Conceptual basis, formalisations and parameterization of the SUNFLO crop model

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Summary

SUNFLO[1] is a process-based model for the sunflower crop which was developped to simulate the grain yield and oil concentration as a function of time (t), environment (E) which includes soil, climate and management practice and genetic diversity (G) (Debaeke *et al.*, 2010; Casadebaig *et al.*, 2011; Lecoeur *et al.*, 2011).

This model is based on a conceptual framework initially proposed by Monteith (1977) and now shared by a large familly of crop models (Jones *et al.*, 2016). In this framework, the daily crop dry biomass (DM_t) is calculated as a difference equation[2] function of incident photosynthetically active radiation (PAR, $MJ.m^{-2}$), light interception efficiency (RIE) and radiation use efficiency (RUE, $g.MJ^{-1}$). The light interception efficiency is based on Beer-Lambert's law[3] as a function of leaf area index (LAI) and light extinction coefficient (k). The radiation use efficiency concept (Monteith, 1994) is used to represent photosynthesis at the crop scale.

Broad scale processes of this framework, the dynamics of $LAI = f(t, G, E)$, photosynthesis ($RUE = f(t, G, E)$) and biomass allocation to grains were split into finer processes (e.g leaf expansion and senescence, response functions to environmental stresses) to reveal genotypic specificity and to allow the emergence of genotype-by-environment interactions. Globally, the SUNFLO crop model has about 50 equations and 64 parameters (43 plant-related traits and 21 environment-related).

[1] model version: commit SHA `897bc320`, repository

[2] $DM_t = DM_{t-1} + PAR \times RIE \times RUE$

[3] $RIE = 1 - exp^{-k\ LAI}$

Inputs

Climate

Climate input data are measured from weather stations close to the field location. Alternatively, predicted data from gridded general circulation models can be used.

label	description	unit
TemperatureAirMin	Daily average of minimum air temperature	°C
TemperatureAirMax	Daily average of maximum air temperature	°C
Radiation	Daily sum of global incident radiation	MJ.m-2
PET	Daily sum of reference evapotranspiration (Penman-Monteith)	mm
Rainfall	Daily sum of rainfall	mm

Soil

Soil is described by two layers (0-30 cm, 30 cm - root depth) and is summarised by its water capacity (mm) and mineralization rate. Soil parameters can be measured from a standard soil analysis or estimated using a soil database (e.g. European Soil Database, ESDB) (Hiederer, 2013). Maximum rooting depth should be superior to the depth of surface layer (300 mm).

label	description	value	unit	reference
RootDepthLimit	Maximum soil rooting depth (> 300 mm)	1000.0	mm	(Lecoeur *et al.*, 2011)
SoilWaterCapacity	Gravimetric water content at field capacity (0 - 300 mm)	19.7	%	-
SoilWaterCapacity	Gravimetric water content at wilting point (0 - 300 mm)	9.7	%	-
SoilWaterCapacity	Gravimetric water content at field capacity (300 mm - root depth)	19.7	%	-
SoilWaterCapacity	Gravimetric water content at wilting point (300 mm - root depth)	9.7	%	-
SoilDensity	Soil bulk density, sieved < 5mm, (0 - 300 mm)	1.3	$g.cm^{-3}$	-
SoilDensity	Soil bulk density, sieved < 5mm, (300 mm - root depth)	1.3	$g.cm^{-3}$	-
StoneContent	Stone content (0 - root depth)	0.1	$[0, 1]$	-
PotentialMineralizationRate	Potential nitrogen mineralization rate	0.5	$kg.ha^{-1}.day^{-1}$	(Valé *et al.*, 2007)

Management

label	description	unit
SowingDate	Sowing date	$date(dd/mm)$
HarvestDate	Harvest date	$date(dd/mm)$
SowingDensity	Plant density	$plant.m^{-2}$
Fertilization	Fertilization date vector	$date(dd/mm)$
Fertilization	Fertilization amount vector	$kg.ha^{-1}$ eq. mineral nitrogen
Irrigation	Irrigation date vector	$date(dd/mm)$
Irrigation	Irrigation amount vector	mm

Cultivar

The values of the genotype-dependent parameters were obtained by measuring the value of phenotypic traits in dedicated field platforms (Casadebaig *et al.*, 2016) and controlled conditions (Casadebaig *et al.*, 2008).

symbol	label	description	value	unit	reference
$TDE1$	ThermalTimeVegetative	Temperature sum to floral initiation	482.00	$C.d$	(Lecoeur *et al.*, 2011)
$TDF1$	ThermalTimeFlowering	Temperature sum from emergence to the beginning of flowering	836.00	$C.d$	(Lecoeur *et al.*, 2011)
$TDM0$	ThermalTimeSenescence	Temperature sum from emergence to the beginning of grain filling	1083.00	$C.d$	(Lecoeur *et al.*, 2011)
$TDM3$	ThermalTimeMaturity	Temperature sum from emergence to seed physiological maturity	1673.00	$C.d$	(Lecoeur *et al.*, 2011)
TLN	PotentialLeafNumber	Potential number of leaves at flowering	29.00	$leaf$	(Lecoeur *et al.*, 2011)
LLH	PotentialLeafProfile	Potential rank of the plant largest leaf at flowering	17.00	$leaf$	(Lecoeur *et al.*, 2011)
LLS	PotentialLeafSize	Potential area of the plant largest leaf at flowering	448.00	cm^{-2}	(Lecoeur *et al.*, 2011)
k	ExtinctionCoefficient	Light extinction coefficient during vegetative growth	0.88	-	(Lecoeur *et al.*, 2011)
LE	WaterResponseExpansion	Threshold for leaf expansion response to water stress	-4.42	-	(Casadebaig *et al.*, 2008)
TR	WaterResponseConductance	Threshold for stomatal conductance response to water stress	-9.30	-	(Casadebaig *et al.*, 2008)
HI	PotentialHarvestIndex	Potential harvest index	0.40	-	(Casadebaig *et al.*, 2011)
OC	PotentialOilContent	Potential seed oil content	55.40	$\% dry$	(Casadebaig *et al.*, 2011)

