_s is the leaf surface relative humidity.

Gross photosynthesis (A) is given as a function of incident quantum flux density (Q_p) and the intercellular partial pressure of CO2 (p_i) and leaf temperature (T_l) in the form of a pair of nested quadratic equations, such that:

$$\begin{cases} \theta M^2 - M(V_T + \alpha Q_p) + V_T \alpha Q_p = 0 \\ \beta A^2 - A\left(M + \frac{k_T p_i}{P}\right) + \frac{M k_T p_i}{P} = 0 \end{cases}$$

Net photosynthesis is defined as:

$$A_n = A - R_T$$

The temperature dependence of V_{max} , k and R_d are given as Q_{10} function:

$$V_T = \frac{V_{max}\, Q_{10}^{\frac{T_l - 25}{10}}}{(1 + e^{0.3\cdot(13 - T_l)})(1 + e^{0.3\cdot(T_l - 36)})}$$

$$R_T = \frac{R_d Q_{10}^{\frac{T_l - 25}{10}}}{1 + e^{1.3\cdot(T_l - 55)}}$$

$$k_T = k Q_{10}^{\frac{T_l - 25}{10}}$$

Finally, the partial pressure of CO, in the intercellular spaces is defined as:

$$p_i = p_s - \frac{1.6 A_n P}{g}$$

These equations can be combined to eliminate p_i and g, and solve A_n analytically as given by Appendix C (Collatz et al. 1992).

IBIS usesthis coupled photosynthesis-stomatal conductance model to calculate net photosynthesis of a leaf at the top of the canopy. The net photosynthesis within the canopy is calculated by scaling it proportional to the APAR within it. Canopy

Adaptation to Agro-Ecosystem

Kucharik and Brye (2003) Adapted IBIS to agro-ecosystem, which requires a few modifications.

Temperature stress is now slightly modified as:

$$V_T = \frac{V_{max}\, Q_{10}^{\frac{T_l - 15}{10}}}{(1 + e^{0.4\cdot(10 - T_l)})(1 + e^{0.4\cdot(T_l - 50)})}$$

A **water stress** factor between 0.0(high stress) and 1.0 (no stress) is calculated using the integralof plant-available water content over each soil layer. The contribution of each layer to the overall plant water stress is weighted by the soil layer root fraction. The value for V_{max} (maximumphotosynthetic rate) is adjusted by this stress factorto reduce plant productivity under water stress conditions, such that:

stressfac (sf): ! sensitivity to soil water stress, default value is "-5"
awc (θ), ! available water content (fraction)
znorm ($\bar{\varphi}$), ! normalizing factor
zwilt (φ) ! function of awc, =1 if awc = 1 (no stress)

$$\bar{\varphi} = 1 - e^{sf}$$

For each soil layer (total=8), calculate available water content as:

$$\theta_i = \frac{wsoi_i \times (1 - wisoi_i) - sWilt_i}{sField_i - sWilt_i}$$

And relative water stress (confined to 0~1) as:

$$\varphi_i = (1 - e^{sf \times \theta_i})/\bar{\varphi}$$

Integrate over soil profile with relative root fraction in each layer to get total water stress.

The latest code implementations can be found at: http://www.sage.wisc.edu/download/IBIS/ibis.html

See “physiology.f” for details (Line 744 – Line 1075).

Yield formation

The daily summation of assimilated C is partitioned between leaf, stem, root, or grain, and is dependent on thephysiological age of the plant.

Harvest index is computed at the endof the growing season as the ratio of carbon allocated to grainto total aboveground biomass, and should not exceed 0.61 for maize.

No additional heat or drought stress was implemented.

A1.2 APSIM

Major documentation

https://www.apsim.info/Documentation/Model,CropandSoil/CropModuleDocumentation.aspx

Biomass production

In APSIM, the daily biomass accumulation (ΔB) is the minimum of radiation (ΔB_r) and water (ΔB_w) limited photosynthesis process such that:

$$\Delta B = min\{\Delta B_r, B_w\}$$

The light-driven biomass production is based on the concept of radiation use efficiency (RUE):

$$\Delta B_r = I \times RUE \times min\{f_{T,photo}, f_{N,photo}, f_{P,photo}\}$$

where$I(MJ\ m^{-2})$ is the canopy intercepted radiation, RUE ($g\ MJ^{-1}$)is crop specific and stage dependent constants; $f_{T,photo}$, $f_{N,photo}$ and $f_{P,photo}$ are temperature, nitrogen and phosphors stresses, respectively.

The **temperature stress**, $f_{T,photo}$, is a multi-linear function of the daily mean temperature, and is defined by parameters x_ave_temp and y_stress_photo in the Maize.xml file:

$$f_{T,photo} = \begin{cases} 0, & if\ T_{mean} \leq T_{min}\ or\ T_{mean} \geq T_{max} \\ 1 - \dfrac{T_{opt\,1} - T_{mean}}{T_{opt\,1} - T_{min}}, & if\ T_{min} < T_{mean} < T_{opt\,1} \\ 1, & if\ T_{opt\,1} \leq T_{mean} \leq T_{opt2} \\ \dfrac{T_{max} - T_{mean}}{T_{max} - T_{opt\,2}}, & if\ T_{opt\,2} < T_{mean} < T_{max} \end{cases}$$

For maize, the default setting of temperature threshold parameters is [T_{min}, $T_{opt\,1}$, $T_{opt\,2}$, T_{max}] = [8, 15, 35, 50], which makes the model unresponsive to hot days for the US Midwest. In this study, we modify these parameters according to literatures so that [T_{min}, $T_{opt\,1}$, $T_{opt\,2}$, T_{max}] = [8, 15, 30, 44]

The **water stressed** biomass production is a calculated as:

$$\Delta B_w = \Delta B_r \times \frac{min(W_s,\ W_d)}{W_d}$$

whereW_s are the actual daily soil water uptake as a result of the demand (i.e. potential transpiration) and soil water availability, and W_d is the soil water demand determined by ΔB_r and transpiration efficiency (TE). Specifically:

$$W_d = \frac{\Delta B_r}{TE}$$

Transpiration efficiency is modulated by the vapor pressure deficit (VPD):

$$TE = TE_c/VPD$$

in which TE_c is a constant of 9 Pa for maize when atmospheric CO_2 is 350 ppm. As the calculation of VPD is temperature dependent, a strong interaction between temperature and water stress exits in the model structure.

Yield formation

In the APSIM Maize module, yield formation is based on the grain number and grain filling rate.

The optimum daily grain growth rate (ΔGR_{opt}; $g\ m^{-2}$) is:

$$\Delta GR_{opt} = GNum \times Rp$$

Where $GNum$ is the grain number, and Rp is the cultivar specific potential rate of grain filling (normally between 8-10 mg per grain per day).

The actual grain number, $GNum$, is limited by a factor, $temp\_fac$, describing the cumulative temperature above 38 °Cbetween flag leaf and start of grain filling:

$$temp\_fac = 1 - \left[\sum_{stage=flag\_leaf}^{start\_of\_grain\_fill} T_{mean}, i - 38\right] \times C_{htstress}$$

where$C_{htstress}$ is coefficient for conversion of heat stress during flowering to heat stress factor on grain number development, and is set as 0.05.

The actual grain growth (ΔGR_{actual}) is:

$$\Delta GR_{actual} = min\{\Delta GR_{opt} \times f_{stress,g}, \quad \Delta GR_{max}\}$$

where the stress factor ($f_{stress,g}$) the product of temperature stress ($rgfill$) and water stress ($\frac{W_s}{W_d}$), and ΔGR_{max} is the maximum daily grain growth determined by the availability of biomass storage and nitrogen.

$rgfill$has a multi-linear function in a similar structure of $f_{T,photo}$, and is constrained by x_temp_grain and y_grain_rate.For $x_{temp_{grain}} = [6.0, 10, 16, 22, 30, 56.3]$, $y_{grain_{rate}} = [0.0, 0.40, 0.75, 1.0, 1.0, 0.0]$. Other values can be linearly interpolated. It should be noted that $rgfill$ is calculated every 3-hours, and then averaged to the daily mean value.

Other stress events

- If the crop hasn't germinated within 40 days of sowing, due to lack of germinating moisture, all plants are killed.
- If cumulative phenological water stress exceed 25, all plants are killed due to water stress prolonging phenology.
- A fraction of plants will be killed by high temperatures immediately following emergence.
- A fraction of plants (0.044) will be killed each day due to water stress once the cumulative water stress factor for photosynthesis exceeds 4.6.

