4. Detailed Information about the Hybrid-Maize Model

Crop simulation models are mathematical representations of plant growth processes as influenced by interactions among genotype, environment, and crop management. They have become an indispensable tool for supporting scientific research, crop management, and policy analysis (Fischer et al., 2000; Hammer et al., 2002; Hansen, 2002). Simulation models serve different purposes, and the intended purpose influences the level of detail needed for mechanistic description of key processes, sensitivity to environment and management, data requirements, and model outputs. All cereal crop models must simulate plant growth and development, biomass partitioning among organs (leaves, stem, root, and reproductive structures), and yield formation. The accuracy of simulating the outcome of these processes across a wide range of environments depends on basic understanding of the key ecophysiological processes and incorporating this knowledge in the mathematical formulations that constitute the model.

Our objective was to develop a model that can provide robust simulation of maize yield potential in different environments with a minimum number of location- or hybrid-specific input parameters (Yang et al., 2004). Agronomists need such robust crop models to improve the efficiency of research that investigates interactions among crop management options in favorable rainfed and irrigated environments, while crop producers and crop consultants need such models for use in computer-based decision-support tools to improve crop management decisions.

The Hybrid-Maize model builds on the strengths of existing models by combining the crop-specific attributes of CERES-Maize (Jones and Kiniry, 1986; Kiniry et al., 1997; Lizaso et al., 2003b) related to phenology and organ growth with explicit photosynthesis and respiration functions from assimilate-driven generic crop models such as SUCROS, WOFOST and INTERCOM (Van Diepen et al., 1989; Kropff and van Laar, 1993; Lindquist, 2001; van Ittersum et al., 2003). Hybrid-Maize also includes additional modifications for several functions based on calibration with experimental data from a field study that produced maize with minimal possible stress—conditions that are required to achieve yield potential (Yang et al., 2004).

Hybrid-Maize simulates maize growth on daily basis from emergence to physiological maturity. It features temperature-driven maize phenological development, vertical canopy integration of photosynthesis, organ-specific growth respiration, and temperature-sensitive maintenance respiration. The functions for crop growth and development in Hybrid-Maize were largely adapted from CERES-Maize, but the inclusion of gross assimilation, growth respiration and maintenance respiration makes the Hybrid-Maize model potentially more responsive to changes in environmental conditions than models such as CERES-Maize. Hybrid-Maize also requires fewer genotype-specific parameters without sacrificing prediction accuracy. A linear relationship between growing degree-days (GDD) from emergence to silking and GDD from emergence to physiological maturity is used for prediction of day of silking when the former is not available.

Detailed descriptions of major model components are provided in the following sections, focusing mainly on the modified or new components in Hybrid-Maize that differ from CERES-Maize or INTERCOM. Default values of user-modifiable parameters used in Hybrid-Maize are listed in Appendix 6.1. Default values of soil physical properties used in Hybrid-Maize are listed in Appendix 6.2. A general comparison with other models is provided in Appendix 6.3.

4.1. Crop Growth and Development Processes

4.1.1. Daily GDD Computation

The model runs on a daily time-step. Growing degree days (GDD) accumulation is the first procedure to be estimated each day. In CERES-Maize, GDD refers to a base temperature of 8 $^{\circ}$C (GDD$_8$). However, such a GDD scheme is inconvenient for practical use because most of the GDD values are reported for maize hybrids by seed companies, and these values predominantly use a base temperature of 10 $^{\circ}$C (GDD$_{10}$). As the conversion of GDD based on one temperature to GDD based on another temperature requires the number of days for the GDD accumulation, there is no simple way to convert GDD$_8$ to GDD$_{10}$. In order to preserve the GDD related growth functions from CERES-Maize, and, at the same time, directly use the available hybrid-specific GDD$_{10}$, the two schemes of GDD co-exist in the Hybrid-Maize: all the GDDs for model inputs and outputs are expressed in GDD$_{10}$, whereas internally GDD$_8$ is used in functions derived from CERES-Maize.

Daily GDD is computed using the single-sine method (http://www.ipm.ucdavis.edu/WEATHER/ddconcepts.html). This method assumes the temperature curve is symmetrical around the maximum temperature. It uses daily minimum (T_{min}) and maximum (T_{max}) temperatures to produce a sine curve over a 24-hour period, and then estimates GDD for that day by calculating the area above the lower threshold (T_L) and below the curve or the upper threshold (T_U). The default upper threshold is 34 $^{\circ}$C (Kropff and van Laar, 1993). GDD$_{10}$ is calculated using $T_L = 10$ $^{\circ}$C, and GDD$_8$ is subsequently calculated by adding 2 to GDD$_{10}$. Six possible relationships can exist between the daily temperature cycle and the upper and lower thresholds. Using two common parameters calculated as

$$T_{mean} = (T_{max} + T_{min})/2 \quad \text{and} \quad \alpha = (T_{max} - T_{min})/2$$

the six possible cases are mathematically described and visualized below.