Phenology

label	description	value	unit	reference
ThermalTimeVegetative	Temperature sum to floral initiation	482.0	$C.d$	(Lecoeur *et al.*, 2011)
ThermalTimeFlowering	Temperature sum from emergence to the beginning of flowering	836.0	$C.d$	(Lecoeur *et al.*, 2011)
ThermalTimeSenescence	Temperature sum from emergence to the beginning of grain filling	1083.0	$C.d$	(Lecoeur *et al.*, 2011)
ThermalTimeMaturity	Temperature sum from emergence to seed physiological maturity	1673.0	$C.d$	(Lecoeur *et al.*, 2011)
SowingDepth	Sowing depth	30.0	mm	NA
TemperatureBase	Base temperature for development and growth process	4.8	C	(Granier and Tardieu, 1998)
Germination	Temperature sum from sowing to germination	86.2	$C.d$	(Casadebaig *et al.*, 2011)
ElongationRate	Reciprocal of hypocotyl elongation rate	1.2	$Cd.mm^{-1}$	(Villalobos *et al.*, 1996)

Emergence

Seed germination and hypocotyl elongation are a function of temperature.

$$Emergence = Germination + (ElongationRate \times SowingDepth)$$

with:

- $Germination = 86$, Thermal time for germination (°C.d);
- $ElongationRate = 1.19$, Hypocotyl elongation rate (°Cd mm-1)
- $SowingDepth = 30$, Default sowing depth (mm).

ThermalTime

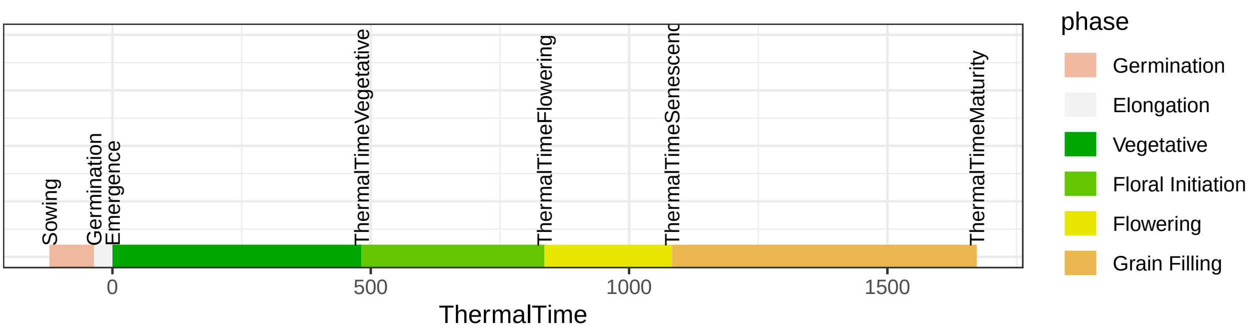
Thermal time accumulation is a function of base temperature, mean air temperature, and water stress.

$$ThermalTime_t = \begin{cases} \int_0^t (T_m - T_b) \times (1 + WaterStressPhenology), & \text{if } T_m > T_b \\ 0, & \text{else} \end{cases}$$

with:

- T_m, daily mean air temperature (°C);
- $T_b = 4.8$, Base temperature (°C) (Granier and Tardieu, 1998);
- $ThermalStressPhenology$, Water stress effect on plant heating

PhenoStages



Phenostages are computed as integers $\in [0, 7]$ corresponding to duration between key phenological stages:

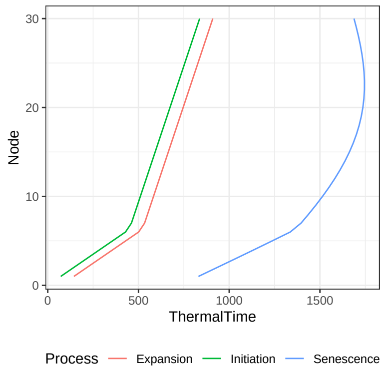
- **0**, begining of simulation - sowing (bare soil)
- **1**, sowing (A0) - emergence (A2)
- **2**, emergence (A2) - floral initiation (E1)
- **3**, floral initiation (E1) - flowering (F1)
- **4**, flowering (F1) - onset of senescence (M0)
- **5**, onset of senescence (M0) - maturity (M3)
- **6**, maturity (M3) - harvest
- **7**, harvest - end of simulation (bare soil)

Leaf Area

label	description	value	unit	reference
PotentialLeafNumber	Potential number of leaves at flowering	29.0	$leaf$	(Lecoeur *et al.*, 2011)
PotentialLeafProfile	Potential rank of the plant largest leaf at flowering	17.0	$leaf$	(Lecoeur *et al.*, 2011)
PotentialLeafSize	Potential area of the plant largest leaf at flowering	448.0	cm^{-2}	(Lecoeur *et al.*, 2011)
Phyllotherm_1	Phyllotherm (leaf <= 6)	71.4	$C.d$	(Rey, 2003)
Phyllotherm_7	Phyllotherm (leaf > 6)	16.3	$C.d$	(Rey, 2003)
PotentialLeafDurationMin	Asymptote of leaf longevity function, base leaf duration	153.0	$C.d$	(Casadebaig, 2008)
PotentialLeafDurationMax	Maximum thermal time between expansion and senescence	851.3	$C.d$	(Casadebaig, 2008)
PotentialLeafDurationWidth	Width of leaf longevity function	0.8	$leaf$	(Casadebaig, 2008)
PotentialGrowthSlope	Rate of leaf growth and senescence processes	0.0	-	(Casadebaig, 2008)

