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3.3 *AquaCrop* parameterization, calibration, and validation guide

This guide is mainly for *AquaCrop* users with an agronomic background and some experience of crop modelling, and for those needing to: simulate the productivity of a crop already parameterized, but not yet validated for their specific conditions; calibrate the model for a crop not yet parameterized; or to improve the parameters already worked out by others and to validate them for the same crop. These users should be acquainted with all Chapter 3 of this publication and the Reference Manual which can be downloaded from the FAO *AquaCrop* website (www.fao.org/nr/water/aquacrop). Users with less experience and background, who need more detailed instructions to run simulations with *AquaCrop* already calibrated for a particular crop, should download the instructions for *Group 1 Users* from the same website.

IMPORTANT DISTINCTIONS OF MODEL PARAMETERS

Conservative vs. user-specific parameters

AquaCrop is designed to be widely applicable under different climate and soil conditions, without the need for local calibration, once it has been properly parameterized for a particular crop species. To this end the model is constructed with parameters falling into two groups. One group is considered conservative, in that the parameters should remain basically constant under different growing conditions and water regimes. The other group encompasses parameters that are dependent on location, crop cultivar, and management practices, and must be specified by the user. A critical stipulation for many of the conservative parameters is that their values are based on data obtained from modern high-yielding cultivars grown with optimal soil fertility without limitation by any mineral nutrient, particularly nitrogen. With some notable exceptions, it is also stipulated that values are based on data obtained when water is not limiting. It follows that, if the conservative parameters already calibrated for a given crop do not provide simulated results, matching measured data for a crop in a particular case, the first thing to check is that mineral nutrients are not limiting the growth of the crop. To keep the model relatively simple, *AquaCrop* does not simulate nutrient cycles and nutritional effects on the crop directly. Instead, a way is provided in the 'Biomass' *tab sheet* to account for nutritional effects after performing a calibration based on the reduction of biomass produced by a nutrient-deficient treatment.

Cultivar classes

For simplicity, the parameters are grouped into two categories, as described above, in reality some of the parameters assigned to the conservative group may vary within small limits for different cultivars of the crop species. This brings up the need for a new term, 'cultivar class', to designate cultivars of a crop with very similar values of conservative parameters, to distinguish them from cultivars of the same species but differing by a limited amount in one or more conservative parameters. Take maize cultivars as an example. The reference HI for a number of maize cultivars has been parameterized at 48 percent (*Hsiao et al., 2009*), and together they comprise one cultivar class. If two or three other cultivars are found to have a higher reference harvest index (e.g., HI=51 percent), they would constitute another cultivar class. It is anticipated that over the long term, plant breeding and biotechnology will alter a number of the conservative parameters, increasing the number of cultivar classes.

INPUT INFORMATION AND DATA FOR VALIDATION AND PARAMETERIZATION

Table 1 lists the required information for using the model to simulate production and water use. The first column lists the absolutely required minimum. If this is the only available information, the simulated results would at best be first order approximations. The second column of the table lists additional information needed to make the simulation more reliable. In this case, agreement between the simulated and observed biomass production and yield should not be considered as validation of the model, unless the agreement is observed for several water regimes and for more than one climate. Essentially, the more exact and detailed information, the more close to reality would be the simulated results.

To validate the model and to parameterize the model, more detailed and exact data are needed, as listed in Table 2. The first column lists the minimum information needed in addition to that in Table 1 for a reasonable validation of the model or initial calibration of the conservative parameters. The second column lists the additional information needed to validate the model for general use, and calibrate the conservative parameters for a wide-range of climate, soil, and water regimes. In the validation and parameterization process, attention must be paid equally to how well the simulated results (canopy cover, biomass, and consumptive water use) agree with the measured values as time progresses through the season, as well as the total biomass, yield and total ET at crop maturity.

ITERATION, ASSESSMENT OF SIMULATION RESULTS, AND REFINING OF PARAMETERS

The common practice is to run simulations with the model starting with estimated or guessed parameter values and than compare the output with the measured experimental data, then adjust the parameters and run the simulation and compare again. This is done repeatedly until the simulated results closely agree with the experimental data. Trial-and-error iterations being the heart of the process, how can the process be streamlined to minimize the time and effort required? Some general rules may be helpful.