(1) Intercepted by both thresholds T_L and T_U:

$$GDD = \frac{1}{\pi}\left((T_{mean} - T_L)(\theta_2 - \theta_1) + \alpha[\cos(\theta_1) - \cos(\theta_2)] + (T_U - T_L)(\frac{\pi}{2} - \theta_2) \right)$$

with

$$\theta_1 = \sin^{-1}[(T_L - T_{mean})/\alpha]$$
$$\theta_2 = \sin^{-1}[(T_U - T_{mean})/\alpha]$$

(2) Intercepted by the upper threshold T_U:

$$GDD = \frac{1}{\pi}\left((T_{mean} - T_L)(\theta_2 + \frac{\pi}{2}) + (T_U - T_L)(\frac{\pi}{2} - \theta_2) - [\cos(\theta_2)] \right)$$

with

$$\theta_2 = \sin^{-1}[(T_U - T_{mean})/\alpha]$$

(3) Entirely between both thresholds T_L and T_U:

$$GDD = T_{mean} - T_L$$

(4) Intercepted by the lower threshold T_L:

$$GDD = \frac{1}{\pi}\left[(T_{mean} - T_L)(\frac{\pi}{2} - \theta_1) + \alpha\cos(\theta_1)\right]$$

with

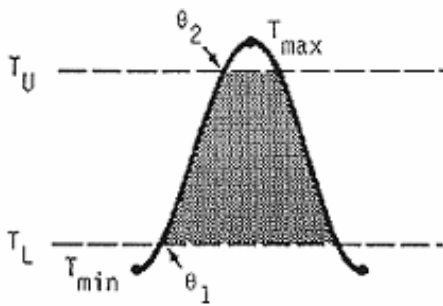$$\theta_1 = \sin^{-1}\left[(T_L - T_{mean})/\alpha\right]$$

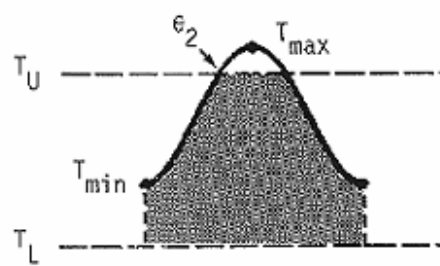(5) Completely above both thresholds T_L and T_U:
$$GDD = T_U - T_L$$

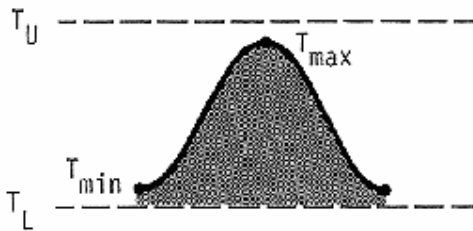(6) Completely below both thresholds T_L and T_U:
$$GDD = 0$$

Case (1)
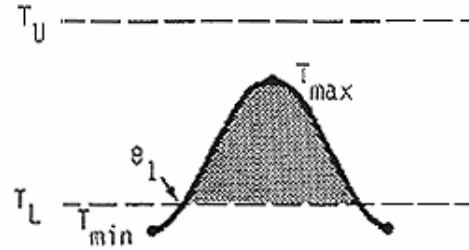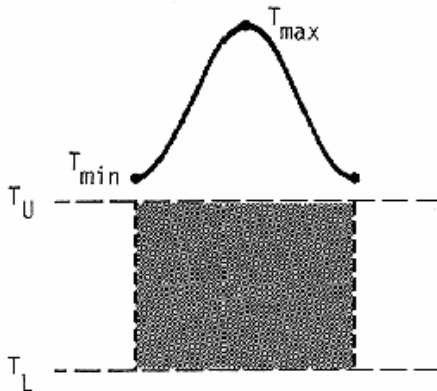

Case (2)

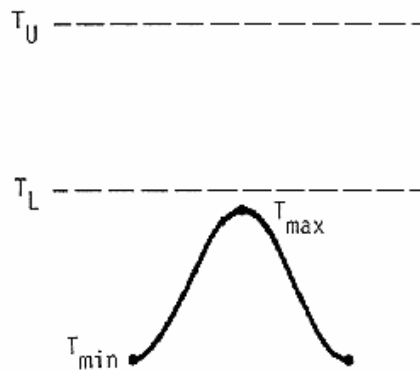Case (3)

Case (4)

Case (5)

Case (6)

4.1.2. Daily CO_2 Assimilation

Daily CO_2 assimilation is computed according to Goudriaan (1986), Kropff and van Laar (1993), and Goudriaan and van Laar (1994). The photosynthetically active radiation (PAR, MJ m^{-2} ground h^{-1}) is assumed to be 50% of the total solar radiation:

$$PAR = 0.5 * I / DL$$

in which I is the daily total incoming radiation (MJ m^{-2} ground d^{-1}) and DL is the daytime length (hours). DL is computed as (Driessen and Konijn, 1992):

$$DEC = -23.45 \cos(2\pi * (DOY + 10) / 365)$$

$$RAD = \pi / 180$$

$$CCOS = \cos(Lat * RAD) * \cos(DEC * RAD)$$

$$SSIN = \sin(Lat * RAD) * \sin(DEC * RAD)$$

$$SSCC = SSIN / CCOS$$

$$DL = 12 [2\pi * arcSin(SSCC)] / \pi$$

in which DOY is day of year, Lat is the latitude of the site, and DEC, RAD, CCOS and SSIN are intermediate variables. For the southern hemisphere, the value of latitude is negative.