LeafInitiationTime, LeafExpansionTime, LeafSenescenceTime

The rate of leaf initiation depends on air temperature and two phyllochrons as preformed lower leaves appear at a lower rate (Rey, 2003).



$$LeafInitiationTime_i = \begin{cases} i \times Phyllotherm_1, & \text{if } i \leq 6 \\ (i-5) \times Phyllotherm_7 + 6 \times Phyllotherm_1, & \text{if } i \leq LeafNumber \end{cases}$$

with:

- $Phyllotherm_1 = 76.43$ (°C d)
- $Phyllotherm_7 = 16.34$ (°C d)

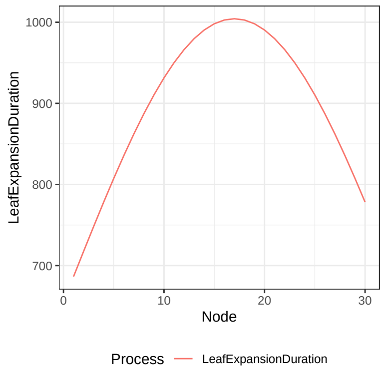
Thermal time at 50% of final leaf area is defined as a function of leaf initiation.

$$LeafExpansionTime_i = LeafInitiationTime_i + 1/a$$

with $a = 0.01379$.

LeafExpansionDuration

The duration of leaf expansion is a function of plant architecture (leaf number and leaf profile).



$$LeafExpansionDuration_i = a + b \times exp^{\frac{-(i-PotentialLeafProfile)^2}{(c \times PotentialLeafNumber)^2}}$$

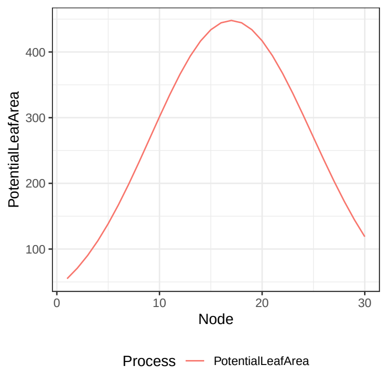
with:

- $a = PotentialLeafDurationMin = 153$ (°C d)
- $b = PotentialLeafDurationMax = 851.3$ (°C d)
- $c = PotentialLeafDurationWidth = 0.78$

$$LeafSenescenceTime_i = LeafExpansionTime_i + LeafExpansionDuration_i$$

PotentialLeafArea

The potential area of individual leaves is a function of plant architecture descriptors (total leaf number, area and position of the largest leaf).

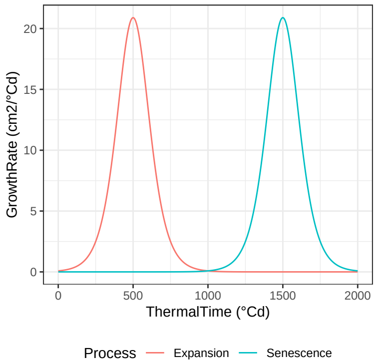


$$PotentialLeafArea_i = PotentialLeafSize \times exp^{a \times (\frac{i-PotentialLeafProfile}{PotentialLeafProfile-1})^2 + b \times (\frac{i-PotentialLeafProfile}{PotentialLeafProfile-1})^3}$$

with:

- $a = -2.05$ and $b = 0.049$, shape parameters
- $PotentialLeafSize$ (cm²) and $PotentialLeafProfile$ (node), genotype-dependent parameters.

LeafExpansionRate, LeafSenescenceRate



Potential expansion or senescence rate of leaf i is a function of thermal time and potential area of the leaf. The illustration uses $i = 10$ as values for $PotentialLeafArea_i$, $LeafExpansionTime_i$ and $LeafSenescenceTime_i$

$$LeafExpansionRate_i = (T_m - T_b) \times PotentialLeafArea_i \times a \times \frac{exp^{-a(ThermalTime - LeafExpansionTime_i)}}{(1 + exp^{-a(ThermalTime - LeafExpansionTime_i)})2}$$

$$LeafSenescenceRate_i = (T_m - T_b) \times LeafArea_i \times a \times \frac{exp^{-a(ThermalTime - LeafSenescenceTime_i)}}{(1 + exp^{-a(ThermalTime - LeafSenescenceTime_i)})2}$$

with:

- $T_m = 25$, mean air temperature (°C)
- $T_b = 4.8$, base temperature (°C)
- $a = 0.01379$

LeafArea, PlantLeafArea

Individual leaf expansion is impacted by water and nitrogen stress during leaf longevity. Leaf senescence is only function of temperature. Active leaf area is the difference between total and senescent leaf area.

$$TotalLeafArea_{it} = \int_0^t LeafExpansionRate_{it} \times WaterStressExpansion_t \times NitrogenStressExpansion_t$$

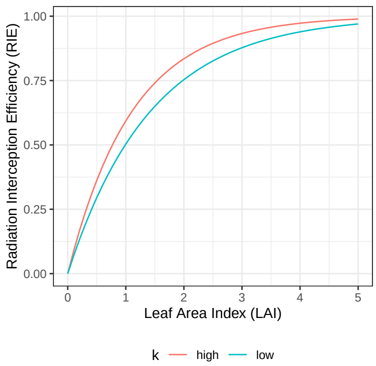
$$SenescentLeafArea_{it} = \int_0^t LeafSenescenceRate_{it}$$

$$PlantLeafArea_t = \sum_{i=1}^{LeafNumber} TotalLeafArea_{it} - SenescentLeafArea_{it}$$

Light Interception

symbol	label	description	value	unit	reference
k	ExtinctionCoefficient	Light extinction coefficient during vegetative growth	0.9	-	(Lecoeur *et al.*, 2011)
-	SowingDensity	Plant density	7.0	$plant.m^{-2}$	NA

Leaf Area Index (LAI)



$$LAI_t = SowingDensity \times PlantLeafArea_t$$

Radiation Interception Efficiency (RIE)

Beer–Lambert law is used to model light interception assuming an homogeneous distribution of leaves for a given soil area (LAI).

$$RIE = 1 - exp^{(-k \times LAI_t)}$$

with:

- k, light extinction coefficient, genotype-dependent parameter.