A1.3 AquaCrop

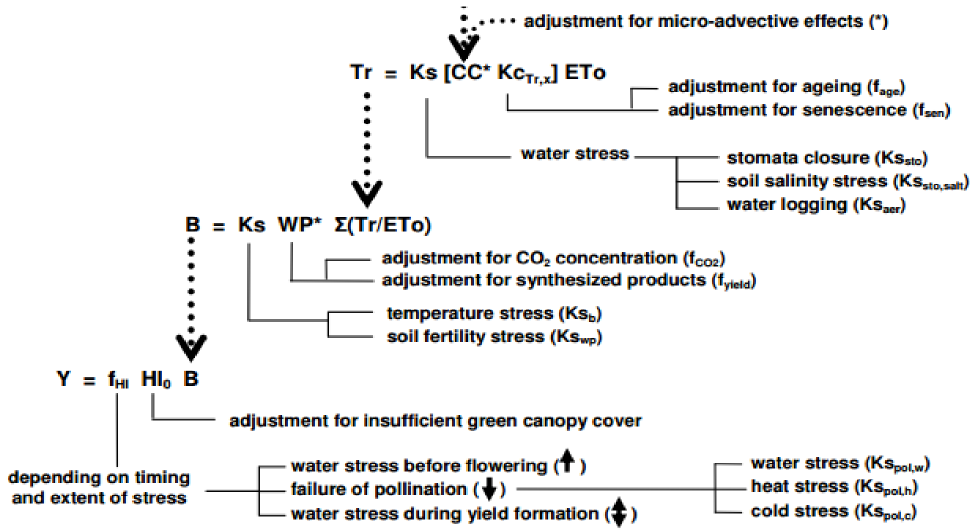
Majordocumentation

http://www.fao.org/nr/water/docs/AquaCropV40Chapter3.pdf

http://www.fao.org/nr/water/docs/AquaCropV40Annexes.pdf

Introduction

AquaCropsimulates crop yield based on the consumption of soil water, and adjusted the process with a range of environmental stresses during different growth stages (Steduto et al., 2009). See the schematic diagram below (re-drawn from AquaCrop V4.0 Chapter 3):



General stress response function

Use convex curve to make a process affected more strongly when water stress becomes severe.

$$Ks = 1 - \frac{exp^{S_{rel} \cdot f_{shape}} - 1}{exp^{f_{shape}} - 1}$$

S_{rel} is relative stress by projecting soil water depletion. The larger f_{shape} is, the more convex the curve will be.

Use logistic shape curve to describe temperature stress.

$$Ks = \frac{S_L S_U}{S_L + (S_U - S_L) exp^{-r(1-S_{rel})}}$$

where$S_L = 0.001$, $S_U = 1$, S_{rel} is relative stress by projecting temperature to the $[T_{min}, T_{max}]$ range; solve r by setting $Ks = S_{rel} = 0.5$.

Biomass production

The daily (dm) and cumulative (B) aboveground biomass production:

$$dm = Ks_b \times WP^* \left(\frac{Tr}{ET_0}\right)$$

$$B = Ks_b \times WP^* \sum \left(\frac{Tr}{ET_0}\right)$$

where Ks_b is stress coefficient when air temperature is too cold; WP^* is the normalized water productivity adjusted for atmospheric CO2/synthesized products/soil fertility, different for C3 and C4; Tr is daily crop transpiration, and ET_0 is the reference evapotranspiration for that day.

Crop transpiration is also affected by water stress (water logging, stomatal closure, soil salinity stress):

$$Tr = Ks_{aer} \times Ks_{sto} \times Ks_{sto,salt} \times CC^* \times Kc_{Tr,x} \times ET_0$$

Ks_{aer} for water logging is linear between 0 (at θ_{sat}) and 1 (at θ_{air} (between θ_{sat} and field capacity)).

Ks_{sto} forstomatal closure is a convex curve between $p_{sto}TAW$ (=1) and wilting point (=0), where TAW is total available soil water in root zone and p_{sto} is fraction of TAW at which stomata start to close.

Yield formation

In AquaCrop, the yield is calculated as:

$$Y = f_{HI} \times HI_0 \times B$$

f_{HI} is the adjustment factor depends on timing and extent of stress:

$$f_{HI} = f_{ante} \times f_{pol} \times f_{post}$$

(1) f_{ante} , water stress before yield formation

When a fruit/grain producing has spent less energy in its vegetation growth, the Harvest Index could increase.

$B_{rel} = \frac{B}{B_0}$ is the relative biomass at the time of flowering

Specify ΔHI_{ante} and given $Range\left(B_{r,up} - B_{r,low}\right) = \frac{ln(\Delta HI_{ante})}{5.62} \leq 1$

$$f_{ante} = \begin{cases} 1 + \dfrac{1 + sin\left((1.5 - Ratio_{low})\pi\right)}{2} \cdot \dfrac{\Delta HI_{ante}}{100} \\ 1 + \dfrac{1 + sin\left((0.5 + Ratio_{up})\pi\right)}{2} \cdot \dfrac{\Delta HI_{ante}}{100} \end{cases}$$

$Ratio_{low} = \frac{B_{rel} - B_{r,low}}{B_{r,top} - B_{r,low}}$, and $Ratio_{up} = \frac{B_{rel} - B_{r,top}}{B_{r,up} - B_{r,top}}$, the top is 1/3 to $B_{r,up}$ and 2/3 to $B_{r,low}$.

(2) f_{pol} , failure of pollination

Pollination is less affected by severe drought or temperature in AquaCrop.

$$f_{pol} = \sum_{i=1}^{n} \left(Ks_{pol,w,i} \times Ks_{pol,c,i} \times Ks_{pol,h,i} \left(1 + \frac{f_{excess}}{100}\right) F_i\right) \leq 1$$

$Ks_{pol,w}$ decreases linearly from 1 at upper threshold $\left(p_{pol}\right)$ to 0 at wilting point.

$Ks_{pol,c}$ is a logistic curve between 0 at air temperature $T_{n,cold} - 5$ and 1 at air temperature $T_{n,cold}$.

$Ks_{pol,h}$ is a logistic curve between 1 at air temperature $T_{x,cold}$ and 0 at air temperature $T_{x,cold} + 5$.

f_{excess} is percentage of excess flowers that can be used to compensate loss after stress ameliorated.

F_i is fractional flowering on day i out of flowering period n. It is derived from the flowering distribution curve given by:

$f_t = 0.00558t^{0.63} - 0.000969t - 0.00383$, where t from 1to 100 is the percentage of flower duration.

(3)f_{post} water stress during yield formation

Positive adjustment when water stress only partially affects leaf expansion.

$$f_{post\uparrow} = 1 + \frac{\sum_{i=1}^{n(exp)} \left(\frac{1-Ks_{exp,i}}{\alpha}\right)}{n(exp)}$$

$Ks_{exp,i}$is water stress coefficient for leaf expansion, $n(exp)$ is days when vegetation growth is possible, α is crop specific parameter with smaller value generate stronger effect.

Negative adjustment when water stress affects crop transpiration.

$$f_{post\downarrow} = \frac{\sum_{i=1}^{n(yield)} \left(\sqrt[10]{Ks_{sto,i}} \cdot \left(1 - \frac{1-Ks_{sto,i}}{b}\right)\right)}{n(yield)}$$

$n(yield)$is days when building up Haverst Index, water stress strongly affect HI when $b \geq 1$ gets closer to 1.

$$f_{post} = \left(\frac{w_1 f_{post\uparrow} + (w_2 - w_1)}{w_2}\right) f_{post\downarrow}$$

A1.4 CropSyst

Majordocumentation

http://modeling.bsyse.wsu.edu/CS_Suite_4/CropSyst/manual/index.htm

Biomass production

Biomass estimation is first based on transpiration and vpd, but use light-dependent biomass production method to compensate cons when vpd close to zero, such that:

$Biomass = min(G_{Tr}, G_R)$

- Water dependent growth

$$G_{Tr} = \frac{Tr_{act} \cdot BTR}{VPD}$$

$BTR$is the above ground biomass-transpiration coefficient crop parameter, Tr_{act} (m/day) is actual transpiration.

This relation will predict infinite growth when VPD approach to zero, unstable. Use radiation method to constrain.