Using L to represent the depth of canopy with L = 0 at the top and L = LAI (leaf area index) at the bottom of the canopy, the PAR interception by the layer of canopy at position L ($PAR_{i,L}$) equals the decrease of PAR at that depth following the Beer's law:

$$PAR_{i, L} = dPAR / dL = PAR * k * \exp(-k * L)$$

in which k is the light extinction coefficient. The default k value of 0.55 is based on data from Lizaso et al. (2003b), Maddonni et al. (2001), and our own measurements made in a field experiment at Lincoln (J.L. Lindquist, unpublished data). This value can be changed under **Settings → Parameter Settings → Crop growth**. The corresponding CO_2 assimilation by that layer (A_L) follows a saturation function of the form:

$$A_L = A_{max} * [1 – \exp(-\varepsilon * PAR_{i, L} / A_{max})]$$

in which ε is the initial light use efficiency (g CO_2 MJ^{-1} PAR) and A_{max} is the maximum assimilation rate (g CO_2 m^{-2} leaf hr^{-1}). The value of ε = 12.5 g CO_2 MJ^{-1} PAR was adapted from Kropff and van Laar (1993) and can be changed under **Settings → Parameter Settings → Resp & Photosyn**. The maximum assimilation rate represents the rate of photosynthesis at light saturation, and is a function of day-time mean temperature (T_{day}, ^{o}C) (Driessen and Konijn, 1992; Kropff and van Laar, 1993). A_{max} is zero below a threshold temperature (T_{zeroA}). From T_{zeroA} upwards A_{max} increases linearly until a plateau ($A_{plateau}$) is reached at a certain temperature ($T_{1, plateau}$). From $T_{1, plateau}$ upwards to another temperature ($T_{2, plateau}$), A_{max} remains at $A_{plateau}$. Above $T_{2, plateau}$, A_{max} decreases linearly. The formulations are:

$$T_{mean} = (T_{max} + T_{min}) / 2$$

$$AMPL = (T_{max} - T_{min}) / 2$$

$$Sunrise = 12 – DL / 2$$

$$Sunset = 12 + DL / 2$$

$$AUX = \pi \ (\text{Sunset} - 14) \ / \ (\text{Sunrise} + 10)$$

$$T_{day} = T_{mean} + (\ \text{Sunset} - 14) * AMPL\ * \sin(AUX) \ / \ (DL * AUX)$$

$$\text{if } T_{day} < T_{1, \text{plateau}}$$

$$A_{max} = (T_{day} - T_{zeroA}) * A_{plateau} \ / \ (T_{1, \text{plateau}} - T_{zeroA})$$

$$\text{else if } T_{day} \leq T_{2, \text{plateau}}$$

$$A_{max} = A_{plateau}$$

else

$$A_{max} = A_{plateau} - 0.2 * (T_{day} - T_{2, \text{plateau}})$$

in which AMPL, sunrise, sunset and AUX are intermediate variables. $A_{plateau} = 7$ g CO_2 m^{-2} leaf hr^{-1} was adapted from Kropff and van Laar (1993), but this value can be changed under **Settings → Parameter Settings → Resp & Photosyn**.

The CO_2 assimilation by the whole canopy in a day (A, g CO_2 m^{-2} ground d^{-1}) is obtained by integration of the A_L along L:

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

Two numerical integration methods are available in the model. The default method is the three-point Gaussian method (Goudriaan, 1986):

$$L_1 = 0.1127 * LAI$$

$$L_2 = 0.5 * LAI$$

$$L_3 = 0.8873 * LAI$$

$$I_1 = k * PAR * \exp(-k * L_1)$$

$$I_2 = k * PAR * \exp(-k * L_2)$$

$$I_3 = k * PAR * \exp(-k * L_3)$$

$$A_1 = Amax * [(1 - \exp(-epsi * I_1 \ / \ Amax)]$$

$$A_2 = Amax * [1 - \exp(-epsi * I_2 \ / \ Amax)] * 1.6$$

$$A_3 = Amax * [1 - \exp(-epsi * I_3 \ / \ Amax)]$$

$$A = (A_1 + A_2 + A_3) \ / \ 3.6 * LAI * DL$$

in which L_1 to L_3, I_1 to I_3, and A_1 to A_3 are intermediate variables. Alternatively, a user can choose the standard Simpson's rule. In this method, the number of integration steps (or intervals) is self progressed until a user-defined maximum negligible gain in A (in %) is reached. In most cases this method is much slower than the three point Gaussian method. Gross CO_2 assimilation rate is then converted to gross carbohydrate production (Carbo$_{gross}$). Because the organ growth functions are on a per plant basis, Carbo$_{gross}$ is also expressed on a per plant basis (g plant^{-1} d^{-1}):

$$\text{Carbo}_{gross} = A \ / \ plantPop * 30 \ / \ 44$$

in which plantPop is plant population density (plants m^{-2}).

4.1.3. Maintenance Respiration and Net Carbohydrate Production

Some of the gross assimilation will be lost to plant maintenance respiration. The rate of maintenance respiration (mResp, g CH_2O respired d^{-1}) differs among different organs, and is affected by the amount of live biomass and temperature. The amount of live biomass of vegetative organs (DM_{live} of leaves, stems, roots) is assumed to be 100% of the organ mass at silking; after silking, the proportion of live biomass of avegetative organ is assumed to be equal to the ratio of green leaf area (at that moment) to the green leaf area at flowering (Kropff and van Laar, 1993). The effect of temperature ($Coef_T$) on mResp follows the Q_{10} function (Kropff and van Laar, 1993):

$$Coef_T = 2^{(T_{mean} - T_{ref})/10}$$

in which T_{mean} is the daily mean temperature, T_{ref} is the reference temperature. As there is unlikely a fixed reference temperature that a plant 'feels', we adapted the approach by Driessen and Konijn (1992) that assumes T_{ref} is the average temperature a plant 'gets used to' in the past 10 days. The duration of this period can be changed under **Settings → Parameter Settings → Resp & Photosyn**.