Biomass production

symbol	label	description	value	unit	reference
r_0	PotentialRUEVegetative	Initial value for RUE during vegetative stage	1.00	$g.MJ^{-1}.m^{-2}$	(Casadebaig *et al.*, 2011
r_{max}	PotentialRUEMax	Maximum value of RUE during flowering stage	3.00	$g.MJ^{-1}.m^{-2}$	(Casadebaig *et al.*, 2011
r_d	PotentialRUEReproductive	Rate of RUE decrease during reproductive stage	4.50	$g.MJ^{-1}.m^{-2}$	(Casadebaig *et al.*, 2011
r_{min}	PotentialRUEMin	Minimum value of RUE at the end of reproductive stage	0.02	$g.MJ^{-1}.m^{-2}$	(Casadebaig *et al.*, 2011

Radiation Use Efficiency (RUE)

The variation of radiation use efficiency during crop development is modeled with a piecewise function. The increase in energy cost of the biomass produced (oil content) is modeled by exponential decrease of RUE during grain filling.

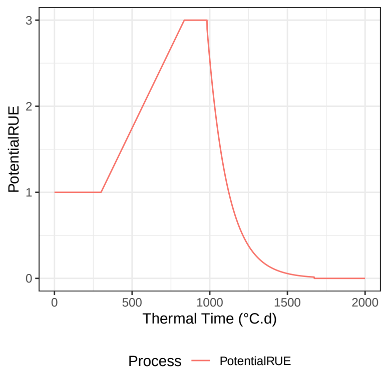
$$PotentialRUE_t = \begin{cases} r_0, & \text{if } ThermalTime < 300 \\ r_0 + 2 \times \frac{ThermalTime-300}{ThermalTimeFlowering-300}, & \text{if } 300 < ThermalTime < ThermalTimeFlowering \\ r_{max}, & \text{if } ThermalTimeFlowering < ThermalTime < ThermalTimeSenescence \\ a \times exp^{b \times (1-\frac{ThermalTime-ThermalTimeMaturity}{ThermalTimeMaturity-ThermalTimeSenescence})}, & \text{if } ThermalTimeSenescence < ThermalTime < ThermalTimeMaturity \\ 0, \text{else} \end{cases}$$

with:

- $r_0 = 1$, vegetative RUE
- $r_{max} = 3$, maximum RUE
- $a = 0.015$, final RUE
- $b = 4.5$, slope of RUE decrease in grain filling stage

The considered abiotic stresses (temperature, water, nitrogen) multiplicatively impact the potential RUE each day.

$$RUE_t = PotentialRUE_t \times ThermalStressRUE_t \times WaterStressRUE_t \times NitrogenStressRUE_t$$



CropBiomass

Intercepted light is the main driver of biomass accumulation ($CropBiomassRate$), based on Monteith (1977) model.

$$CropBiomass_t = CropBiomass_{t-1} + (PAR_t \times RIE_t \times RUE_t)$$

with:

- $PAR_t = Radiation_t \times 0.48$, Photosynthetically active radiation

Crop Performance

Harvest index and oil content value at harvest time are predicted using a linear regression based on a subset of simulated state variables.

Harvest Index

factor	process	symbol	description	unit	formula	integration
water	photosynthesis	NETR_EF	Edaphic water deficit (discrete)	d	$sum(ET/PET < 0.6)$	vegetative
water	photosynthesis	NETR_FM	Edaphic water deficit (discrete)	d	$sum(ET/PET < 0.6)$	flowering
water	photosynthesis	NETR_MH	Edaphic water deficit (discrete)	d	$sum(ET/PET < 0.6)$	filling
-	photosynthesis	STDM_F	Aerial Biomass at flowering	$g.m^{-2}$	$max(TDM$	flowering
water	transpiration	STR_FH	Sum of water loss through transpiration	mm	$sum(TR)$	reproductive
temperature	phenology	TT_FH	Thermal time since flowering (4.8 C basis)	$C.d$	$sum(TM - 4.8)$	reproductive
genotype	allocation	HI	Potential harvest index	-	-	-

The following coefficients are used to predict harvest index at harvest time (Casadebaig *et al.*, 2011).

```
Coefficients:
            Estimate   Std. Error t value Pr(>|t|)
(Intercept)  9.370e-02  6.996e-02   1.339 0.182276
STDM_F      -1.552e-04  6.376e-05  -2.434 0.015982 *
NETR_EF     -2.828e-03  1.335e-03  -2.118 0.035650 *
NETR_FM     -2.557e-03  1.174e-03  -2.178 0.030813 *
NETR_MH     -1.940e-03  4.995e-04  -3.884 0.000148 ***
STR_FH      -3.907e-04  1.696e-04  -2.304 0.022464 *
TT_FH        1.274e-04  3.190e-05   3.992 9.80e-05 ***
HI           8.189e-01  1.540e-01   5.317 3.34e-07 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
Adjusted R-squared: 0.3036 F-statistic: 11.84 on 7 and 167 DF,  p-value: 3.311e-12
```