Rule 1: The better one understands the principles underlying the model, its flow diagram, and the flow of calculation steps, the more capable one would be in identifying the likely input or

TABLE 1 Information and data needed for simulation of crop growth, yield and water productivity with *AquaCrop*.

	1. Absolute minimum	2. Additional for reliable simulation
Crop	Grain yield, and indication of the proportion of grain dry weight to above-ground biomass, i.e. rough idea of harvest index (HI) Planting and harvesting dates (can be approximate), and estimated crop life-cycle length Seeding rate and germination percentage	Above-ground biomass at harvest Date of emergence (either the start of or nearly full emergence) and date of grain maturity Plant density; estimated maximum rooting depth Maximum green leaf area index (LAI) or indication of the extent of maximum canopy cover or canopy cover at a given time
Climate and ET	Ten-day or monthly mean values of: minimum and maximum temperature, and indication of fraction of sunny days, and wind and humidity regimes. Latitude and elevation Alternatively, pan evaporation data with information on the type of pan and whether the pan is set in a dry or green surrounding, to estimate reference evapotranspiration (ET_o) Daily rainfall data (10-day or monthly mean not recommended although better than none)	Weekly or 10-day mean values of: daily solar (global) radiation or sunshine hours, minimum and maximum temperature, minimum and maximum relative humidity, and wind run Daily rainfall Evapotranspiration (ET) estimated by long-term water balance
Soil and fertility	Textural class of the soil and indication of variation with depth Indication of land slope and soil-water holding capacity Indication of native fertility of the soil General fertilization practice	Texture of the various layers (or horizons) of the soil, and any layer restrictive to root growth and its depth Kind, rate and time of fertilization
Irrigation and water in soil	Water application method and approximate irrigation schedule Rough idea of soil-water content at planting based on rainfall of past months and the crop grown before the current one	Actual irrigation dates and rough amounts Estimate of soil-water content at planting based on some measurement or close observation

parameter to adjust, and in what direction. To this end, any time taken to read the three initial publications on *AquaCrop* (Steduto *et al.;* Raes *et al.;* Hsiao *et al.,* all 2009) is worthwhile.

Rule 2: Always pay attention to the graphic display of the *Climate-Crop-Soil water tab sheet* on the simulation run page, as well as the output numbers of the *Production* and the *Climate and water balance tab sheets*. By switching the simulation run to advance in time steps, one can see how the crop and soil water change step-by-step. The graphic display is particularly useful for water limited conditions to see whether the crop canopy cover (CC), transpiration relative to potential transpiration, and acceleration of canopy senescence are reasonable or need adjustment.

TABLE 2 Additional information and data needed for parameterization and validation of *AquaCrop*. The required data include those not mentioned here but listed in Column 2 of Table 1.

	1. Minimal additional beyond Column 2 of Table 1	2. Additional for reliable parameterization
Crop	Periodic measurements of leaf area index (LAI) or canopy cover over the season Periodic measurements of above-ground biomass over the season Date when foliage canopy begins to turn visibly yellow Measured rooting depth Signs of water stress and dates	Data as in Column 1 but obtained at several locations and climates on different soil types
Climate and ET	Daily maximum and minimum temperature and humidity Daily solar radiation and wind run ET by soil water balance (optional)	Data as in Column 1 but obtained at several locations and climates for different soil types Measured daily ET
Soil and fertility	Must have one treatment with optimal soil fertility Field capacity and permanent wilting point of soil horizons Infiltration rate or saturated hydraulic conductivity of the soil	Data as in Column 1 but obtained at several locations and climates for different soil types
Irrigation and water in soil	Must include a well-watered (full irrigation) treatment and water-stress treatments Amount of water applied at each of the irrigations Measured or good estimate of soil-water content for different soil depths at planting Periodic measurements of soil-water contents at various depths of the root zone (optional alternative to soil-water balance)	Data as in Column 1 but obtained at several locations and climates for different soil types Must include treatments with water stress at different times and different severities

Rule 3: Differentiate the input information and measured or observed data according to their reliability and exactness, and make rational adjustment to the vague or rough estimates of input first to see if the simulated results better match the measured results, before changing the model parameters. In later Sections, many of the uncertainties of the input information or data, and the measurements taken on crops, are mentioned and discussed to decide which inputs can be altered based on a rational evaluation of its likely range of uncertainty.