Each organ has a specific coefficient of maintenance respiration ($Coef_{resp}$, g CH_2O respired g^{-1} DM d^{-1}), which is the respiration rate per unit of live biomass at T_{ref}. Suggested values for maize plants at 25°C are: 0.03, 0.015, 0.01 & 0.01 g CH_2O respired g^{-1} DM d^{-1} for leaf, stem, root and grain, respectively, as compiled by Penning de Vries et al. (1989) and as also used by Kropff and van Laar (1993). However, those values were derived nearly two decades ago, based on a combination of theoretical considerations, experimental measurements, and model studies (Penning de Vries et al., 1989; van Ittersum et al., 2003). We suspected that those earlier values are too large for modern maize hybrids because Earl and Tollenaar (1998) provided evidence that recent maize hybrids had smaller respiration losses than older hybrids, which also agrees with the measurements conducted by Kiniry et al. (1992). Therefore, the default values of mResp in the Hybrid-Maize model were obtained by calibrating the model prediction of dry matter yields against observed yields of 1999 in a high-yield field experiment at Lincoln. The average of the maintenance respiration coefficients obtained from this calibration (0.007 g g^{-1} d^{-1}) was comparable to the whole-plant respiration value of 0.008 g g^{-1} d^{-1} at silking observed by Kiniry et al. (1992). Default values used in Hybrid-Maize are: 0.010, 0.006, 0.005, and 0.005 g CH_2O g^{-1} DM d^{-1} for leaf, stem, root and grain maintenance respiration, respectively. They can be changed under **Settings → Parameter Settings → Resp & Photosyn**.

The mResp for each organ is computed as

mResp = DM_{live} * $Coef_{resp}$ * $Coef_T$

and the total losses from maintenance respiration for a plant equal the summation of all organs. The net production of carbohydrate (Carbo, g CH_2O d^{-1} $plant^{-1}$) is then computed:

Carbo = $Carbo_{gross}$ – ΣmResp

Carbo is the amount of assimilates that is available for growth of all organs, during which a further loss of carbohydrate will occur due to growth respiration.

4.1.4. Growth Stages

In Hybrid-Maize, the entire maize growth from emergence to physiological maturity is divided into four stages, following largely CERES-Maize (Jones and Kiniry, 1986), but with a merger of stages 1 and 2 into one stage. The four periods used in the Hybrid-Maize model are:

Stage 1: from emergence to tassel initiation

Stage 2: from tassel initiation to silking

Stage 3: from silking to effective grain filling

Stage 4: from effective grain filling to physiological maturity.

In Hybrid-Maize, the end of Stages 1 and 2 is determined differently from CERES-Maize. The end of Stage 2 is when GDD_{10} reaches $GDD_{10silking}$ (GDD_{10} from emergence to silking). $GDD_{10silking}$ is either a direct user input or estimated from the total GDD_{10} of a hybrid. Refer to section 4.3 for detailed discussion on estimation of $GDD_{10silking}$.

The duration of Stage 2 in terms of GDD equals P3 whose value is determined at the end of Stage 1:

$TLNO = GDD_8 / 21 + 6$

$P3 = (TLNO - 2) * 38.9 + 96 - GDD_8$

in which GDD_8 is for the duration of Stage 1, and TLNO is the total number of leaves that will eventually appear.

As the total duration of Stages 1 and 2 is known (i.e., when GDD_{10} reaches $GDD_{10silking}$) and the duration of Stage 2 is a function of the duration of Stage 1, the duration of Stage 1 is then determined by an iteration procedure in the model, in which one day is added to Stage 1 until the GDD_{10} at the end of Stage 2 reaches $GDD_{10\ silking}$.

Stage 3 ends when the GDD_8 accumulated during this stages reaches 170, and Stage 4 ends when the GDD_{10} reaches $GDD_{10total}$, which is a hybrid-specific value entered by the user (see 2.3.4.).

4.1.5. Leaf Growth and Senescence

Leaves grow both in number and total area until flowering, and most of the functions describing this were adapted from CERES-Maize (Jones and Kiniry, 1986). The growth of leaf number is a function of daily temperature:

if cumPh < 5

$PC = 0.66 + 0.068 * cumPh$

if cumPh $\geq$ 5

$PC = 1$

$TI = GDD_8 / (38.9 * PC)$

$cumPh = cumPh + TI$

$XN = cumPh + 1$

in which TI is the fraction of daily increase in leaf number, cumPh is the number of fully expanded leaves, XN is the leaf number of the oldest expanding leaf, and PC is an intermediate variable. At emergence cumPh = 1 and XN = 3.

The daily expansion of leaf area (PLAG) and growth of leaf biomass is driven by temperature, and the choice of functions depends on growth stage. For Stage 1 (from emergence to tassel initiation):

if XN < 4

$$PLAG = 3 * XN * TI$$

if XN ≥ 4

$$PLAG = 3.5 * XN^2 * TI$$

PLA = PLA + PLAG

leafWtToday = PLA / SLA

leafWtGrow = leafWtToday – leafWt

in which PLA (cm^2 $plant^{-1}$) is the total leaf area per plant, SLA (cm^2 g^{-1}, ≤ 400 cm^2 g^{-1}) is the specific leaf area, leafWtToday (g $plant^{-1}$) is the leaf biomass after update, and leafWt is the leaf biomass of the previous day, leafWtGrow (g $plant^{-1}$) is the daily growth in leaf biomass. For Stage 2 (from tassel initiation to flowering):