Oil Content

factor	process	symbol	description	unit	formula	integration
genotype	allocation	OC	Potential seed oil content	% dry	-	-
water	photosynthesis	SFTSW_FM	Edaphic water deficit (continuous)	-	$sum(1-FTSW)$	flowering
water	photosynthesis	SFTSW_MH	Edaphic water deficit (continuous)	-	$sum(1-FTSW)$	filling
nitrogen	nutrition	SNAB_MH	Absorbed nitrogen	$kg.ha^{-1}$	$max(NAB)$	filling
nitrogen	photosynthesis	NNNIE_EM	Nitrogen excess (discrete)	d	$sum(NNI > 1.2)$	flowering
temperature	photosynthesis	NHT_MH	Thermal stress, heat (discrete)	d	$sum(TM > 34)$	filling
-	photosynthesis	MRUE_MH	Photosynthesis	$g.MJ^{-1}.m^{-2}$	$mean(RUE)$	filling
-	interception	LAD_MH	Leaf area duration	-	$sum(LAI)$	filling
management	-	DENS	Plant density	$plant.m^{-2}$	-	-

The following coefficients are used to predict oil content at harvest time (Andrianasolo *et al.*, 2014).

```
Coefficients:
               Estimate Std. Error t value Pr(>|t|)
(Intercept)  -18.702220   3.898791  -4.797 2.26e-06 ***
OC             0.996473   0.059631  16.711  < 2e-16 ***
SFTSW_FM       0.111097   0.026317   4.221 2.99e-05 ***
SFTSW_MH       0.126438   0.041208   3.068 0.002297 **
NNNIE_EM      -0.068492   0.015455  -4.432 1.20e-05 ***
SNAB_MH       -0.035815   0.010669  -3.357 0.000862 ***
NHT_MH        -0.235708   0.049564  -4.756 2.75e-06 ***
LAD_MH         0.007082   0.009191   0.771 0.441441
MRUE_MH       21.052693   2.900957   7.257 2.01e-12 ***
DENS           0.831619   0.172779   4.813 2.10e-06 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 2.516 on 408 degrees of freedom
Multiple R-squared:  0.5022,	Adjusted R-squared:  0.4913
F-statistic: 45.74 on 9 and 408 DF,  p-value: < 2.2e-16
```

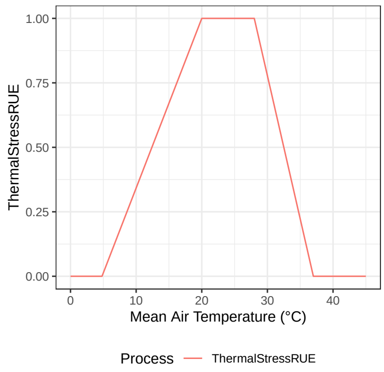
Crop Yield

At harvest time, crop yield is computed as the proportion of total aerial biomass allocated to seeds (i.e. crop yield is not defined before harvest).

$$CropYield_{harvest} = CropBiomass_{harvest} \times HarvestIndex_{harvest}$$

Thermal stress

ThermalStressRUE



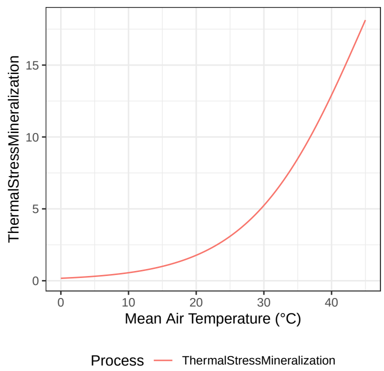
The impact of temperature on photosynthesis is modeled with a piecewise linear function, with four thresholds defined below (Villalobos *et al.*, 1996).

$$ThermalStressRUE_t = \begin{cases} T_m \times \frac{1}{T_{ol} - T_b} - \frac{T_b}{T_{ol} - T_b}, & \text{if } T_b < T_m < T_{ol} \\ 1, & \text{if } T_{ol} < T_m < T_{ou} \\ T_m \times \frac{1}{T_{ou} - T_c} - \frac{T_c}{T_{ou} - T_c}, & \text{if } T_{ou} < T_m < T_c \\ 0, & \text{else} \end{cases}$$

with:

- $T_b = 4.8$, base temperature (°C)
- $T_{ol} = 20$, optimal lower temperature (°C)
- $T_{ou} = 28$, optimal upper temperature (°C)
- $T_c = 37$, critical temperature (°C)

ThermalStressMineralization



A logistic function is used to describe the effect of air temperature on net nitrogen mineralization (Valé, 2006; Valé *et al.*, 2007). The parameterization does not change with soil type.

$$ThermalStressMineralization_t = \frac{T_c}{1 + (T_c - 1) \times exp^{(-0.119 \times (T_m - T_b))}}$$

with:

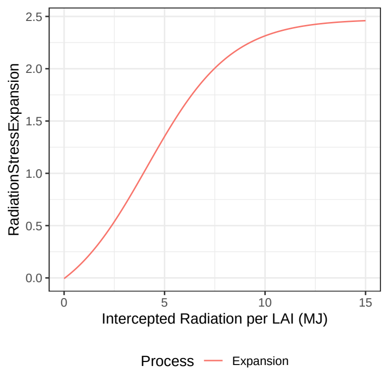
- $T_b = 15$, base temperature (°C)
- $T_c = 36$, critical temperature (°C)

ThermalStressAllocation

Predictors based on temperature are used in linear models of harvest index and oil content and are described in the *Crop Performance* section.