- Radiation dependent growth

$$G_R = LtBC \times PAR \times FCC_{green} \times T_{lim}$$

$$T_{lim} = \begin{cases} 1.0, & if\ T_{ave} > T_{opt} \\ 0.0, & if\ T_{ave} < T_{base} \\ \dfrac{T_{ave} - T_{base}}{T_{opt} - T_{base}}, & otherwise \end{cases}$$

$LtBC$is a coefficient representing the conversion of photosynthetically active radiation (PAR) to above ground biomass input parameter. It is assumed that temperature effects, after cumulative degree-days is larger than the threshold, are accounted for in the radiation conversion factor $LtBC$. Cropsyst thus does not have explicit heat stress from high temperature.

Yield formation

The harvested yield is a calculated as the product of harvestable biomass and the HI:

$$Yield = Biomass_{hrv} \times HI$$

where the actual HI is:

$$HI = \begin{cases} HI_{unstressed} \cdot SF_{flowering} \cdot SF_{filling} \cdot duration_{filling}, & Cereals/Grains \\ HI_{unstressed} \cdot aveStress_g^{Sg}, & Others?\ Soybean\ etc? \\ others, & Tea, Potato \end{cases}$$

$aveStress_f$, $aveStress_{gf}$, $aveStress_g$is mean water stress during flowering, grain filling and throughout growth (from emergence).

Sf, Sgf, Sg, are the harvest index adjustment parameters for water stress sensitivity during flowering (Sf), grain filling (Sgf) and throughout growth for all other crops respectively (Sg). Range [0, 1] is calibrated, 0 indicate no stress effect.

$duration_{filling}$ is the simulated grain filling period duration divided by the typical duration of the grain filling period.

For heat stress also see:

http://adam-digital-compendium.pik-potsdam.de/risk-damage-maps/crop-risk-maps/adaptation-in-guadiana/materials-and-methods/

- Cereals/Grains

$$SF_{flowering} = \begin{cases} 1.0\ (no\ effect), & if\ Sf = 0\ or\ aveStress_f > 0.75(stress\ threshold) \\ \left(\dfrac{aveStress_f}{0.75}\right)^{Sf}, & otherwise \end{cases}$$

$$SF_{filling} = \begin{cases} 1.0\ (no\ effect), & if\ Sf = 0\ or\ aveStress_{gf} > 0.75(stress\ threshold) \\ \left(\dfrac{aveStress_{gf}}{0.75}\right)^{Sgf}, & otherwise \end{cases}$$

In addition, grain yield based on translocation is determined as biomass at flowering, times the translocation factor, times the mean flowering stress. The maximum of the two is compared with the unstressed yield from then biomass harvest index equation and the minimum is taken as the predicted yield.**This is only post correction!**

- Other crops

No explicit equation for $avgStress_g$is found in the documentation or literatures.

Alternative way of Heat Stress around anthesis (Morionda et al. 2011)

Morionda et al. (2011) incorporated an alternative way of accounting heat stress around the anthesis-silking stage.

Heat stress reduce harvest index from -5 to +12 days from the onset of anthesis

$$HTS = 1 - \frac{T_{am} - T_{cr}}{T_{lim} - T_{cr}}$$

whereHTS is heat stress, T_{am} is mean *8 am- 2pm* temperature, T_{cr} is temperature above which grain-set starts to decline, T_{lim} is the temperature at 0% grain-set.

$$HTS_{tot} = \sum_{i=1}^{Nf}(HTS_i \times Fd_i)$$

whereFd_i is the fraction of total flowers opening on day i.

Adjusted scalar to harvest index is:

$$f(HTS) = 1 - \frac{HTS_{cr} - HTS_{tot}}{HTS_{cr}}$$

$HTS_{cr}$is the critical fractional grain-set below which harvest index is reduced from its non-stressed value.$HTS_{cr} = 0.85$is used for wheat in Morionda et al. (2011).

A1.5 DayCent

Majordocumentation

For DayCent 4.5, see:

http://www.nrel.colostate.edu/projects/daycent-downloads.html

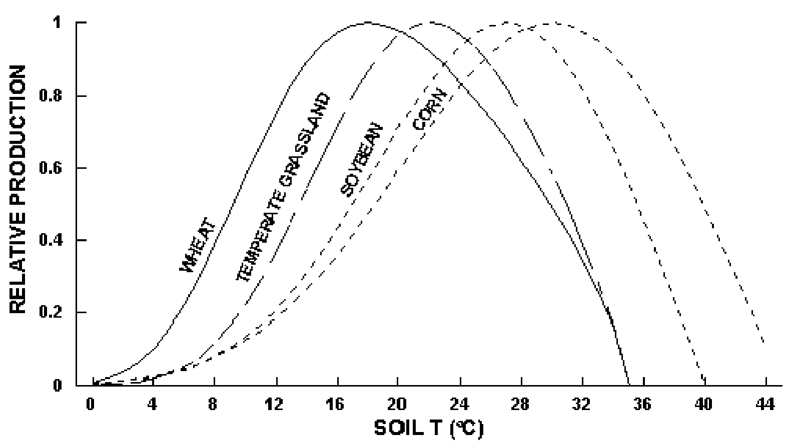
For Century 4.0, see:

https://www.nrel.colostate.edu/projects/century/MANUAL/html_manual/man96.html#GRASS

Biomass production

DayCent inherits from Century 4.0. It is not specifically designed for cropping systems, but is capable to simulate crop growth on relatively coarse scale. Biomass accumulation starts with the net primary production (NPP). Plant production is a function of genetic potential, phenology, nutrient availability, water/temperature stress, and solar radiation. NPP is allocated to plant components (e.g., roots vs. shoots) based on vegetation type, phenology, and water/nutrient stress. Nutrient concentrations of plant components vary within specified limits depending on vegetation type and nutrient availability relative to plant demand (Metherell, 1993).

Temperature stress.Plant growth rates will depend on the combined temperature response of photosynthesis and respiration. For most temperate species the lower limit at which the rate of development is perceptible is between zero and 5 ℃. Development increases in rate up to an optimum of 20 to 25 ℃ and then declines to an upper limiting temperature between 30 and 35 ℃. For tropical species the base, optimum and maximum temperatures are approximately 10℃ higher (Monteith, 1981). In the DayCent model the temperature response curve can be parameterized for each crop using a generalized Poisson density function as shown below:



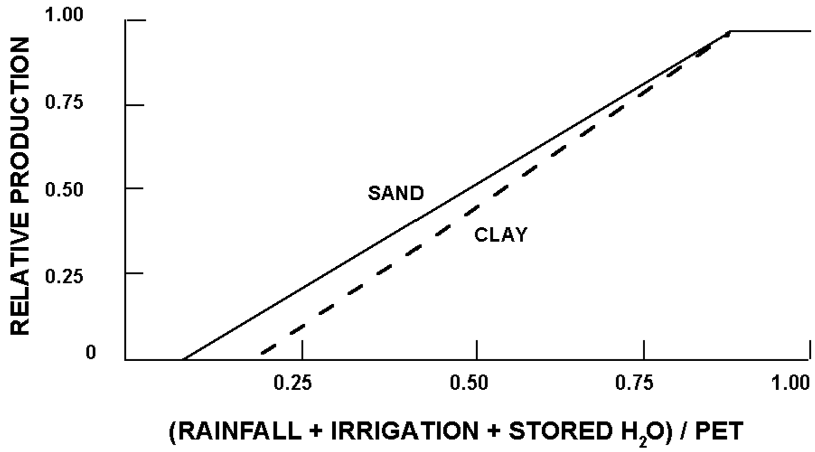
The relative production (i.e.T_{stress}) with generalized Poisson density function is:

$$T_{stress} = \left(\frac{T_{lim} - T_{mean}}{T_{\mathrm{lim}} - T_{opt}}\right)^{cLeft} \times exp\left[\frac{cLeft}{cRight} \cdot \left(1 - \left(\left(\frac{T_{lim} - T_{mean}}{T_{\mathrm{lim}} - T_{opt}}\right)^{cRight}\right)\right)\right]$$

whereT_{mean} is the daily mean temperature, T_{lim} is the maximum temperature for photosynthesis, T_{opt} is the optimum temperature for photosynthesis; $cLeft$ and $cRight$ are curvature parameters for the left and right of the Poisson density function, respectively. For C4 crops, $T_{lim} = 45$℃, $T_{opt} = 29$℃, $cLeft = 1$, $cRight = 2.5$.

Moisture stress.The moisture status effect reduces growth when:

$$\frac{soil\ water\ in\ the\ plant\ root\ zone + Precipitation + Irrigation}{Potential\ evapotranspiration} < 0.8$$



The slope of the linear relationship is dependent on the field capacity, which varies with soil texture

Yield formation

For crops, the root to shoot carbon allocation can be computed using the Great Plains equation or as a function of **soil water** and soil nutrient functions. Explicit equations, however, are not found after an extensive search for the literatures. Roughly, the proportion of NPP allocated to roots increases as precipitation decreases, and can be made a function of time since planting for crops.