if XN ≤ 12

$$PLAG = 3.5 * XN^2 * TI$$

$$leafWtGrow = 0.00116 * PLAG * PLA^{0.25}$$

$$stemGrow = leafWtGrow * 0.0182 * (XN - XNTI)^2$$

if 12 < XN ≤ (TLNO – 3)

$$PLAG = 595 * TI$$

$$leafWtGrow = 0.00116 * PLAG * PLA^{0.25}$$

$$stemGrow = leafWtGrow * 0.0182 * (XN - XNTI)^2$$

if XN > (TLNO - 3)

$$PLAG = 595 * TI / (XN + 5 - TLNO)^{0.5}$$

$$leafWtGrow = 0.00116 * PLAG * PLA^{0.25}$$

$$stemGrow = 10.85 * TI$$

in which XNTI is the value of XN at the end of Stage 1. Note that both PLAG and leafWtGrow are the values projected based on temperature, but whether they can be realized depends on availability of net carbohydrate from photosynthesis. Leaf growth stops at the end of Stage 2 when silking occurs.

Leaf senesces occurs naturally in the course of development as well as due to competition for light and stress by low temperature, even under optimal water and nutrient conditions. The

functions of leaf senescence before silking are largely adapted from CERES-Maize (Jones and Kiniry, 1986), but the functions after silking are significantly different from CERES-Maize.

During Stage 1, the accumulated leaf senescence caused by natural development (SLAN, cm^2 $plant^{-1}$) is computed as

$$SLAN = GDD_8 * PLA / 10000$$

and during Stage 2 as

$$SLAN = PLA / 1000$$

Daily leaf senescence due to competition for light and temperature stress (PLAS, cm^2 $plant^{-1}$ d^{-1}) is computed from the a stress rate factor (LSR, 0~1):

if $LAI < LAI_{critical}$

$$SLFC = 1$$

else

$$SLFC = 1 - 0.008 * (LAI - LAI_{critical}) \qquad 1 \geq SLFC \geq 0$$

if $T_{mean} > 6$

$$SLFT = 1$$

else

$$SLFT = 1 - (6 - T_{mean}) / 6 \qquad 1 \geq SLFT \geq 0$$

if $SLFC \leq SLFT$

$$LSR = 1 - SLFC$$

else

$$LSR = 1 - SLFT$$

in which SLFC and SLFT are the leaf stress factors due to competition for light and low temperature, respectively. LSR = 0 means no stress and 1 full stress. Leaf area senesced in a day (PLAS, cm^2 $plant^{-1}$ d^{-1}) is computed as

$$PLAS = PLAG * LSR$$

The actual leaf senescence is determined by comparing the accumulated PLAS with SLAN; whichever is larger is then taken as the actual leaf senescence. Green leaf area and LAI can then computed as the difference of PLA and total leaf senescence.

Leaf senescence after silking is described by

$$sumDTT8 = \Sigma[DTT_8 / (1 - LSR)]$$

$$SF = LAI_{mature} * (sumDTT_8 / P5)^{SG}$$

in which DTT_8 is daily accumulation of GDD_8, $sumDTT_8$ is the DTT_8 accumulation after silking, and SF (0 to 1) is the fraction of senesced leaf of the maximum green leaf area, which is achieved at silking, LAI_{mature} is the fraction of LAI at maturity of the maximum LAI, and SG is a 'stay-green' factor, which controls how fast leaf senesces proceeds after silking. LAI refers to green leaf area, and green leaf area is PLA minus total senesced leaf area. Since leaf area is on a per

plant basis in the model, converting from green leaf area to LAI requires multiplication with plant density.

LAI_{mature} and SG are likely to be cultivar-specific and affected by management conditions such as water and nutrient conditions. The default values for LAI_{mature} and SG are 0.7 and 4, respectively. They apply to high-yielding maize in well-managed field, but they can be changed under **Settings** → **Parameter Settings** → **Crop growth**.

4.1.6. Stem and Cob Growth

Stem growth starts from the beginning of Stage 2 until the end of Stage 3, when effective grain filling starts. As adapted from CERES-Maize (Jones and Kiniry, 1986) with modifications, the choice of functions describing stem growth (stemGrow, g plant^{-1} d^{-1}) depends on the development stage:

if $XN \leq (TLNO - 3)$

$$stemGrow = leafWtGrow * 0.0182 * (XN - XNTI)^2$$

if $XN > (TLNO - 3)$

$$stemGrow = 10.85 * TI$$

after silking:

$$stemGrow = 0.22 * DTT_8$$

As in CERES-Maize, the start of cob growth is not specified, but the function for cob growth (cobGrow, g plant^{-1} d^{-1}) starts from silking with an initial cob biomass set at 16.7% of the stem biomass at silking:

$$cobGrow = 0.088 * DTT_8$$

Cob growth stops at the end of Stage 3 when effective grain filling starts.

The functions of stem growth after silking and cob growth were modified from those in CERES-Maize based on field measurements in experiment at Lincoln (Yang et al., 2004). Essentially, cob growth was reduced by 60% compared with that in CERES-Maize, and stem growth after silking was increased accordingly. This was based on the observation that CERES-Maize grossly overestimated measured cob dry matter. The modified functions more accurately predicted measured cob harvest index (ratio of cob dry matter to cob+grain dry matter) over a range of experimental conditions.