Radiation stress

RadiationStressExpansion



Competition for light affects leaf expansion, allowing to model the plant area response to sowing density (Rey, 2003).

$$RadiationStressExpansion_t = s \times (a + \frac{b}{1 + exp^{(\frac{c - \frac{IPAR_t}{LAI_t}}{d})}})$$

with:

- $IPAR_t = PAR_t \times RIE_t$, light intercepted by the crop;
- $s = 2.5$, scaling parameter for density effect;
- $a = -0.14$; $b = 1.13$; $c = 4.13$; $d = 2.09$

Water stress

symbol	label	description	value	unit	reference
LE	WaterResponseExpansion	Threshold for leaf expansion response to water stress	-4.4	-	(Casadebaig *et al.*, 2008)
TR	WaterResponseConductance	Threshold for stomatal conductance response to water stress	-9.3	-	(Casadebaig *et al.*, 2008)
-	RootDepthLimit	Maximum soil rooting depth (> 300 mm)	1000.0	mm	(Lecoeur *et al.*, 2011)
θ_{fc}	SoilWaterCapacity	Gravimetric water content at field capacity (0 - 300 mm)	19.7	%	-
θ_{wp}	SoilWaterCapacity	Gravimetric water content at wilting point (0 - 300 mm)	9.7	%	-
θ_{fc}	SoilWaterCapacity	Gravimetric water content at field capacity (300 mm - root depth)	19.7	%	-
θ_{wp}	SoilWaterCapacity	Gravimetric water content at wilting point (300 mm - root depth)	9.7	%	-
-	SoilDensity	Soil bulk density, sieved < 5mm, (0 - 300 mm)	1.3	$g.cm^{-3}$	-
-	SoilDensity	Soil bulk density, sieved < 5mm, (300 mm - root depth)	1.3	$g.cm^{-3}$	-
-	StoneContent	Stone content (0 - root depth)	0.1	$[0,1]$	-
θ_0	SoilWaterInitial	Initial value for soil water capacity in surface layer (0 - 300 mm)	1.0	$[0,1]$	-
θ_0	SoilWaterInitial	Initial value for soil water capacity in root layer (300 mm - rooting depth)	1.0	$[0,1]$	-
-	RootDepthMaximum	Maximum species rooting depth	1800.0	mm	(Casadebaig, 2008)
NA	NA	Scaling factor for phenology reponse to water deficit	0.1	-	(Casadebaig, 2008)
-	RootGrowthRate	Root growth rate	0.7	$mm.Cd^-1$	(Lecoeur *et al.*, 2011)
K_c	CropCoefficient	Crop coefficient for potential crop transpiration	1.2	-	(Lecoeur *et al.*, 2011)

RootGrowth

Root growth is a linear function of temperature and stops at estimated maximum soil rooting depth.

$$RootDepth = \begin{cases} RootGrowthRate \times T_m, & \text{if } RootDepth < RootDepthLimit \\ RootDepthLimit, & \text{else} \end{cases}$$

with:

- $RootGrowthRate = 0.7$, root elongation rate (mm °Cd-1)
- $RootDepthMax = 1800$, maximum root depth (mm)

WaterSupply

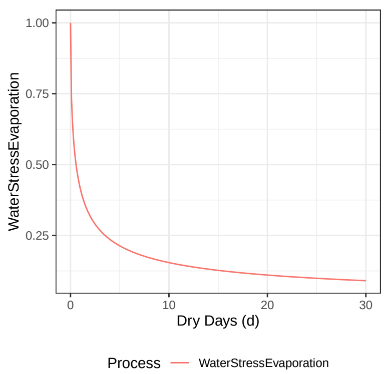
The water balance model treats the soil as a reservoir with three dynamic layers: surface layer (0-30 cm), root layer (30-rooting front), and soil layer (rooting front - soil depth) (Sarr *et al.*, 2004). Rainfall, irrigation and evaporation only impacts the balance of the surface layer. Water movement in the soil is assumed to be only vertical, with runoff and lateral flow being ignored. Drainage occurs when the water content of a layer exceeds its water retention capacity (defined by the $SoilWaterCapacity$ parameter).

$$WaterAvailable_t = Rainfall_t + Irrigation_t - Evaporation_t - Transpiration_t - Drainage_t$$

Soil evaporation is modeled with the same approach as crop transpiration.

$$Evaporation_t = (1 - RIE) \times PET \times WaterStressEvaporation$$

The relative soil evaporation is based on Ritchie (1981) two-stage model, where soil evaporation is reduced as a function ($WaterStressEvaporation$) of the number of days since last water input (x)



$$WaterStressEvaporation = \sqrt{x+1} - \sqrt{x}$$

with:

$$dx/dt = \begin{cases} 1, & \text{if } Rainfall + Irrigation <= 4 \\ 0, & \text{else} \end{cases}$$

Crop transpiration rate correspond to the water demand scaled by the reduction of transpiration under water deficit (control of stomatal conductance).

$$Transpiration_t = WaterDemand_t \times WaterStressConductance_t$$

WaterDemand

Water demand is a function of crop light interception and potential evapotranspiration.

$$WaterDemand_t = RIE_t \times PET_t \times K_c$$

with $K_c = 1.2$, crop coefficient

WaterStress

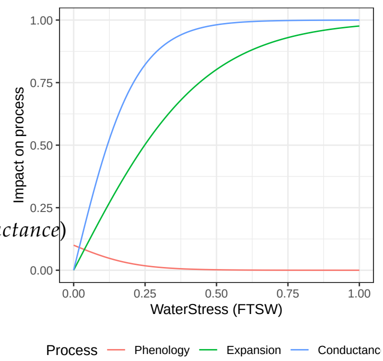
The fraction of transpirable soil water ($FTSW$, Sinclair, 2005) accounts for the amount of soil water available to the plant within the root zone. $FTSW$ is used to drive function representing various physiological responses to water deficit in the model.

$$WaterStress_t = FTSW_t = \frac{WaterAvailable_t}{WaterTotal_t}$$

Total water available for the crop depends on rooting depth and soil texture and density.

$$WaterTotal_t = RootDepth_t \times SoilWaterCapacity \times SoilDensity \times (1 - StoneContent)$$

with $SoilWaterCapacity = \theta_{fc} - \theta_{wp}$, the difference between the gravimetric water content at field capacity and at wilting point.