Rule 4: When simulated results and measured data do not agree, the problem could also be in the measured data. If simulated results coincide with measured data obtained in several different studies, but not with that of another study, the data in the other study are more suspect and additional data sets should be sought to complete the validation or parameterization.

LOCATION AND USER SPECIFIC PARAMETERS AND INPUT

Climate and soil are location specific, and crop cultivar, timing of crop cycle, water management and agronomic practices are user specific.

Climate data and reference evapotranspiration (ET_o)

AquaCrop simulates in daily time steps because plant responses to water status are highly dynamic and cannot be easily represented as weekly or 10-day means. The model runs with 10-day or monthly mean temperature and ET_o files, through interpolations. The results are, however, obviously approximations, and should not be used to calibrate or validate the model except as the last resort. ET_o is a key input for *AquaCrop* as the model calculates daily crop transpiration (Tr) and soil evaporation (E) using daily ET_o values.

ET_o is to be calculated using the FAO Penman-Monteith equation from full daily weather data sets, as described by Allen *et al.* (1998). A programme to do this calculation, named ET_o Calculator (FAO, 2009) is available on the FAO website. The ET_o Calculator has the advantage of allowing approximations when one or several kinds of the required weather data are missing, also following the approximation procedure of Allen *et al.* (1998). This makes it possible for a user to run rough simulations, even when the weather data are minimal, but can be easily misused. For validation and parameterization, such approximation should not be relied upon. The rougher the approximation of ET_o, the less reliable would be the simulated results and derived *AquaCrop* parameters. For example, ET_o Calculator can use daily maximum and minimum temperature, relative humidity, wind run, and sunshine hours in place of radiation, to calculate ET_o, and also can calculate ET_o simply from daily minimum and maximum temperature data and general information on site location such as whether it is arid or humid and windy or calm. Obviously, the ET_o calculated from the sunshine hours would be somewhat less reliable than that calculated with daily radiation, and the ET_o simply estimated with the daily minimum and maximum air temperature would be essentially worthless for the purpose of model validation and parameterization. Thus, it must be understood that reliable climatic data are critical in *AquaCrop*.

Growing degree day (GDD)

AquaCrop is designed for use under different climatic conditions and hence should be parameterized in the growing degree day (GDD) mode to account for different temperature regimes. This may be difficult, however, because many users may only have data for their specific locations with their limited temperature range. In this case, it is best to select data obtained when cold temperature is not a limiting factor and run the model first in the calendar time mode for parameterization. After arriving at reasonably acceptable parameter values, by switching the model to the GDD mode, the parameters are automatically converted to units in terms of GDD. The challenge is then to define: (1) the base temperature and upper temperature to calculate the GDD, and (2) the temperature thresholds for biomass accumulation and for pollination and fruit set of the specific crop. These are to be discussed later.

Soil water characteristics

In *AquaCrop*, the extent of water limitation is expressed as a fraction of the total available water (TAW) in the root zone, with TAW defined as the water held in the soil between its field capacity (FC) and permanent wilting point (PWP). In the case that the soil has layers differing in FC and PWP, the different values for the layers encompassing the maximum rooting depth need to be entered into the model.

Accurate FC and PWP are only important to specify the local conditions if water is a significant limiting factor. If the simulation is for conditions where water is either not limiting or only minimally limiting, approximate FC and PWP would do, but the water-stress functions (threshold and curve shape) derived cannot be relied on for conditions limited more by water deficits. Approximate FC and PWP may be estimated simply from the textural class of the soil. In *AquaCrop* there are default soil files for a number of textural classes. In each file the relevant water parameters are given in the 'Characteristics of soil horizons' *tab sheet*. More accuracy is required to calibrate the model for the various water-stress functions using data obtained when water is limiting.

Spatial heterogeneity of the soil can be a problem for accurate simulation for a given water limiting location, because FC and PWP, and hence TAW, can vary sufficiently from area-to-area in a field, reducing the accuracy of the simulated results for the field. If data are available for different parts of a field, simulation should be run for each part of the field that differs in soil water characteristics.