4.1.7. Root Growth

The functions for root growth from emergence until it stops shortly after silking were adapted from Kropff and van Laar (1993). Root growth rate is measured by a dry matter allocation coefficient (AC_{root}) to roots from the net assimilation. AC_{root} is assumed to be highest at emergence and decreases during the course of crop development until root growth stops. The course of crop development is measured by development stage (DS) on a scale ranging from 0 to 2, with 1 at silking. DS is computed as

$$DS = GDD_{10} / GDD_{10silking} \qquad if\ GDD_{10} \leq GDD_{10silking}$$

or:

$$DS = 1 + (GDD_{10} - GDD_{10silking}) / (GDD_{10\ total} - GDD_{10silking})$$

Then AC_{root} is computed as

$$AC_{root} = ACE_{root} - DS * ACE_{root} / DS_{stop}$$

in which ACE_{root} is the AC_{root} at emergence (=biomass allocation coefficient for root at emergence), and DS_{stop} is the development stage when root growth stops. The default values for ACE_{root} and DS_{stop} are 0.35 and 1.15, respectively. They can be modified under **Settings →** **Parameter Settings → Crop growth**. Besides, a small fraction of total root biomass is lost each day. The default value for this daily root death rate (fraction) is 0.005 as in CERES-Maize, which can also be modified under **Settings → Parameter Settings → Crop growth**.

4.1.8. Adjustment of Growth Rates for Leaf, Stem, Cob and Roots

So far, the growth rates for leaf, stem, cob and root have been determined independent from the quantity of daily net assimilation (NetAssim) and without including growth respiration costs, which occur during the conversion from carbohydrate to organ-specific substances. The default coefficients of growth respiration of the five organs were adapted from Kropff and van Laar (1993):

leaf: 0.47 g CH_2O g^{-1} DM

stem: 0.52 g CH_2O g^{-1} DM

root: 0.45 g CH_2O g^{-1} DM

grain: 0.49 g CH_2O g^{-1} DM

They can be modified under **Settings → Parameter Settings → Resp & Photosyn**. Taking a leaf for example, for accumulation of 1 g leaf dry matter, 0.47 g carbohydrate is lost during the conversion. In other words, growth of 1 g leaf dry matter requires total 1.47 g carbohydrate.

In Stage 1, only leaves and roots grow and the following three constrains are imposed:

(1) in case of insufficient daily NetAssim, root growth must be satisfied,

(2) if leafWtGrow is less than 0.5*NetAssim, then 0.5*NetAssim is allocated to leaf, and

(3) the maximum NetAssim allocated to roots is 0.5*NetAssim. Growth in leaf area is then adjusted accordingly.

In Stage 2, stem starts to grow. The growth rates of leaf and stem are equally adjusted after meeting the need for root. Note that the need for root decreases continuously from emergence. In Stage 3, stem and cob grow, as well as root (for part of this period). The growth rates of stem and cob are equally adjusted after meeting the need for root.

4.1.9. Grain Filling

Grain filling was adapted from CERES-Maize with modifications and is an active process in which the daily filling rate is determined by temperature. When daily NetAssim is insufficient to meet the potential grain-filling rate, translocation of carbohydrate from stem and/or leaf will occur as long as there are carbohydrate reserves in these two organs. The amount of carbohydrate

reserves in leaf and stem is determined at the start of effective grain filling. For leaf, the amount is equivalent to 15% of the leaf biomass. For stem, the amount is equivalent to 60% of the dry matter accumulation from silking to start of effective grain filling (the remaining 40% goes to cob growth). The request for translocation is first to stem; after the reserve in stem is exhausted, the reserve in leaf will be used, but each day only up to 0.5% of leaf biomass can be translocated. The efficiency of carbohydrate translocation is 0.26 as observed by Kiniry et al. (1992). The cost of translocation is the cause for occasional negative daily accumulations of dry matter during grain filling. If there is more NetAssim than needed to satisfy daily demand for grain filling, the surplus will be stored in stem as part of the carbohydrate reserve for future translocation.

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

$$grainGrow = RGfill * GPP * G5 * FillEffi * 0.001$$

in which G5 is the potential grain filling rate (mg d^{-1} kernel^{-1}), GPP is the number of viable grain per plant (assuming one ear per plant), FillEffi is the filling efficiency related to plant density, RGfill (0 to 1) is the temperature driven filling scale.

G5 is a cultivar-specific genetic coefficient in CERES-Maize. For high yielding maize hybrids in North America, a default value of 8.7 mg d^{-1} is used in Hybrid-Maize, which can be modified under **Settings → Parameter Settings → Crop growth**.

GPP is set at start of effective grain filling, and is determined by:

$$PSKER = sumP * 1000 / IDURP * 3.4 / 5$$

$$GPP = G2 * (PSKER - 195) / (1213.2 + PSKER - 195)$$

in which sumP (g CH$_2$O plant^{-1}) is the dry matter accumulation equivalent to the formation of grain from silking to the start of effective grain filling, IDURP is the duration in days of this period, PSKER is the average daily dry matter accumulation (g d^{-1}) during this period, and G2 is the potential number of kernels per ear. G2 is a cultivar-specific genetic coefficient in CERES-Maize. For high yielding maize hybrids grown at plant densities common in North America (25-35,000 plants/acre or 60 to 85,000 plants/ha), a default value of 675 kernels ear^{-1} is used in Hybrid-Maize. This value can be modified under **Settings → Parameter Settings → Crop growth**.

FillEffi is for adjusting the potential grain filling rate based on plant population, and its function was derived from a high-yield maize experiment at Lincoln, Nebraska (Yang et al., 2004):

$$FillEffi = 1.47 – 0.09 * D + 0.0036 * D^2$$

in which D is plant population (plants m^{-2}).