A1.6 DSSAT-CSM-CERES

Biomass production

CERES has evolved frequently through time. The version we documented here is CERES 4.0 (López-Cedrón et al., 2005, 2008).

As in most simple crop models, CERES-Maize usesthe RUE concept to estimate potential biomass accumulation per plant (PCARB) and reduces to a minimum the number of equations needed to calculate net photosynthesis:

$$PCARB = RUE \times \frac{IPAR}{PLTPOP}$$

where$IPAR$ is PAR intercepted by the canopy, and $PLTPOP$ is plant population.

The actual daily biomass production per plant (CARBO) is limited by temperature, water stress or nitrogen:

$$CARBO = PCARB \times min(PRFT, SWFAC, NFAC, 1.0)$$

The **temperature limiting** function, $PRFT$, is a multilinear function of daytime temperature ($\frac{T_{max} + T_{mean}}{2}$) with the following cardinal temperatures: Tbase=6.2, Topt1=16.5, Topt2=33, Tlim=44°C.

The **water stres**s is activated when potential transpirational demand (EP_0) equals or exceeds the potential root water uptake ($TRWUP$):

$$SWFAC = \frac{TRWUP}{EP_0}$$

where TRWUP is calculated following Ritchie (1998) as:

$$TRWUP = \sum_{i=1}^{N} \frac{k_1 \cdot e^{k_2(SW_i - LL_i)}}{k_3 - ln(RLV_i)} \times RLV_i \times \Delta Z_i$$

where for each layer i, RLV is the root length density (cm/cm^3); k_1 = 0.00132; k_2 = 45.0 if the drained lower limit (LL) of the soil water (plant wilting point or soil water contentat 1.5 MPa suction) in the soil layer is > 0.30 cm^3 cm^{-3}, and k_2 = 130 LL if the LL for the soil layer is <0.30 cm^3 cm^{-3}; k_3=7.01.SW and LL are the volumetric soil water content and the lower limit of plant-available water (cm cm^{-1}), respectively; and Z_i is the depth of the ith layer (cm).

Yield formation

In CERES-4.0, grain growth rate per day (GROGRN) depends on temperature (**RGFILL** (relative rate of grain fill) is a temperature function), number of grains per plant (GPP), potential kernel growth rate per day (G3, mg $kernel^{-1}$ d^{-1}) and soil water stress factor on photosynthesis (**SWFAC**):

$$GROGRN = RGFILL \times GPP \times G3 \times 0.001 \times (0.45 + 0.55 \times SWFAC)$$

RGFILL follows a linear daily average temperature (Tavg) function with the following cardinal temperatures: Tbase=5.5, Topt1=16, Topt2=39, Tlim=48.5°C.

GPP is a function of PSKER and limited by the potential number of kernels (G2), and PSKER is directly related to the values of CARBO during stage 4 and therefore linearly influenced by the actual SWFAC effects on CARBO:

$$GPP = min\left(G2 \times \frac{PSKER}{7200} + 50, G2\right)$$

It should be noted that GROGRN is actually influenced by SWFAC in a quadratic way. Algorithms are mostly given in Lopez-Cedron et al. (2005, 2008).

A1.7 DSSAT-CSM-IXIM

Biomass production

CSM-IXIM is a new maize simulation model with detailed representation of leaf level canopy assimilation (Lizaso et al., 2005, 2011). Daily input solar radiation is fractioned into hourly components, separated in direct and diffuse fraction, and transformed into hourly intensities of PAR. Leaf area is separated into sunlit and shaded fraction and light absorption is calculated for each component.

Leaf expansion is affected by temperature and water stress. Under water stress, leaf rolling reduces the effective light capture of canopies by:

$$Fla = \frac{SF_w + (h-14)}{\{25 + (100-25) \cdot exp[-3.5(1-AT)]\} \times (5 - 4 \cdot SF_w)}$$

andSF_w is the 0~1 most limiting **water stress** factor (TURFAC in CERES), h is the hour of the day, AT is atmospheric transmission of radiation describing sky cloudiness.

Leaf level CO_2 assimilation (sunlit/shaded) follows a nonrectangular hyperbola function (Thornleyand Johnson 1990):

$$\theta \cdot A_g^2 - (\emptyset \cdot APAR + A_{sat}) \cdot A_g + \emptyset \cdot APAR \cdot A_{sat} = 0$$

$$=> A_g = \frac{\emptyset \cdot APAR + A_{sat} - \sqrt{(\emptyset \cdot APAR + A_{sat})^2 - 4\theta \cdot \emptyset \cdot APAR \cdot A_{sat}}}{2\theta}$$

Parameter	Definition	Unit
A_g	grossCO_2assimilation rate	$\mu mol\ CO_2 m^{-2} s^{-1}$
$APAR$	absorbed photosynthetic photon flux density (PPFD)	$\mu mol\ quanta\ m^{-2} s^{-1}$
A_{sat}	saturated assimilation rate	$\mu mol\ CO_2 m^{-2} s^{-1}$
$\emptyset$	quantum efficiency of CO_2 assimilation	$\mu mol\ CO_2 (\mu mol\ quanta)^{-1}$
θ	ratio of the diffusion resistance to the total resistance	

Leaf aging effect was simulated internally through changes in A_{sat}, $\emptyset$, θ with sigmoidal functions.

Temperature effect on assimilation was described by multiplying a cubic function to A_{sat}, $\emptyset$, θ:

$$p_t = a + bt + ct^2 + dt^3$$

wherea, b, c, d are parameters to be calibrated for each A_{sat}, $\emptyset$, θ.

Roughly, A_{sat}, $\emptyset$, θ have constant value between 15-40 °C, but decrease beyond this range.

Hourly gross canopy assimilation is calculated by integrating assimilation over sunlit and shaded leaves:

$$A_{can} = \sum_{l=1}^{n} A_{sun}(l) \times LAI_{sun}(l) + A_{sha} \times LAI_{sha}(l)$$

This will be further converted into hourly glucose by:

$$A_{day_g} = \frac{30}{44} \times 44 \times 0.0036 \times \sum_{h=1}^{24} A_{can}(h)$$

The daily potential growth rate (PGR, g plant^{-1} day^{-1}) is adjusted by maintenance and growth respiration:

$$PGR = \frac{A_{day_g} - R_m}{RD_g \times PD}$$

Where RD_g is weighted growth respiratory demand, PD is plant density.

Yield formation

Carbon partitioning to different organs is a function of time (see figure below), a noticeable feature is under **drought**and N stress conditions, partitioning of daily assimilates gives roots a greater proportion at the expense of shoots or ear.

As described in Lizaso et al. (2011), the reduction coefficient of assimilates partitioned to the shoot, based on a similar concept developed by Penning de Vries and van Laar (1982), is:

$$FS = 0.46 + 0.72 \times exp[-2.83 \times (1 - \mathrm{SF})]$$

where SF is the most limiting of water or N stress factors (from 0.0 as full stress to 1.0 as no stress).The FS parameter assumes that partitioningto shoots could be reduced by up to 50% under extreme stress conditions (SF=0). With no stress, FS is constrained to 1.$SF_{\mathrm{W}}$is the zero-to-one most-limiting water stress factor (TURFAC) as used in CERES

Ear growth starts 250 GDD before silking follows a sigmoidal function such that:

$$F_e = \frac{P_e \cdot PGR}{1 + exp[-0.02 \cdot (tt - 225)]}$$

whereF_e is the fraction of daily dry mass partitioned to the ear, PGR is the daily plant growth rate (g plant–1 d–1), P_e is an ear partition parameter, and tt is the thermal time after the onset of ear growth (°C d). Ear tissues (ovaries first,

kernels after fertilization, cob, rachis, husks) continue to grow indistinctly until the end of the lag phase (170 GDD after 50% silking). Assimilates in excess of grain sink capacity are allocated into stems.

The grain fillingalgorithm is not explicitly documented.

A1.8EPIC

Major documentation

http://epicapex.tamu.edu/files/2015/05/EpicModelDocumentation.pdf

Biomass production

Daily potential increase in biomass (t/ha) is given by:

$$\Delta B_p = 0.001 \times BE \times PAR \times (1 + \Delta HRLT)^3$$

whereBE is the crop parameter for converting energy to biomass (kg/MJ), $\Delta HRLT$ is change in day length (h/d).