Saturated hydraulic conductivity (K_{sat}) of the top soil determines the internal drainage in the soil profile, losses from deep percolation and the amount of water infiltrated in the root zone and the surface runoff after an irrigation or rainfall. Surface runoff is only important if the amount of water applied per irrigation is excessive or the rainfall is intense and heavy. In such situations, the measured K_{sat} should be used for simulation. If measured value is unavailable, the default value provided by *AquaCrop* for the given soil textural class (based on the difference in soil-water content (θ) between saturated soil and FC) should be adjusted according to general knowledge of the local condition.

Initial soil water content

Another local specific factor is the initial water content of the soil for the maximum rooting depth at start of the simulation run. If the values are not measured, estimates may be made based on knowledge of the local climate, particularly rainfall, and the preceding crop or weed history. For example, for a climate with winter rainfall, sufficient to completely charge the soil profile, and dry summer, and the field is kept fallow and weed free, one may assume the deeper layers of the soil to be at FC but reduce soil-water content of the upper layer of the soil by estimating the extent of soil evaporation taking place before the simulation starting time. If weather data before the starting time of simulation are available, *AquaCrop* can be used to make that estimate by setting the start time as the end of the last significant rain. If weeds are present, however, some estimates would have to be made on canopy cover (CC) of the weed in order for *AquaCrop* to simulate a reasonable profile of initial soil-water content.

Crop phenology

Many of the differences among crop cultivars are related to the timing of developmental stages. The timing to reach a particular stage, or its duration for the local cultivar, needs to be specified by the user. These stages are: time to 90 percent seedling emergence, to the beginning of flowering, to the beginning of canopy senescence, and to physiological maturity, and the duration of flowering.

Time to 90 percent emergence

The particular choice of time to 90 percent emergence is explained later, under **Initial canopy size per seedling**. In nearly all the cases, this time is likely to be estimated and not determined by actual counting of the seedlings. It should be adjusted to have a good match between the simulated and measured canopy cover (CC) at the seedling stage and in early season. The adjustment, however, should be taken only after the relevant conservative parameters (initial canopy size per seedling and canopy growth coefficient) are well parameterized and the plant density is ascertained.

Time to start of flowering and duration of flowering

For determinate crops with their short flowering duration (e.g. 15 days), it is important to have an accurate time for start of flowering. For indeterminate crops with their long flowering duration, the timing can be more approximate. In cases where there is no significant water stress, the model is constructed in such a way that timing of flowering does not matter.

Time to maximum canopy cover

This parameter is provided in *AquaCrop* to allow simulation runs when the conservative parameter, canopy growth coefficient (CGC) of the crop, is not known, and should be used only as a last resort. See the later section **Canopy growth coefficient** for more explanation.

Time to canopy senescence

In *AquaCrop*, the timing to the start of canopy senescence is defined as the time when green leaf area falls to or below LAI = 4 as a result of yellowing of leaves, under optimal conditions with no water stress. By this definition, if the plant density is low and the maximum LAI is less than 4.0, canopy senescence starts once there is significant senescence of lower leaves. But if the maximum LAI is considerably higher than 4.0, enough of the lower leaves must senesce to reduce LAI to 4.0 before the canopy is considered to be at the beginning of senescence.

Time to physiological maturity

Different crop species may each have its own specific definition of physiological maturity (e.g. black layer formation in maize grains). To be general, however, *AquaCrop* uses as default the time when canopy cover is reduced to 5 percent of the achieved maximum canopy cover as the time of maturity. Users can change the maturity time according to their own data on the Canopy development *tab sheet*. Clearly, maturity is closely linked to the time of canopy senescence, and this may be one practical way to estimate maturity time if no detailed determination of maturity is made. Seed companies usually supply information on the life-cycle duration of their cultivars. This, however, can be very general, in terms of short, medium, or long season. The information can also be given in degree days, but unfortunately defined in ways different from that used in *AquaCrop*. For accuracy, experimental observations or data are necessary to determine the time to maturity. It would be justified to take the time when only a little green leaf area remains in the canopy as the time of maturity.

Rooting depth and deepening rate

Root development is highly site specific because of differences in soil physical (temperature, mechanical impedance, and aeration) and chemical (pH, salinity, and high levels of aluminum or manganese) characteristics, which strongly affect root growth. When soil conditions are all highly favourable, the root-deepening rate is likely to be in the range of 20 to 25 mm per day for many crops. The probable exceptions are crop species known for their shallow roots.

