

Conceptual basis, formalisations and parameterization of the SUNFLO crop model

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Summary

SUNFLO¹ is a process-based model for the sunflower crop which was developed 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; Lecoecur *et al.*, 2011).

This model is based on a conceptual framework initially proposed by Monteith (1977) and now shared by a large family of crop models (Jones *et al.*, 2016). In this framework, the daily crop dry biomass (DM_t) is calculated as a difference equation² 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 law³ 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 <i>et al.</i> , 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 <i>et al.</i> , 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 |
|-------------|--------------------------|--|-----------|------------------------|-----------------------------------|
| <i>TDE1</i> | ThermalTimeVegetation | Temperature sum to floral initiation | 482.00 | <i>C.d</i> | (Lecoeur <i>et al.</i> , 2011) |
| <i>TDF1</i> | ThermalTimeFlowering | Temperature sum from emergence to the beginning of flowering | 836.00 | <i>C.d</i> | (Lecoeur <i>et al.</i> , 2011) |
| <i>TDM0</i> | ThermalTimeSenescence | Temperature sum from emergence to the beginning of grain filling | 1083.00 | <i>C.d</i> | (Lecoeur <i>et al.</i> , 2011) |
| <i>TDM3</i> | ThermalTimeMaturity | Temperature sum from emergence to seed physiological maturity | 1673.00 | <i>C.d</i> | (Lecoeur <i>et al.</i> , 2011) |
| <i>TLN</i> | PotentialLeafNumber | Potential number of leaves at flowering | 29.00 | <i>leaf</i> | (Lecoeur <i>et al.</i> , 2011) |
| <i>LLH</i> | PotentialLeafProfile | Potential rank of the plant largest leaf at flowering | 17.00 | <i>leaf</i> | (Lecoeur <i>et al.</i> , 2011) |
| <i>LLS</i> | PotentialLeafSize | Potential area of the plant largest leaf at flowering | 448.00 | <i>cm⁻²</i> | (Lecoeur <i>et al.</i> , 2011) |
| <i>k</i> | ExtinctionCoefficient | Light extinction coefficient during vegetative growth | 0.88 | - | (Lecoeur <i>et al.</i> , 2011) |
| <i>LE</i> | WaterResponseExpansion | Threshold for leaf expansion response to water stress | - 4.42 | - | (Casadebaig <i>et al.</i> , 2008) |
| <i>TR</i> | WaterResponseConductance | Threshold for stomatal conductance response to water stress | - 9.30 | - | (Casadebaig <i>et al.</i> , 2008) |
| <i>HI</i> | PotentialHarvestIndex | Potential harvest index | 0.40 | - | (Casadebaig <i>et al.</i> , 2011) |
| <i>OC</i> | PotentialOilContent | Potential seed oil content | 55.40 | <i>% dry</i> | (Casadebaig <i>et al.</i> , 2011) |

Phenology

| label | description | value | unit | reference |
|-----------------------|--|--------|---------------------|-----------------------------------|
| ThermalTimeVegetative | Temperature sum to floral initiation | 482.0 | C.d | (Lecoeur <i>et al.</i> , 2011) |
| ThermalTimeFlowering | Temperature sum from emergence to the beginning of flowering | 836.0 | C.d | (Lecoeur <i>et al.</i> , 2011) |
| ThermalTimeSeed | Temperature sum from emergence to the beginning of grain filling | 1083.0 | C.d | (Lecoeur <i>et al.</i> , 2011) |
| ThermalTimeMaturity | Temperature sum from emergence to seed physiological maturity | 1673.0 | C.d | (Lecoeur <i>et al.</i> , 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 <i>et al.</i> , 2011) |
| ElongationRate | Reciprocal of hypocotyl elongation rate | 1.2 | Cd.mm ⁻¹ | (Villalobos <i>et al.</i> , 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.

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

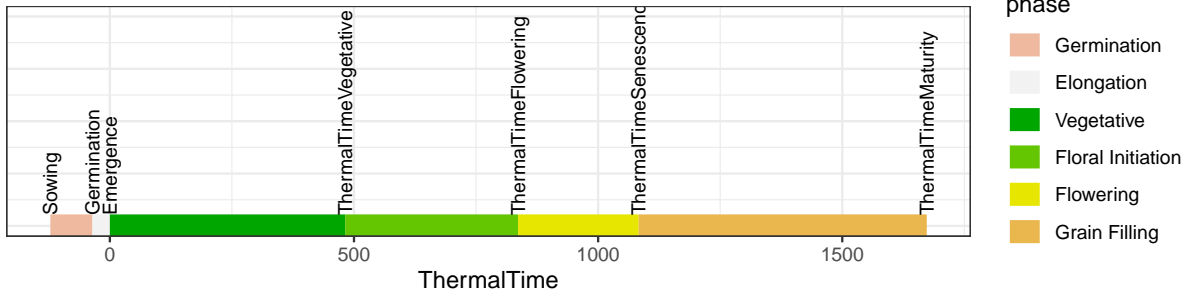
with:

- 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, beginning 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 (Mo)
- 5, onset of senescence (Mo) - 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 <i>et al.</i> , 2011) |
| PotentialLeafProfile | Potential rank of the plant largest leaf at flowering | 17.0 | leaf | (Lecoeur <i>et al.</i> , 2011) |
| PotentialLeafSize | Potential area of the plant largest leaf at flowering | 448.0 | cm ⁻² | (Lecoeur <i>et al.</i> , 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 | Minimum 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).

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

with:

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

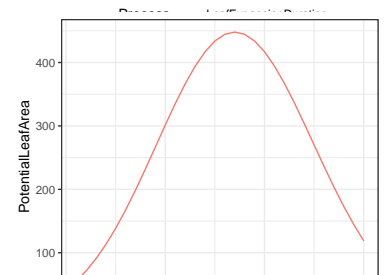
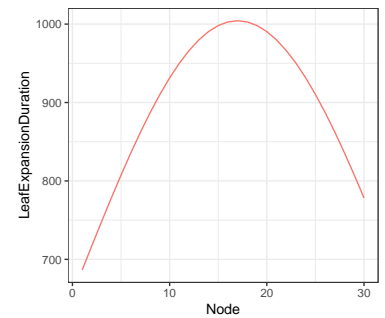
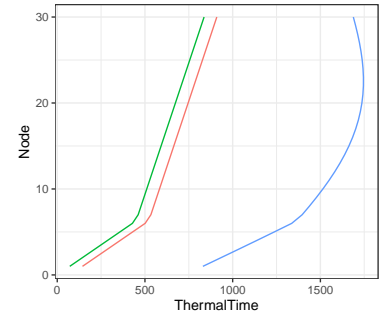
$$LeafSenescenceTime_i = LeafExpansionTime_i + LeafExpansionDuration_i$$

PotentialLeafArea

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

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

with:



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 <i>et al.</i> , 2011) |
| - | SowingDensity | Plant density | 7.0 | $plant.m^{-2}$ | NA |

Leaf Area Index (LAI)

$$LAI_t = SowingDensity \times PlantLeafArea_t$$

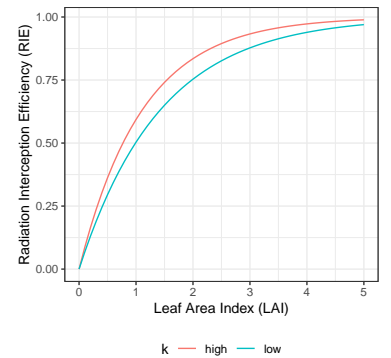
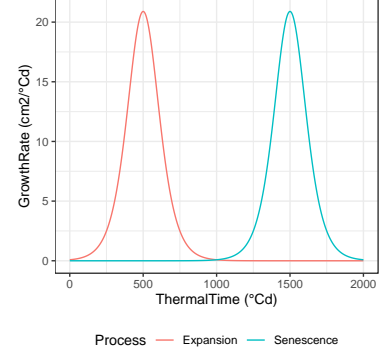
Radiation Interception Efficiency (RIE)

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 | Potential RUE Vegetative | Initial value for RUE during vegetative stage | 1.00 | $g.MJ^{-1}.m^{-2}$ | (Casadebaig et al., 2011) |
| r_{max} | Potential RUE Maximum | Maximum value of RUE during flowering stage | 3.00 | $g.MJ^{-1}.m^{-2}$ | (Casadebaig et al., 2011) |
| r_d | Potential RUE Reproductive | Rate of RUE decrease during reproductive stage | 4.50 | $g.MJ^{-1}.m^{-2}$ | (Casadebaig et al., 2011) |
| r_{min} | Potential RUE Minimum | Minimum value of RUE at the end of reproductive stage | 0.01 | $g.MJ^{-1}.m^{-2}$ | (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.