The biomass constraint is calculated by using the lowest value from among the stress factors estimated such that:

$$\Delta B = \Delta B_p \times min(WS, TS, NS, PS, AS)$$

Water stressof i-th day limits biomass production in proportion to transpiration reduction:

$$WS_i = \frac{\sum_{l=1}^{M} u_{i,l}}{Ep_i}$$

where$u_{i,l}$ is the water use (mm/d) in *l*-th soil layer, and Ep_i is the potential plant water evaporation rate.

Also includesaeration stress describing excessive water.

Temperature stress is a function of soil surface temperature TG:

$$TS = sin\left(\frac{\pi}{2} \times \frac{TG - T_{base}}{T_{opt} - T_{base}}\right)$$

For maize, $T_{base} = 8, T_{opt} = 25$; for soybean, $T_{base} = 10, T_{opt} = 29$.

Yield formation

The harvest index is affected by **water stress** according to:

$$HIA_i = HIA_{i-1} - HI_0 \cdot \left(1 - \frac{1}{WSYF \times FHU_i \times (0.9 - WS_i)}\right)$$

where HIA is the adjusted harvest index, WSYF is crop specific drought sensitivity, FHU is a function of crop stage.

Notice HIA may increase slightly on days with $WS_i > 0.9$.

$$FHU_i = \begin{cases} sin\left(\frac{\pi}{2} \times \frac{HUI_i - 0.3}{0.3}\right), & 0.3 \leq HUI_i \leq 0.9 \\ 0, & otherwise \end{cases}$$

FHU_imakes water stress only affect harvest index between 0.3 and 0.9 of maturity (represented by heat unit index, HUI), with greatest effect occurring at 0.6.

For maize, $HI_0 = 0.5, WSYF = 0.05$; for soybean, $HI_0 = 0.31, WSYF = 0.01$.

A1.9HYBIRD-Maize

Major documentation

http://hybridmaize.unl.edu/assets/usermanual/User%20Manual.pdf

Biomass production

The CO_2 assimilation by the whole canopy in a day (g CO_2 m^{-2} day^{-1}):

$$A = DL \times \int_{L=0}^{LAI} A_{max} \left[1 - exp\left(-\varepsilon \times PAR_{i,L}/A_{max}\right)\right]$$

The maximum assimilation rate (A_{max}) is a function of **day-time mean temperature** (T_{day}).

$$A_{max} = \begin{cases} 0, & if\ T_{day} \le T_{zeroA} \\ A_{plateau} \times \dfrac{T_{day} - T_{zeroA}}{T_{1,plateau} - T_{zeroA}}, & if\ T_{zeroA} < T_{day} \le T_{1,plateau} \\ A_{plateau}, & if\ T_{1,plateau} < T_{day} \le T_{2,plateau} \\ \max\left(A_{plateau} - 0.2 \times \left(T_{day} - T_{2,plateau}\right), 0\right), & if\ T_{day} \ge T_{2,plateau} \end{cases}$$

$A_{plateau}$ = 7 g CO_2 m^{-2} leaf hr^{-1}

This setting makeA_{max} not much less sensitive to heat stress than cold.

Water stress index (WS), following APSIM, will linearly limit CO2 assimilation (claimed to be described in User's manual, Section 4.1.2, but not really available) and leaf area expansion, as well as an acceleration factor for leaf area senescence after silking(see Yang et al., 2013, Page70).

The maximum water uptake ($Uptake_{max}$, cm d^{-1}) from each soil layer is estimated as:

$$Uptake_{max} = (PSI_{leaf} - PSI) / (R_{plant} + R_{root}) * WUweight$$

in which PSI_{leaf} is the leaf water suction at permanent wilting point, R_{plant} is the resistant of plant to water flow. If $Uptake_{max}$ >$Water_{avail}$ then $Uptake_{max}$ =$Water_{avail}$.

Available water (cm) for each soil layer is calculated as:

$$Water_{avail} = \left(Theta - Theta_{pwp}\right) \times 10$$

Integrate water uptake at each soil layer as the actual transpiration:

$$Transp_{actual} = \min(Uptake_{total}, Transp_{max})$$

Finally, the water stress (WS) is estimated as:

$$WS = 1 - \frac{Transp_{actual}}{Transp_{max}}$$

Gross carbohydrate production ($Carbo_{gross}$) is expressed on a per plant basis (g CH_2Oplant^{-1} day^{-1}):

$$Carbo_{gross} = A/plantPop \times 30/44$$

where$plantPop$ is plant population density (plants m^{-2}).

The net production of carbohydrate (Carbo, g CH_2O d^{-1} $plant^{-1}$) is then computed by minus maintenance respiration from $Carbo_{gross}$. $Carbo$is then allocated to different organs, and adjusted for growth respiration as well.

Yield formation

Actual grain filling rate (g CH_2O plant^{-1} day^{-1}) is computed as:

$$grainGrow = RG_{fill} \times G_{PP} \times G_5 \times Fill_{eff} \times 0.001$$

In which RG_{fill} is the temperature driven filling scale, G_{PP} is the number of viable grain per plant (default is 676 for high yield hybrids), G_5 is the potential grain filling rate (mg kernel^{-1} day^{-1}), $Fill_{eff}$ is filling efficiency determined by plant population density.

Temperature dependent function $\boldsymbol{RG_{fill}}$ is calculated as a sum of 8 consecutive 3-hour interval filling scales:

$$RG_{fill} = \begin{cases} \sum_{i=1}^{8} \frac{1}{8} \times [1 - 0.0025 \times (TTMP_i - 26)^2], & TTMP_i \geq 6 \\ 0, & otherwise \end{cases}$$

$$TTMP_i = T_{min} + TMfac_i \times (T_{max} - T_{min})$$

$$TMfac_i = 0.931 + 0.114 \times i - 0.0703 \times i^2 + 0.0053 \times i^3$$

When daily net CO_2 assimilation is insufficient to meet the grain-filling rate, translocation of carbohydrate from stem and/or leaf will occur as long as there is carbohydrate reserve in these two organs (Yang et al., 2013).

Otherwise, the surplus will be stored in stem as part of the carbohydrate reserve for future translocation.

Water stress will indirectly affect grain filling through regulating G_{PP} (User manual P66):

$$G_{PP} = G2 - 676 / (PSKER / 1000)$$

$$PSKER = sumP / (1 + GRRG) * 1000 / IDURP * 3.4 / 5$$

in which both the cumulative net assimilation ($sumP$) and the duration in days of the 340 sumDTT8 period are both influenced by water stress.

A1.10GLAM

Biomass

Above-groundbiomass (W) is determined by a separate prognostic equation:

$$\frac{\partial W}{\partial t} = T_T \times min\left(\frac{E_T}{VPD}, E_{TN,max}\right)$$

whereT_T is transpiration rate, $E_T$is the normalized transpiration efficiency, $E_{TN,max}$ is the maximum transpiration efficiency (g/kg).Transpiration (T_T) and evaporation rates (E) are determined by considering separately the limitations imposed by plant/soil structure, energy availability, and water availability.

While the calculation of transpiration and evaporation is a little complex (see section 2.3 in Challinor et al., 2004), **water stress** will affect biomass accumulation in two ways: (i) limit leaf area expansion (Eq.3, 4 in Challinor et al., 2004) and hence the physiologically limited transpiration (T^p_{Tpot}); and (ii) the partitioning of available soil water according to demand expansion (Eq.19 in Challinor et al., 2004).

High temperature could reduce transpiration efficiency (Challinor et al., 2009).
Between temperature T_{crt} and T_{lim}, E_T is reduced linearly from its non-temperature-limited value of E_{Tf} to 0:

$$E_T = E_{Tf} \times \left(1 - \frac{T - T_{crt}}{T_{lim} - T_{crt}}\right)$$

By default, $T_{crt} = 35$ and $T_{lim} = 47$ (but see Osborne et al. 2012 for much lower values, 25/30)

Yield formation

Daily increase in harvest index begins after pod filling, and is a constant $\frac{\partial H_I}{\partial t}$.

Yield is calculated as: $Y = H_I \times W$

Challinor et al. (2005) introduced the algorithm of **heat stress** on flowering and pod set:

The first stage of the simulation of high temperature stress is the identification of episodes of high temperature. This is done by comparing the mean 8 a.m.–2 p.m. (solar time) temperature (T_{AM}) to a predefined critical value (T^{min}_{cr}). From this, all hightemperature episodes are identified and characterized by their duration (d) and the centered time at which they occur.