On deep soils with no layers restricting root growth, as default *AquaCrop* stops root deepening once the time for canopy senescence is reached (for no stress conditions). There is a notion in the literature that roots do not grow or deepen beyond the pollination stage of a crop. Good data on various crops show, however, that roots deepen after pollination, albeit at a slower rate. For soils of limited depth, but also with no growth-restricting layer in between, roots deepen at the normal rate in *AquaCrop* but stop abruptly when the bottom of the soil is reached.

In cases where the observed rooting is too shallow; although the soil is deep, some characteristic of the soil or soil layer may be inhibiting root growth. To approximate the situation with *AquaCrop* there are two possible means. One is simply to reduce the average deepening rate throughout the soil profile, by setting the maximum root depth at the beginning of canopy senescence at a point so that the root depth observed at a particular time matches that displayed by *AquaCrop*. The other approximation is only applicable to situations where root growth is inhibited more as the soil depth increases. By raising the shape factor of the root depth vs. time curve to the 2.5 to 3.0 range in the *Root deepening tab* under *Development* of the Crop file, the deepening rate would start high and slows with time as the roots go deeper. *AquaCrop* also offers the possibility of specifing the soil depth of a restrictive layer blocking root zone expansion as a soil characteristic in the *Restrictive soil layer* tab sheet.

CONSERVATIVE PARAMETERS

Temperature effects

Most temperature effects on crops are accounted for by using the GDD in place of calendar time as the driver, for which the setting of base and upper (cutoff) temperature are critical, and also by the use of ET_o. In addition, three temperature effects should be accounted for by other means. These are inhibitory effects, of low temperature on the conversion of transpiration to biomass production and on pollination, and of high temperature on pollination.

Base and upper temperature

The base temperature may be thought of as the lower threshold for crop growth and development. The upper temperature is the limit above which further increase in temperature has no effect on the rate of progression. The GDD calculation in *AquaCrop* is according to 'Method 2' as described by McMaster and Wilhelm *(*1997*)*, but with an important modification, that no adjustment is made of the minimum temperature when it drops below the base temperature. The base and upper temperature are usually selected in modelling work by trial and error by running simulation models for data collected in different temperature regimes. In terms of guiding principles, C_4 species are generally more cold sensitive than C_3 species, winter crops are obviously more cold tolerant than spring and summer crops, and crops with higher base temperature would benefit from warmer temperature (higher upper temperature). Base temperature for crops, such as barley and wheat, are generally taken to be 0 °C in most crop models, whereas for C_4 summer crops such as maize it is 8 or 10 °C. Upper temperature has been set at 30 °C for maize and 32 °C for cotton, but at 26 °C for wheat in *AquaCrop*.

If the experimental data used to test *AquaCrop* were obtained in a climate where the temperature does not often fall around the base temperature or above the upper temperature, the exact value of these two thresholds, as long as they are reasonable, would not likely make much difference in the simulated results. On the other hand, the difference may be large if the temperature often hovers around the base temperature or rises substantially above the upper temperature. In this case, it is necessary to refine the threshold values, best by securing data sets of the crop grown in other temperature regimes and by trial-and-error to arrive at the most reasonable temperature thresholds.

Low temperature effect on converting transpiration to biomass production

When simulating periods around the base temperature using *AquaCrop*, it was found that the model overpredicted production, probably because transpiration, mostly a physical process, is less inhibited by cold than photosynthesis, a complex metabolic process. It was then decided to apply a logistic function to arbitrarily reduce the amount of biomass produced per unit of normalized transpiration according to the magnitude of GDD each day, with an upper threshold GDD where the reduction begins, and a lower GDD fixed at GDD = 0, where conversion is reduced to zero. Generally, the upper threshold should probably be set in the range of 6 to 10 GDD.

Low and high temperature effects on pollination

These effects are also dealt with by arbitrary reductions using logistic functions, with temperature as the independent variable. The reduction starts at the upper threshold temperature for the cold effect, and the lower threshold for the high temperature effect. Pollination is completely inhibited when the temperature drops to 5 °C below the upper threshold for the cold effect, and when the temperature rises 5 °C above the lower threshold for the high temperature effect. Generally these inhibiting temperatures fall outside the temperature regimes favouring the growth and production of a given crop class.