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

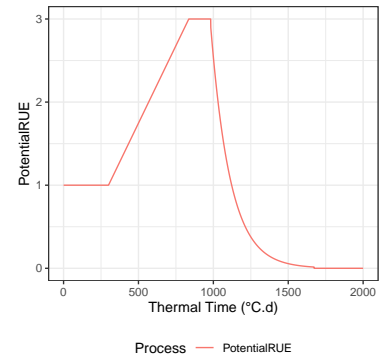
with:

- $PAR_t = Radiation_t \times 0.48$, 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) | <i>d</i> | $sum(ET/PET - 0.6)$ | vegetative |
| water | photosynthesis | NETR_FM | Edaphic water deficit (discrete) | <i>d</i> | $sum(ET/PET - 0.6)$ | flowering |
| water | photosynthesis | NETR_MH | Edaphic water deficit (discrete) | <i>d</i> | $sum(ET/PET - 0.6)$ | filling |
| - | photosynthesis | STDM_F | Aerial Biomass at flowering | $g.m^{-2}$ | $max(TDM$ | flowering |
| water | transpiration | STR_FH | Sum of water loss through transpiration | <i>mm</i> | $sum(TR)$ | reproductive |
| temperature | phenology | TT_FH | Thermal time since flowering (4.8 C basis) | <i>C.d</i> | $sum(TM - 4.8)$ | 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 | % <i>dry</i> | - | - |
| 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) | <i>d</i> | $sum(NNI > 1.2)$ | flowering |
| temperature | photosynthesis | NHT_MH | Thermal stress, heat (discrete) | <i>d</i> | $sum(TM > 34)$ | 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

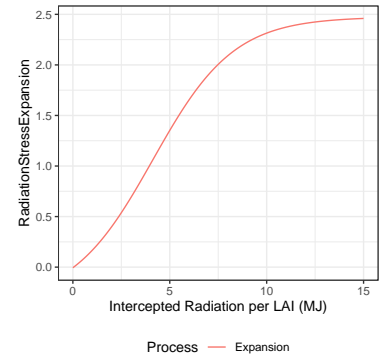
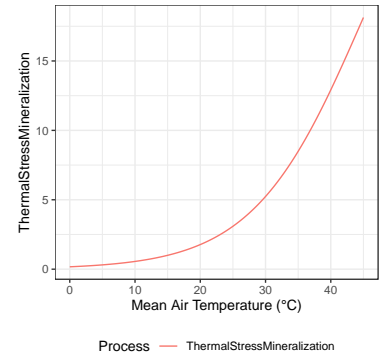
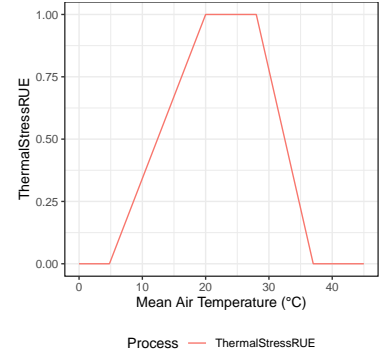
RadiationStressExpansion

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

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

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 | WaterResponseExpans | Threshold for leaf expansion response to water stress | - 4.4 | - | (Casadebaig <i>et al.</i> , 2008) |
| TR | WaterResponseConduct | Threshold for stomatal conductance response to water stress | - 9.3 | - | (Casadebaig <i>et al.</i> , 2008) |
| - | RootDepthLimit | Maximum soil rooting depth (> 300 mm) | 1000.0 | mm | (Lecoeur <i>et al.</i> , 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] | - |
| - | RootDepthMax | 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 <i>et al.</i> , 2011) |
| K_c | CropCoefficient | Crop coefficient for potential crop transpiration | 1.2 | - | (Lecoeur <i>et al.</i> , 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 ($mm \text{ } ^\circ C^{-1}$)
- $RootDepthMax = 1800$, maximum root depth (mm)

WaterSupply

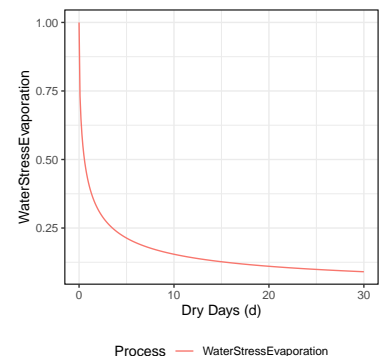
The water balance model treats the soil as a reservoir with three dynamic layers: surface layer (0-30 cm), root layer (30-rooting front), and soil layer (rooting front - soil depth) (Sarr *et al.*, 2004). Rainfall, irrigation and evaporation only impacts the balance of the surface layer. Water movement 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:

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

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*).