Refer to Morionda et al. (2011) for clean explanations on the detailed algorithms.

A1.11MAIZSIM

Major documentation

https://github.com/ARS-CSGCL-DT/MAIZSIM

Biomass

In MAIZSIM, canopy transpiration and photosynthesis are simulated at leaf level using the sun/shade method by (De Pury and Farquhar, 1997).

CO2 assimilation is limited either by Rubisco activity or by electron transport (Appendix in Yang et al. 2009):

$$A = min(A_c, \quad A_j)$$

$$A_c = \{(V_p + g_s C_m - R_m), \ (V_{cmax} - R_d)\}$$

$$A_j = \left\{\left(\frac{xJ}{2} + g_{bs} C_m - R_m\right), \ \left(\frac{(1-x)J}{3} - R_d\right)\right\}$$

Stomatal conductance is limited by **water stress** such that (Eq-4 in Yang et al. 2009):

$$f(w_l) = \frac{1 + exp(s_f \Psi_f)}{1 + exp[s_f(\Psi_f - \Psi_l)]}$$

whereΨ_l is bulk leaf water potential, Ψ_f is a reference potential (= -1.2 MPa), and s_f is a sensitivity parameter (= 2.3) (Tuzetet al., 2003).Need to find out how Ψ_l is calculated. It is calculated by the 2DSOIL model (Timlin et al. 2002), implemented in *carbon_partitioning.FOR*. Pay attention to the calculation of leaf water potential (PSIL).

Leaf level photosynthesis is scaled up to the whole canopy by integrating sun/shade leaf area index (LAI).

Simulation of LAI is temperature constrained ($\beta\_function$), algorithms are detailed described in Kim et al. (2012).

Implemented in `voidCPlant::calcGasExchange(constTWeather& weather)`

And in `voidCPlant::update(constTWeather& weather, doublePredawnLWP)` daily increase in carbon pool was converted from the CO2 assimilation as:`double c_pool2 = assimilate*CH2O_MW/CO2_MW;`

C allocation & Yield

Theoretically follow Grant et al. (1989).

Implemented in `voidCPlant::C_allocation(constTWeather& w)`

Hourly available carbohydrate for allocation is computed as:

$$C_{supply} = C_{pool} \times GRO_{fac} \times \boldsymbol{T_{effect}}$$

$$T_{effect} = \begin{cases} 0, & T_{air} > T_d = 48.6 \\ \dfrac{1 - exp[-0.2035 \times (T_d - T_{air})]}{1 + exp(2.3252 - 0.1854 \times T_{air})}, & T_{air} < T_d \end{cases}$$

C_{supply} is adjusted to meet grain filling demand by transferring mass between organs and $C_{reservior}$.

Partitioning to shoot is determined by the fraction factor:

$$FRAC = min(0.925, 0.67 + 0.33 \times scale)$$

$$shootPart = Y_g \times FRAC \times (C_{supply} - maintRespiration)$$

in which calculation is gCH_2O based and Y_g is synthesis efficiency, ranging from 0.7 to 0.76 for maize. The remaining part goes to root.

Water stress will limit C_{supply} by allocating more carbohydrate to root, as is implemented by GLYCIM (Acock et al., 1982). That's why we see `shootPart_real = max(0, shootPart-(w.pcrs-rootPart_old));` in carbon allocation function.

Grain filling demand is calculated as:

$$C_{demand} = maxKernelNo \times maxKernelFillRate \times T_{effect,2} \times C\_content$$

And the **temperature response function $\boldsymbol{T_{effect,2}}$** is $1.0 - 0.0025 \times (T_{air} - 26.0)^2$ in Grant et al. (1989), but is same as T_{effect} listed above in the latest version. This should be treated with caution!If hourly growth increments allocated to the grain exceed the maximum filling rate, the excess is allocated to the soluble reserve fraction of the stalk.

A1.12MONICA

Major documentation

http://monica.agrosystem-models.com/

Biomass production

Crop growth in MONICA follows a generic approach derived from the SUCROS model. Daily net dry matter production by photosynthesis and respiration is driven by global radiation and temperature. Atmospheric CO_2 concentration affects the crop's maximum photosynthesis rate and stomatal resistance, which in turn influences transpiration (Nendel et al. 2009). For the former, Mitchell et al. (1995) presented a set of algorithms based on the ideas of Farquhar and von Caemmerer (1982) and Long (1991) for the calculation of the photosynthesis rate (kg CO_2 ha^{-1} h^{-1}):

$$A = \frac{(C_i - \Gamma^*) \cdot V_{cmax}}{C_i + K_c \cdot \left(1 + \frac{O_i}{K_o}\right)}$$

whereC_i (intercellular CO2 concentration) and O_i (intercellular O2 concentration) are temperature dependent (Long et al. 1991), Γ^* is compensation point of photosynthesis, V_{cmax} is maximum saturated Rubisco carboxylation rate.

$$V_{cmax} = 98 \cdot \frac{A_{max}}{34.668} \cdot K(T)_{V_{cmax}}$$

whereA_{max} is crop-specific and $\boldsymbol{K(T)_{V_{cmax}}}$ is a temperature function with optimum around 30-40 degreeC.

Gross CO_2 assimilation is calculated by estimating the sky cover duration:

$$A_g = O_r \cdot A_0 + (1 - O_r) \cdot A_c$$

A_0 *and* $A_c$are CO_2 assimilation under cloudy/clear sky, and is scaled up from A with LAI and a few other variables.

Drought stress. The reduction factor for drought is calculated by the relation of actual to potential transpiration:

$$\zeta_W = \frac{T_a}{T_p}, if\ \zeta_W < threshold\ \overline{\zeta_W}$$

Stress modified CO_2 assimilation is:

$$A_{gm} = A_g \times \zeta_W$$

Biomass of organ (root, leaf, shoot and fruit) W_i is:

$$\frac{dW_i}{dt} = A_{gm} \cdot a_i \cdot dt - M_{photo} - M_{dark}$$

wherea_i is partitioning coefficient, depending on growth stages; M_{photo} *and* M_{dark} is maintenance respiration during the photo period and in darkness as a function of organ dry mass, temperature and daylength.

Yield formation

Compute dry matter yield based on storage organ biomass (W_s) and harvest index (HI): $W_s \times HI$.

Heat stress reduces the assimilate flow to the storage organ, such that:

$$W_s = A_{gm} \cdot a_s \cdot \zeta_H$$

In which a_s is assimilation partitioning coefficient for the storage organ.

Heat stress. Heat stress mainly affects the production of ovules during bloom, and is derived from the smallest value of stress factor during the sensitive phase:

$$\zeta_H = min(F_{H1}, \cdots, F_{Hn})$$

$$F_H = 1 - \left(\frac{T_{photo} - T_{critH}}{T_{limH} - T_{critH}}\right) \cdot rF$$

whererF is fraction of flowers opened on specific day, and for other limit and critical temperature parameter, see Moriondo et al. (2011). $T_{photo}$is air temperature during the daylight period computed as:

$$T_{photo} = T_{max} - (T_{max} - T_{min})/4.$$

A1.13PEGASUS

Major documentation

Publically available description only available in Deryng et al. (2011, 2014)

Biomass production

Daily net biomass production $\mathcal{P}$ based on LUE model is limited by temperature, soil moisture and nutrient:

$$\mathcal{P} = \varepsilon \cdot APAR \cdot f_T \cdot f_W \cdot f_N$$

whereε (mol C mol quanta^{-1}) is the light use efficiency coefficient, APAR (mol quanta m^{-2} s^{-1}) is the daily average absorbed photosynthetically active radiation and is expressed using Beer-Lambert's law for light interception.

The **temperature stress** factor (f_T) is similar to that of Agro-IBIS, but has wider range of optimum state, representing an envelope of individual cultivar (mathematical realization to be confirmed with the author).

Water limitation is a linear combination of irrigated $A_i$and harvested A_h (irrigated + rain-fed) area, such that:

$$f_W = \frac{A_i}{A_h} max\left(0.9, U_p\right) + \left(1 - \frac{A_i}{A_h}\right) U_p$$

$U_p$is the potential plant water uptake rate as a nonlinear function of relative soil available water capacity (SWAR 0~1):

$$U_p = 1 - e^{-6 \times SWAR}$$

Nutrient limitation derived from regression between yield gap and N fertilizer application, is also a substitution for many other management failures.

Yield formation

Carbon assimilated is allocated to four vegetation pools: leaves, stem, roots and storage organs by:

$$\frac{dC_x}{dt} = \alpha_x \mathcal{P} - \beta_x C_x$$

whereC_x is the carbon content in organs x, α_x and β_x are the allocation and turnover fractions depend on development stages.