WaterStressExpansion, WaterStressConductance, WaterStressRUE

Leaf expansion and plant transpiration rates are exponentially reduced with increased water deficit. The same response curve is used for transpiration ($WaterStressConductance$) and photosynthesis ($WaterStressRUE$).

$$WaterStressProcess_t = -1 + \frac{2}{1 + exp^{(a \times WaterStress_t)}}$$

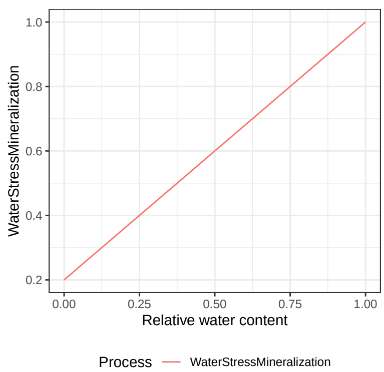
with $a \in [-15.6; -2.3]$, genotype-dependant response parameter

WaterStressPhenology

Accelerated crop developement under water deficit is modeled as a function plant sensitivity to water deficit.

$$WaterStressPhenology_t = a \times (1 - WaterStressConductance_t)$$

with $a = 0.1$, scaling parameter for water-stress plant heating



WaterStressMineralization

The effect of soil water content on net mineral nitrogen mineralization is described by a linear function (Mary *et al.*, 1999; Valé, 2006).

$$WaterStressMineralization = (1 - y_0) \times RelativeWaterContent + y_0$$

with:

- $y_0 = 0.2$, relative nitrogen mineralization rate at wilting point
- $RelativeWaterContent = \frac{\theta - \theta_{wp}}{\theta_{fc} - \theta_{wp}}$, relative water content in surface layer.

Nitrogen stress

symbol	label	description	value	unit	reference
v_0	PotentialMineralizationRate	Potential nitrogen mineralization rate	0.5	$kg.ha^{-1}.day^{-1}$	(Valé *et al.*, 2007)
y_0	WaterResponseMineralization	Relative nitrogen mineralization rate at wilting point	0.2	-	(Mary *et al.*, 1999)
-	SoilNitrogenInitial	Initial value for nitrogen residuals in surface layer (0 - 300 mm)	10.0	$kg.ha^{-1}$	-
-	SoilNitrogenInitial	Initial value for nitrogen residuals in root layer (300 mm - rooting depth)	20.0	$kg.ha^{-1}$	-
a	PlantNitrogenCritical	Critical plant nitrogen concentration threshold	4.5	%	(Debaeke *et al.*, 2012)
b	PlantNitrogenCritical	Slope for critical nitrogen dilution curve	0.4	-	(Debaeke *et al.*, 2012)
a	PlantNitrogenMaximum	Maximum plant nitrogen concentration threshold	6.5	%	(Debaeke *et al.*, 2012)
b	PlantNitrogenMaximum	Slope for maximum nitrogen dilution curve	0.4	-	(Debaeke *et al.*, 2012)
-	NitrogenResponseExpansion	Threshold for leaf expansion response to nitrogen stress	0.6	-	(Brisson *et al.*, 2009)
-	NitrogenResponseExpansion	Minimum value of leaf expansion response to nitrogen stress	0.3	-	(Brisson *et al.*, 2009)

NitrogenSupply

The mineral nitrogen content of the soil layers (kg ha^{-1}) depends on nitrogen fertilization, mineralization, leaching, denitrification, and plant uptake. The amount of nitrogen added to the surface layer from fertilization depends on a threshold of water input (5 mm) for solubilization and nitrogen use efficiency[4], which is modeled as a linear function of crop growth rate (g m^{-2} °Cd^{-1}) (Limaux *et al.*, 1999). Leaching is the product of drained water (*Drainage*) and the nitrogen concentration from the soil layer concerned.

[4] $NUE = 30 + 0.34 \times CropBiomassRate \times 100$

$$SoilNitrogenContent_t = Fertilization_t + Mineralization_t - Leaching_t - Denitrification_t - NitrogenUptake_t$$

Nitrogen mineralization takes place in surface layer and is impacted by relative soil water content and temperature.

$$MineralizationRate_t = PotentialMineralizationRate \times WaterStressMineralization_t \times ThermalStressMineralization_t$$

Denitrification occurs when the surface soil layer is water saturated and is function of air temperature (Sinclair and Muchow, 1995).

$$DenitrificationRate_t = 6 \times exp^{(a \times T_m - b)}$$

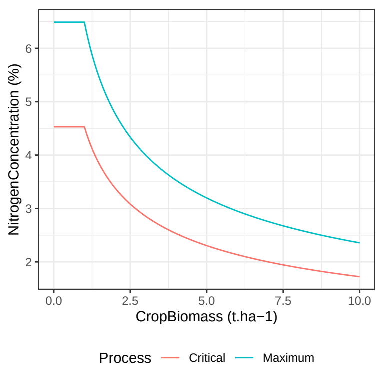
with:

- T_m, daily mean air temperature (°C);
- $a = 0.07738$ and $b = 6.593$ (Sinclair and Muchow, 1995)

Soil nitrogen is absorbed in the transpirational stream (mass flow).

$$NitrogenSupply_t = NitrogenUptake_t$$

$$NitrogenUptakeRate_t = TranspirationRate_t \times SoilNitrogenConcentration_t$$



NitrogenDemand

Crop nitrogen demand is driven by the nitrogen dilution in the biomass produced. Two thresholds (critical and maximal) for plant nitrogen concentration (% dry matter) were thus experimentally defined by monitoring nitrogen accumulation in relation to crop biomass for various fertilization levels (0–160 kg ha^{-1}) in field (Debaeke *et al.*, 2012).

$$CropNitrogenConcentration = min(a, a \times CropBiomass^{-b})$$

with:

- $CropBiomass$, daily shoot biomass (t ha^{-1});
- $CropNitrogenConcentrationCritical$ is defined with $a = 4.53$ and $b = 0.42$;
- $CropNitrogenConcentrationMaximum$ is defined with $a = 6.49$ and $b = 0.44$;