RGfill is computed as a sum of eight consecutive 3-hour interval filling scales (RGfill$_i$):

$$TMFAC_i = 0.931 + 0.114 * i - 0.0703 * i^2 + 0.0053 * i^3$$

$$TTMP_i = Tmin + TMFAC_i * (Tmax - Tmin)$$

if TTMP$_i$ > 6

$$RGfill_i = [1- 0.0025 * (TTMP_i - 26)^2] / 8$$

else

$$RGfill_i = 0$$

in which i ranges from 1 to 8.

4.1.10. Initiation of a Simulation Run

Five variables, i.e., leafWt, PLA, rootWt, cumPh, and XN, need to be initiated at emergence before the first step of computations. Their initial values are derived by assuming a 100-seed weight of 32 g, and 1/3 of the seed weight is lost during germination, and 1/3 emerges as leaf, and the remaining 1/3 is root. cumPh = 1, and XN = 3. The leaf area is converted from leaf area via $PLA = 267 * leafWt^{0.8}$.

4.2. Water Balance and Soil Water Dynamics

Soil water dynamics are computed as water balance between inputs from precipitation and/or irrigation and water losses through evaporation from soil surface and crop transpiration (water fixed by biochemical reactions is relatively small and thus ignored). The crop is assumed to take up water only from the rooting zone, with increasing rooting depth until silking. The whole rooting zone is divided into layers of 10 cm plus the top layer of the planting depth. For the top soil layer, precipitation and/or irrigation are the water inputs; for other layers the water drained from above layers provides the input. The soil holds water only up to field capacity so that excess water drains to the subsequent soil layer underneath. The crop takes up water only when soil water content is above the permanent wilting point. The formulations in this section are largely based on Driessen and Konijn (1992).

4.2.1. Rooting Depth and Water Uptake Weighing Factor

Crop rooting depth increases while the crop grows until DS reaches 1.15 (i.e., shortly after silking, see 4.1.7.). At this point, the rooting depth is supposed to be at the maximum ($Depth_{rootmax}$) as specified in the input settings (see 2.3.6.). The increase of rooting depth ($Depth_{root}$) from emergence to the time when root growth stops is assumed to be a linear function of DS:

$$Depth_{root} = DS * Depth_{rootmax} / 1.15 + Depth_{planting}$$

Although rooting depth increases steadily before root growth stops, root biomass concentrates more in a shallow layer near the soil surface and declines sharply with depth. The proportion of water uptake by roots from each layer is assumed to follow the root biomass distribution. For the top layer of the planting depth, its water uptake weighing factor (WUweight, total = 1) is assumed to be 0.05; for other layers WUweight is estimated as in CERES-Maize (Jones and Kiniry, 1986):

$$WUweight_{absolute} = exp[(-VDC * (Depth) / (Depth_{root})]$$

$$WUweight = 0.95 * WUweight_{absolute} / \sum WUweight_{absolute}$$

where $WUweight_{absolute}$ is the absolute water uptake weight of the layer, VDC is the vertical distribution coefficient that determines the shape of the exponential function, Depth is the depth of a layer (to its lower end), $Depth_{root}$ is the current rooting depth. The greater the VDC, the greater the WUweight for shallower layers. The default value of VDC is 4 according to CERES-Maize.

4.2.2. Maximum Evaporation and Maximum Transpiration

Maximum evaporation from soil surface is estimated by the following steps. First, water evaporation from well-watered soil surface ($Evap_{pot}$, cm d^{-1}) is set to be 30% of the potential evapotranspiration (ET_{ref}, cm d^{-1}), which is an input from weather data, i.e,:

$$Evap_{pot} = 0.3 * ET_{ref}$$

This value is based on Driessen & Konijn (1992) and Steele et al. (1996). Next, the relative humidity of the thin soil mulch layer (RHS, in fraction) is estimated by:

$$RHS = \exp[-2.1649 * 10^{-4} * PSI_{mulch} / (273 + T_{mean})]$$

in which T_{mean} (^{o}C) is the air mean temperature, PSI_{mulch} (cm) is the water potential of the mulch layer. PSI_{mulch} is estimated as:

$$PSI_{mulch} = (PSI_{evapsoil} + PSI_{drysoil}) / 2$$

and

$$PSI_{drysoil} = -(273 + T_{mean})*10^4 / 2.1649 * \ln(RHA)$$

$$PSI_{evapsoil} = \exp(GAM^{-1} * \ln(Porosity/Theta))^{1/2}$$

in which $PSI_{evapsoil}$ (cm) is the soil water potential of the top 30 cm which is assumed to the contributor to water evaporation, and $PSI_{drysoil}$ (cm) is the soil water potential in the very thin soil layer at top that is likey to be air-dry, GAM is a soil texture-specific constant (cm^{-2}, see Appendix 6.2.), Porosity (in fraction, see Appendix 6.2.) and Theta (volumetric water content, in fraction) are for the top 30 cm of soil. Then the evaporation from bare soil is estimated through:

$$Evap_{baresoil} = Evap_{pot} * (RHS - RHA) / (1 - RHA)$$

Finally, the maximum evaporation from soil under canopy ($Evap_{max}$, cm d^{-1}) is calculated as:

$$Evap_{max} = Evap_{baresoil} * \exp(-LAI * k)$$

The maximum transpiration by the crop ($Transp_{max}$, cm d^{-1}) is estimated based on ET_{ref} and the $Evap_{max}$ under closed canopy (i.e., LAI ≈ 5):