Crop yield (t Ha^{-1}), calculated in fresh matter, is proportional to the amount of dry biomass accumulated in the storage organs at harvesting date (C_{so}) and limited by heat stress around anthesis (f_{HSA}):

$$Y_e = \frac{EF}{0.45 \times DF} \times C_{so} \times f_{HSA}$$

Daily **heat stress** scalar (f_{HSAd}) is calculated as:

$$f_{HSAd} = \begin{cases} 1, & if\ T_{eff} < T_{cr} \\ 1 - \dfrac{T_{eff} - T_{cr}}{T_{lim} - T_{cr}}, & if\ T_{cr} \le T_{eff} < T_{lim} \\ 0, & if\ T_{eff} > T_{lim} \end{cases}$$

where$T_{cr} = 32\ for\ maize, 35\ for\ soybean$, $T_{eff} = (T_{max} + T_{mean})/2$, $T_{lim} = 45\ for\ maize, 40\ for\ soybean.$

$$f_{HSA} = \frac{1}{TSP} \sum_1^{TSP} f_{HSAd}$$

in which TSP is the thermal sensitive period (calendar days), from $min\{0.45\ GPL,\ anthesis\}$ to $max\{0.7\ GPL,\ anthesis\}$; and GPL is growing period length defined as emergence to maturity.

A1.14STICS

Major documentation

Brisson, N. (2008). Conceptual basis, formalisations and parameterization of the STICS crop model. Editions Quae.

Biomass production

In STICS the calculation of the daily production of shoot biomass (DLTAMS) relies on the radiation use efficiency (RUE) concept:

$$DLTAMS_i = \left[EBMAX_i \cdot RAINT_i - COEFB_G \cdot RAINT_i^{\,2}\right] \times FTEMP_i \cdot SWFAC_{i-1} \cdot INNS_{i-1} \cdot EXOBIOM_{i-1} \cdot FCO_2 + DLTAREMOBIL_{i-1}$$

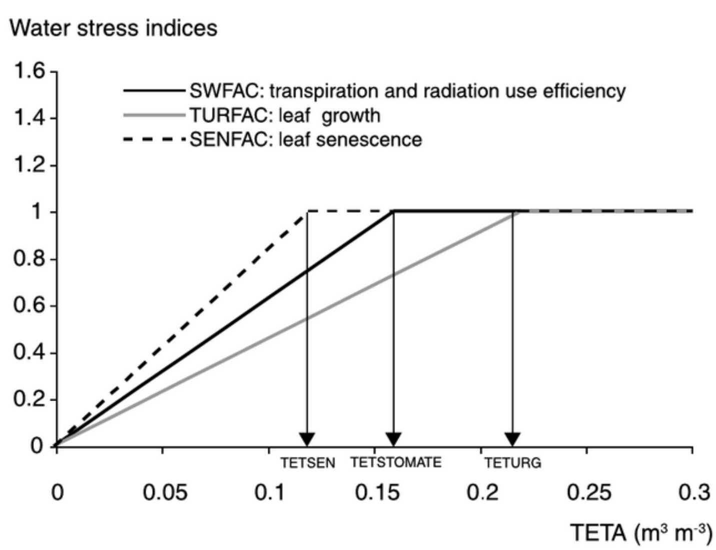
Parameter definitions are given in the table below.

Abbreviation	Definition	Unit
EBMAX	maximum value of radiation use efficiency	g MJ^{-1}
RAINT	PAR intercepted by the canopy	MJ m^{-2}
$COEFB_G$	parameter of radiation effect on conversion efficiency	
FTEMP	temperature-related RUE reduction factor	
SWFAC	index of stomatal water stress	
INNS	index of N stress active on growth in biomass	
EXOBIOM	water logging stress on RUE and transpiration	
FCO_2	species-specific CO2 effect on RUE	
DLTAREMOBIL	amount of reserves remobilized	g m^{-2} day^{-1}
TETA	available soil water content above wilting point	m^3 m^{-3}
TETSTOMATE	soil water threshold limiting photosynthesis and trans	m^3 m^{-3}
TCULT	crop surface temperature (daily average)	°C
$TEOPT_p$	begin thermal optimal plateau for net photosynthesis	°C
$TEOPTBIS_p$	end thermal optimal plateau for net photosynthesis	°C

Stomatal**water stress** for photosynthesis is calculated as:

$$SWFAC = \begin{cases} \dfrac{TETA}{TETSTOMATE}, & if\ TETA < TETSTOMATE \\ 1, & if\ TETA \geq TETSTOMATE \end{cases}$$

in which $TETSTOMATE$ depends on root density, the stomatal functioning of the plant, and the evaporative demand.



The **Temperature stress** on photosynthesis is calculated as:

$$FTEMP = \begin{cases} 1 - \left[\dfrac{TCULT - TEOPT_p}{TEMIN_p - TEOPT_p}\right]^2, & if\ TCULT < TEOPT_p \\ 1, & if\ TEOPT_p \leq TCULT < TEOPTBIS_p \\ 1 - \left[\dfrac{TCULT - TEOPTBIS_p}{TEMAX_p - TEOPTBIS_p}\right]^2, & if\ TCULT \geq TEOPTBIS_p \end{cases}$$

In which $TCULT$ is calculated with iterations as described in Figure 6.11.
Daily accumulation of $DLTAMS$ gives the aboveground biomass, $MASEC$.

Yield formation

Daily grain filling is calculated as:

$$DLTAGS_i = [IRCARB_i \times MASEC_i - IRCARB_{i-1} \times MASEC_{i-1}] \times FTEMPREMP_i$$

Total harvestable biomass is adjusted by **frost damage**:

$$MAFRUIT_i = \left(\sum\nolimits_{j=IDRP}^{i} DLTAGS_j\right) - \frac{PGRAINGEL_i}{100}$$

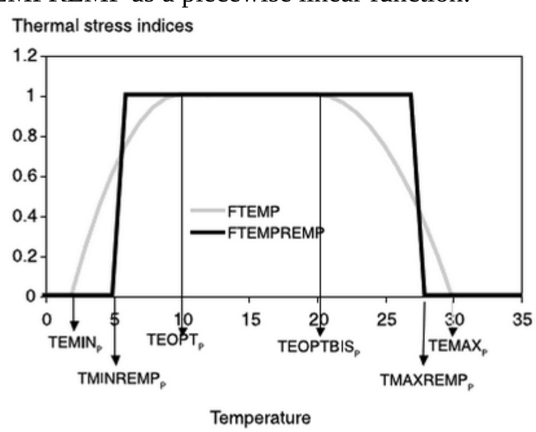
where definitions of variables are given in the table below:

Abbreviation	Definition	Unit
DLTAGS	growth rate of the grains	t ha^{-1} day^{-1}
IRCARB	carbon harvest index	g grain g plant^{-1}
MASEC	aboveground dry matter	t ha^{-1}
FTEMPREMP	temperature related grain filling reduction factor	
MAFRUIT	dry matter of harvested organs	t ha^{-1}
IDRP	day of stage DRP; beginning of grain/fruit filling	julian day
PGRAINGEL	frozen grain weight	g m^{-2}

Harvest index $IRCARB$ increases linearly until hit the maximum ($IRMAX_p$):

$$IRCARB_i = min\left(VITIRCARB_p \times (i - IDRP), IRMAX_p\right)$$

Thermal stress is described by FTEMPREMP as a piecewise linear function:



Frozen damage to grains is simulated by:

$$PGRAINGEL_i = \sum_{j=IDRP+1}^{i} \left(PGRAIN_{j-1} \times NBGRAINGEL_j\right)$$

$$PGRAIN_i = min\left(\frac{MAFRUIT_i}{NBGRAINS_i} \times 100, PGRAINMAXI_v\right)$$

The calculation of stressed grain number is:

$$NBGRAINGEL_i = NBGRAINS_{i-1} \times (1 - FGELFLO_i)$$

$$NBGRAINS_i = NBGRAINS_{IDRP} - \sum_{j=IDRP+1}^{i} NBGRAINGEL_j$$

where the definition of each variable is given in the table below:

Abbreviation	Definition	Unit
PGRAIN	grain weight	g
NBGRAINS	grain number	grains m^{-2}
FGELFLO	frost index acting on grain/fruit numbers	

Empirical approach to simulate canopy temperature

The canopy temperature, TCULT is the average of TCULTMAX and TCULTMIN. When using the empirical approach to estimate TCULT, we assume TCULTMIN equals TMIN and estimate TCULTMAX based on a relationship between midday surface temperature and daily evaporation:

$$TCULTMAX = max\left\{TMAX,\ \ TMAX + \left[\frac{RNET}{2.46} - ET - 1.27\right] / \frac{1.68}{ln\frac{1}{Z_0}}\right\}$$

$$Z_0 = max\left(0.13 \times C_{height},\ \ 0.001\right)$$

where RNET is the net daily radiation in MJ m-2, ET is the daily evapotranspiration in mm and C_{height} is the canopy height (m), 2.46 is the conversion factor for evapotranspiration,1.27 and 1.68 are empirical parameters.