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

$$WaterStressConductance_t = \frac{1}{1 + \exp(4.5 \times a \times WaterStress_t)}$$

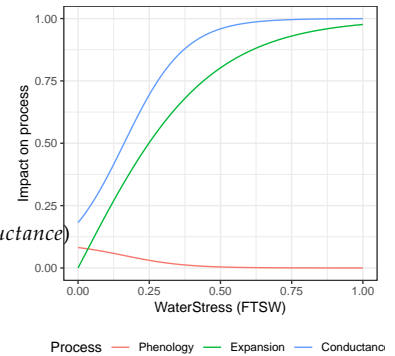
with $a \in [-15.6; -2.3]$, genotype-dependant response parameter

WaterStressPhenology

Accelerated crop development 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



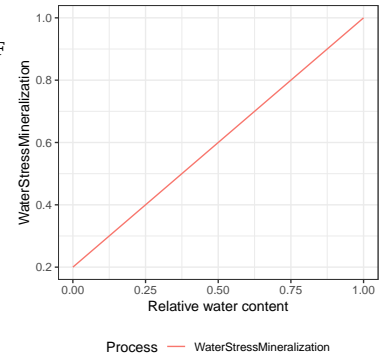
WaterStressMineralization

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 <i>et al.</i> , 2007) |
| y_0 | WaterResponseMineralization | Relative nitrogen mineralization rate at wilting point | 0.2 | - | (Mary <i>et al.</i> , 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 <i>et al.</i> , 2012) |
| b | PlantNitrogenCritical | Slope for critical nitrogen dilution curve | 0.4 | - | (Debaeke <i>et al.</i> , 2012) |
| a | PlantNitrogenMaximum | Maximum plant nitrogen concentration threshold | 6.5 | % | (Debaeke <i>et al.</i> , 2012) |
| b | PlantNitrogenMaximum | Slope for maximum nitrogen dilution curve | 0.4 | - | (Debaeke <i>et al.</i> , 2012) |
| - | NitrogenResponseExpansion | Expansion coefficient for leaf expansion response to nitrogen stress | 0.6 | - | (Brisson <i>et al.</i> , 2009) |
| - | NitrogenResponseExpansion | Expansion value of leaf expansion response to nitrogen stress | 0.3 | - | (Brisson <i>et al.</i> , 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 efficiency⁴, which is modeled as a linear function of crop growth rate ($g\ m^{-2}\ ^\circ C d^{-1}$) (Limaux *et al.*, 1999). Leaching is the product of drained water (*Drainage*) and the nitrogen concentration from the soil layer concerned.

$$^4NUE = 30 + 0.34 \times CropBiomassRate \times 100$$

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

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 ($^\circ C$);
- $a = 0.07738$ and $b = 6.593$ (Sinclair and Muchow, 1995)

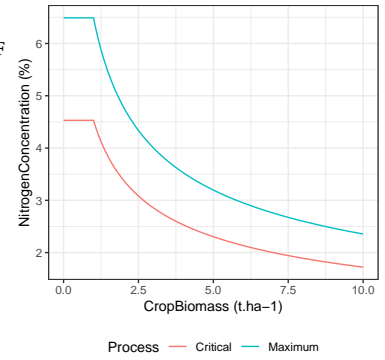
Soil nitrogen is absorbed in the transpirational stream (mass flow).

$$NitrogenSupply_t = NitrogenUptake_t$$

$$NitrogenUptakeRate_t = TranspirationRate_t \times SoilNitrogenConcentration_t$$

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).



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

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.

$$\text{NitrogenDemand}_t = \text{CropNitrogenConcentrationCritical}_t \times \text{CropBiomass}_t$$

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 (*NNitrogenDemand*, kg ha⁻¹).

$$\text{NitrogenStress}_t = \frac{\text{NitrogenSupply}_t}{\text{NitrogenDemand}_t} = \text{NNI}$$

NitrogenStressExpansion

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

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

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.

$$\text{NitrogenStressRUE}_t = \frac{\text{NitrogenSupplyRate}_t}{\text{NitrogenDemandRate}_t}$$

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 | %(<i>drymatter</i>) |

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 | ET | 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 | FHT | Thermal stress, high temperature (continuous) | - | $sum(1 - HTRUE)$ |
| species | temperature | FLT | Thermal stress, low temperature (continuous) | - | $sum(1 - LTRUE)$ |
| species | temperature | FTRUE | 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 | SFHRU | 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 | SFNRU | 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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