$$Evap_{LAI=5} = Evap_{baresoil} * \exp(-5 * k)$$

$$Transp_{max} = (ET_{ref} - Evap_{LAI=5}) * [1 - \exp(-LAI * k)]$$

4.2.3. Actual Evaporation

Actual evaporation, which is assumed to be from the top 30 cm of soil, is calculated through the following steps. First, the hydraulic conductivity of the soil mulch layer (K_{mulch}, cm d^{-1}) is estimated as:

$$K_{mulch} = K_{sat} * \exp(-alfa * PSI_{mulch}) \qquad \text{if } PSI_{mulch} <= PSI_{max}$$

or:

$$K_{mulch} = AK * PSI_{mulch}^{-1.4}$$

where K_{sat} is the saturated hydraulic conductivity (cm d^{-1}) of the soil, alfa is a soil texture-specific geometry constant (cm^{-1}, see Appendix 6.2.), PSI_{max} is a soil texture-specific boundary potential

(cm, see Appendix 6.2.), AK is a soil texture-specific empirical constant ($cm^{-2.4}$ d^{-1}, see Appendix 6.2.). Next the depth of the soil mulch layer ($Depth_{mulch}$, cm) is estimated by

$$Depth_{mulch} = K_{mulch} * (PSI_{drysoil} - PSI_{evapsoil})/(Evap_{max} + K_{mulch})$$

followed by a sequence of calculations:

$$RH_{mulch} = \exp(-2.1649 * 10^{-4} * PSI_{mulch} / (273 + T_{mean}))$$

$$Theta_{mulch} = Porosity * \exp\{-GAM*[\ln(PSI_{mulch})]^2\}$$

$$Diff_{air} = 2.38 + 0.0192 * T_{mean}$$

$$DMDA = 0.9 * (Porosity - Theta_{mulch}) - 0.1$$

$$VP_{sat} = 6.11 * \exp(17.4 * Tmean / (239 + Tmean))$$

$$Flux_{vapor} = Diff_{air} * DMDA * VP_{sat} * (RH_{mulch} - RHA) / Depth_{mulch}$$

$$Supply_{water} = K_{evapsoil} * ((PSI_{mulch} - PSI_{evapsoil}) / 30 - 1);$$

if $Supply_{water} > Flux_{vapor}$

$$Supply_{vapor} = Flux_{vapor}$$

else

$$Supply_{vapor} = Supply_{water}$$

where RH_{mulch} is rhe relative humidity in the mulch layer (in fraction), $Theta_{mulch}$ is the volumetric moisture content of the mulch layer (in fraction), $Diff_{air}$ is the air diffusion coefficient, DMDA is the ratio of the diffusion coefficient of the mulch layer to that of free soil, VP_{sat} is the saturated vapor pressure of the air (mbar), $Flux_{vapor}$ is the vapor flux through the mulch layer (cm d^{-1}), $Supply_{water}$ is the water supply (cm d^{-1}) from layers below 30 cm, and $Supply_{vapor}$ is the vapor supply for evaporation (cm d^{-1}).

Finally the evaporation from the soil under canopy is estimated as:

if $Supply_{vapor} > Evap_{max}$

$$Evap_{actual} = Evap_{max}$$

else

$$Evap_{actual} = Supply_{vapor}$$

4.2.4. Actual Transpiration and Water Stress Coefficient

Actual transpiration ($Transp_{actual}$, cm d^{-1}) is estimated from the maximum water uptake by roots from all layers where roots have reached in comparison with maximum transpiration ($Transp_{max}$). For the top layer, which is the planting depth, the maximum water uptake is estimated by the next steps. First, the available water ($Water_{avail}$, cm) is estimated by:

$$Water_{avail} = (Theta_{planting} - Theta_{pwp}) * Depth_{planting}$$

in which $Theta_{planting}$ is the volumetric water content of planting depth, $Theta_{pwp}$ is the volumetric water content of planting depth at permanent wilting point. Then the soil water potential ($PSI_{planting}$) of this layer is estimated from $Theta_{planting}$ in the same way as for PSIevapsoil in

Section 4.2.2. Then the hydraulic conductivity of this layer ($K_{planting}$) is estimated from $PSI_{planting}$ in the same ways as for K_{mulch} in Section 4.2.3. After that, the root resistance to transpiration (R_{root}, d^{-1}) is estimated as:

$$R_{root} = 13 / (Depth_{root} * K_{planting})$$

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

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

in which PSI_{leaf} is the leaf water suction at permanent wilting point (=17000 cm), R_{plant} (d^{-1}) is the resistant of plant to water flow (=9690 d^{-1}). If $Uptake_{max} > Water_{avail}$ then $Uptake_{max} = Water_{avail}$.

Water uptake for other layers is computed similarly. Then the total maximum water uptake ($Uptake_{total}$, cm d^{-1}) is compared with $Transp_{max}$:

if $Uptake_{trotal} >= Transp_{max}$

$Transp_{actual} = Transp_{max}$

else

$Transp_{actual} = Uptake_{total}$

Finally the water stress coefficient (Stress, in fraction) is estimated as:

$$Stress = 1 - Transp_{actual} / Transp_{max}$$

The stress coefficient ranges from 0 to 1 and is used as a reduction factor for CO_2 assimilation (see 4.1.2.). A value of Stress=0 indicates no water stress on crop growth so that CO_2 assimilation is not reduced, whereas at Stress=1 CO_2 assimilation stops completely.