The critical crop nitrogen uptake is defined as the minimum nitrogen uptake necessary to achieve maximum biomass accumulation.

$$NitrogenDemand_t = CropNitrogenConcentrationCritical_t \times CropBiomass_t$$

NitrogenStress

Nitrogen stress index (Nitrogen Nutrition Index, NNI, see Lemaire and Meynard, 1997), is based on the ratio of actually absorbed nitrogen (*NitrogenSupply*, kg ha^{-1}) to the critical nitrogen amount needed to satisfy the demand (N*NitrogenDemand*, kg ha^{-1}).

$$NitrogenStress_t = \frac{NitrogenSupply_t}{NitrogenDemand_t} = NNI$$

NitrogenStressExpansion

The impact of nitrogen deficit on leaf expansion is a linear function of nitrogen stress index (Brisson *et al.*, 2009).

$$NitrogenStressExpansion_t = \begin{cases} 1.75 \times NNI - 0.75, & \text{if } NNI > 0.6 \\ 0.3, & \text{else} \end{cases}$$

NitrogenStressRUE

The impact of nitrogen deficit on photosynthesis (RUE) is the ratio of daily nitrogen uptake rate to the daily critical nitrogen amount needed to satisfy the demand.

$$NitrogenStressRUE_t = \frac{NitrogenSupplyRate_t}{NitrogenDemandRate_t}$$

Outputs

Timed variables

symbol	label	description	unit
TN	TemperatureAirMin	Minimum air temperature	C
TX	TemperatureAirMax	Maximum air temperature	C
TM	TemperatureAirMean	Mean air temperature	C
GR	Radiation	Global incident radiation	$MJ.m^{-2}$
ETP	PET	Reference evapotranspiration	mm
RR	Rainfall	Rainfall	mm
TTA2	ThermalTime	Temperature sum from emergence	$C.d$
PhenoStage	PhenoStage	Phenological stages index	-
FTSW	WaterStress	Fraction of transpirable soil water	-
FHTR	WaterStressConductance	Transpiration response to water stress	-
FHRUE	WaterStressConductance	Photosynthesis response to water stress	-
ETRETM	WaterSupplyDemandRatio	Water supply:demand ratio	-
FTRUE	ThermalStressRUE	Photosynthesis response to thermal stress	-
NAB	NitrogenAbsorbed	Absorbed nitrogen	$kg.ha^{-1}.d^{-1}$
NNI	NitrogenNutritionIndex	Nitrogen nutrition index	-
FNRUE	NitrogenStressRUE	Photosynthesis response to nitrogen stress	-
LAI	LAI	Leaf area index	-
RIE	RIE	Radiation interception efficiency	-
RUE	RUE	Radiation use efficiency	-
TDM	CropBiomass	Crop aerial dry biomass	$g.m^{-2}$
GY	CropYield	Grain yield	$q.ha^{-1}$
OC	OilContent	Grain oil content	$\%(drymatter)$

Indicators

level	factor	symbol	description	unit	formula
climate	light	SGR	Photosynthetically active radiation	$MJ.m^{-2}$	$sum(GR * 0.48)$
climate	water	SRR	Rain	mm	$sum(RR)$
climate	water	SPET	Potential evapotranspiration	mm	$sum(PET)$
climate	water	SCWD	Climatic water deficit	mm	$sum(RR - PET)$
species	temperature	TT	Thermal time (4.8 C basis)	$C.d$	$sum(TM - 4.8)$
species	temperature	D_SE	Duration of sowing - emergence phase	d	-
genotype	temperature	D_EF	Duration of vegetative phase	d	-
genotype	temperature	D_FM	Duration of flowering phase	d	-
genotype	temperature	D_MH	Duration of grain filling phase	d	-
species	temperature	NHT	Thermal stress, high temperature (discrete)	d	$sum(TM > 28)$
species	temperature	NLT	Thermal stress, low temperature (discrete)	d	$sum(TM < 20)$
species	temperature	SHT	Thermal stress, high temperature (continuous)	-	$sum(1 - HTRUE)$
species	temperature	SLT	Thermal stress, low temperature (continuous)	-	$sum(1 - LTRUE)$
species	temperature	SFTRUE	Thermal stress impact on photosynthesis	-	$sum(1 - FTRUE)$
species	water	SFTSW	Edaphic water deficit (continuous)	-	$sum(1 - FTSW)$
species	water	MET	Edaphic water deficit (continuous)	-	$mean(ET/PET)$
species	water	NET	Edaphic water deficit (discrete)	d	$sum(ET/PET < 0.6)$
genotype	water	SFHTR	Water stress impact on crop transpiration	-	$sum(1 - FHTR)$
genotype	water	SFHRUE	Water stress impact on crop photosynthesis	-	$sum(1 - FHRUE)$
species	nitrogen	SNAB	Absorbed nitrogen	$kg.ha^{-1}$	$diff(range(NAB))$
species	nitrogen	SNNI	Nitrogen deficit (continuous)	-	$sum(1 - NNI)$
species	nitrogen	SFNRUE	Nitrogen stress impact on photosynthesis	-	$sum(1 - FNRUE)$
genotype	-	LAI	Leaf area index	-	$max(LAI)$
genotype	-	LAD	Leaf area duration	-	$sum(LAI)$
genotype	light	SIR	Intercepted radiation	$MJ.m^{-2}$	$sum(RIE * GR * 0.48)$
genotype	-	MRUE	Photosynthesis	$g.MJ^{-1}.m^{-2}$	$mean(RUE)$
genotype	-	STDM	Aerial Biomass	$g.m^{-2}$	$max(TDM)$
genotype	-	GY	Grain yield	$q.ha^{-1}$	$max(GY)$
genotype	-	OC	Grain oil content	$\%(drymatter)$	$max(OC)$

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