A1.15SWAT (with new EPIC crop growth model)

Major documentation

http://swat.tamu.edu/media/99192/swat2009-theory.pdf

Biomass production

In SWAT, photosynthesis is simulated by intercepting and converting light into biomass according to a plant specific radiation use efficiency (Neitsch et al., 2011). The maximum increase in daily biomass (kg/ha) without stress is:

$$\Delta bio = RUE \cdot H_{phosyn}$$

where H_{phosyn} is the amount of intercepted photosynthetically active radiation on a given day (MJ m^{-2}):

$$H_{phosyn} = 0.5 \times H_{day} \times \left(1 - exp(-k_l \cdot LAI)\right)$$

and RUE is the radiation-use efficiency of plant ((kg/ha)/(MJ m^{-2})), and is adjusted to atmospheric [CO_2] and VPD.

Following Stockle and Kiniry (1990), adjusted RUE is:

$$RUE = \begin{cases} RUE_{vpd=1} - \Delta rue_{dcl} \cdot (vpd - vpd_{thr}), & if\ vpd > vpd_{thr} \\ RUE_{vpd=1}, & if\ vpd \leq vpd_{thr} \end{cases}$$

where $RUE_{vpd=1}$ is radiation-use efficiency at vpd=1.0 KPa, Δrue_{dcl} is the rate of decline parameter, $vpd_{thr} = 1.0\ KPa$ for all crops.

Actual biomass accumulation is limited by water, temperature, nitrogen and phosphorus:

$$\Delta bio_{act} = \Delta bio \cdot \gamma_{reg} = \Delta bio \cdot \{1 - max(wstrs, tstrs, nstrs, pstrs)\}$$

Water stress (0 indicate no stress) is simulated by comparing actual to potential plant transpiration:

$$wstrs = 1 - \frac{E_{t,act}}{E_t} = 1 - \frac{W_{actualup}}{E_t}$$

Temperature stress (0 indicate no stress) is based on daily average temperature (similar shape to old EPIC):

$$tstrs = \begin{cases} 1, & if\ T_{av} \leq T_{base} \\ 1 - exp\left[\frac{-0.1054 \cdot \left(T_{opt} - T_{av}\right)^2}{(T_{av} - T_{base})^2}\right], & if\ T_{base} < T_{av} \leq T_{opt} \\ 1 - exp\left[\frac{-0.1054 \cdot \left(T_{opt} - T_{av}\right)^2}{\left(2 \cdot T_{opt} - T_{av} - T_{base}\right)^2}\right], & if\ T_{opt} < T_{av} \leq 2 \cdot T_{opt} - T_{base} \\ 1, & if\ T_{av} \geq 2 \cdot T_{opt} - T_{base} \end{cases}$$

Yield formation

Biomass allocation to yield is based on the actual HI, calculated as:

$$HI = HI_{opt} \cdot \frac{100 \cdot fr_{PHU}}{100 \cdot fr_{PHU} + exp(11.1 - 10 \cdot fr_{PHU})}$$

where HI is the potential harvest index for a given day, fr_{PHU} is the fraction of potential heat units accumulated for the plant on given day of growing season.

The yield (grain/stem/leaves) is calculated as:

$$yld = bio_{ag} \times HI_{act}$$

Actual harvested index is affected by **water deficit** such that:

$$HI_{act} = (HI - HI_{min}) \cdot \frac{\gamma_{wu}}{\gamma_{wu} + exp(6.13 - 0.883 \cdot \gamma_{wu})} + HI_{min}$$

$$\gamma_{wu} = 100 \times \frac{\sum_{i=1}^{m} E_a}{\sum_{i=1}^{m} E_0}$$

whereγ_{wu} is the water deficiency factor by accumulating actual/potential ET over growing season.

In our test, γ_{wu} will not limit HI much when $6.13 - 0.883 \cdot \gamma_{wu} < 0$. Therefore 6.13 and 0.883 should be calibrated to fit field observation.

A1.16WOFOST

Major documentation

http://www.wageningenur.nl/en/Expertise-Services/Research-Institutes/alterra/Facilities-Products/Software-and-models/WOFOST/Documentation-WOFOST.htm

https://github.com/ajwdewit/WOFOST

Biomass production

WOFOST is a carbon-driven crop growth model, and has a complex hierarchical structure. WOFOST can simulate crop growth by following different approaches: (i) a potential mode, where crop growth is purely driven by temperature and solar radiation; (ii) a water-limited mode, and (iii) a nutrient-limited mode.

Dry matter accumulation is estimated by the rate of gross CO2 assimilation of the canopy. Daily gross CO2 assimilation is obtained by integrating assimilation rates over the leaf layers and over the day. Part of the assimilated CO2 is used for maintenance of respiration and respiration growth, while the rest is partitioned between plant organs.

Daily growth rate (kg Dry Matter ha^{-1} day^{-1}) is obtained as:

$$\Delta W = C_e \cdot (A - R_m)$$

whereC_e is conversion efficiency of assimilation (kg Dry Matter kg^{-1} CH_2O), A and R_m is gross assimilation and maintenance respiration rate.

Potential gross assimilation is integrated from leaf level CO_2 assimilation($AMAX$). All in ***cropsi.for***

Actual leaf CO_2 assimilation rate $AMAX$is interpolated by development stages (DVS)

$$AMAX = \boldsymbol{AFGEN}(AMAXTB, ILAMAX, DVS)$$

Adjust $AMAX$ with sub-optimal average **daytime temperature** ($DTEMP = \frac{T_{max} + T_{mean}}{2}$):

$$AMAX = AMAX * AFGEN(TMPFTB, ILTMPF, DTEMP)$$

Use subroutine ***TOTASS*** to calculate total gross CO_2 assimilation rates (DTGA, g CO_2 m^{-2} d^{-1})

DTGA is adjusted with **low nighttime temperature**(7-day moving average of minimum temperature) by:

$$DTGA = DTGA * AFGEN(TMNFTB, ILTMNF, TMINRA)$$

Not high nighttime temperature effect on respiration, but the infrastructure makes it easy to incorporate.

Potential gross assimilation (PGASS) is obtained by converting assimilation into CH_2O (kg CH_2O $ha^{-1}d^{-1}$) as:

$$PGASS = DTGA * 30/44$$

Final gross assimilation, adjusted $PGASS$ with **water stress** (actual to potential transpiration) is:

$$GASS = PGASS * \frac{TRA}{TRA_{max}}$$

Daily aboveground dry matter (ADMI) is computed by multiplying assimilation with conversion coefficient:

$$ADMI = CVF * (GASS - MRES) * (1 - FR)$$

whereCVF is conversion factor, $MRES$ is maintenance respiration, FR is fraction allocated to root. Integration over growing period gives overall biomass.

Yield formation

No explicit modeling for harvest index, but harvestable dry matter is simulated with allocation to storage organ as a function of time.Daily allocation is:

$$GWSO = ADMI * AFGEN\ (FOTB, ILFO, DVS)$$

Integration over growing period gives final yield.

PS:$\boldsymbol{AFGEN}(TB, IL, \hat{x})$ function

Multi-linear interpolation with “TB”a one-dimensional array with paired data (x1, y1, x2, y2, etc.), “IL” length of TB, $\hat{x}$ value at which interpolation should take place:

$$\hat{y} = y_{n-1} + (\hat{x} - x_{n-1}) \times \frac{y_n - y_{n-1}}{x_n - x_{n-1}}$$

$AMAXTB$, $TMPFTB$ and $TMNFTB$ values for maize and soybean can be found at:

https://github.com/ajwdewit/WOFOST/blob/1a9a58e50f5da52c6eff616eb93e1a85bbebd482/cropd/grain_maize.crp

https://github.com/ajwdewit/WOFOST/blob/1a9a58e50f5da52c6eff616eb93e1a85bbebd482/cropd/soybean.w41