Canopy cover and related parameters

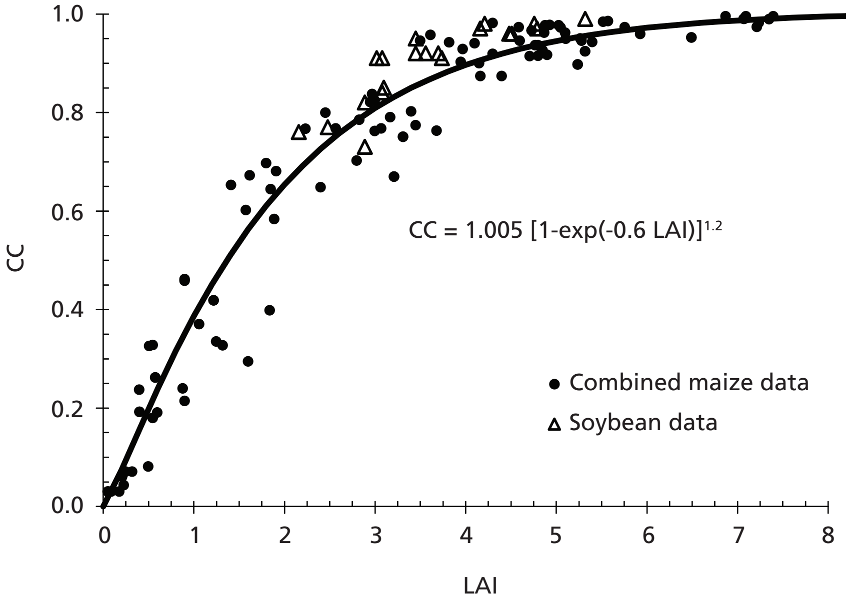
Converting leaf area index (LAI) data to canopy cover (CC)

AquaCrop simulates transpiration in terms of canopy cover (CC) of the crop, but often experimental studies measure LAI but not canopy cover, especially in earlier studies. During the parameterization of *AquaCrop* for maize (Hsiao *et al.,* 2009), a conversion equation, $CC = 1.005\ [1 - \exp(-0.6\ LAI)]^{1.2}$ was arrived at and used to analyse the literature of maize and soybean data (Figure 1).

Crops differing substantially in canopy architecture would have CC-LAI relationships different than that of Figure 1. Several recent reports on such relationships may be found in the scientific literature.

It should be noted that, during the canopy senescence phase, there is no simple way to measure CC, which refers to only green cover, because green and yellow leaves intermingle and some leaves are partly green and partly yellow. Hence, converting measured LAI to CC is the only way to obtain CC values during this crop phase.

FIGURE 1 Canopy cover (CC) in relation to leaf area index (LAI), based on data obtained for maize (combined data of several treatments and years) and soybean. The curve, described by the equation (*Hsiao et al., 2009*), represents the regression line revised slightly at the extreme low and high ends of LAI according to theoretical expectations.



Initial canopy size per seedling (cc_o)

Initial canopy cover per unit land area (CC_o) is computed from the mean initial canopy size per seedling (cc_o) and the plant density, that is, $CC_o = cc_o$ x plant density. CC_o is taken to be the canopy cover on the day of 90 percent emergence. At this stage, the average seedling is likely to be at the start of autotrophy and its growth begins to obey the equation for the first half of the canopy expansion (Equation 3 of Section 3.1).

Ideally, cc_o should be measured on seedlings of the chosen species, about 3 to 4 days after emergence, when the leaf or leaves turn fully green. At this stage, instead of measuring CC, the green leaf area of a seedling can be measured and used to approximate cc_o with a small downward adjustment (e.g. cc_o being 10 percent or 15 percent less than leaf area per seedling). The alternative is to derive cc_o indirectly, from data of CC taken at different times and plant density using the CC growth equations of *AquaCrop*. This approach is described fully later, when the parameterization of CGC is discussed. Regarding cc_o, one guiding principle is that for the variety of crop species, initial canopy size per seedling (cc_o) is generally correlated with mass per seed. Take an example of three crops, the relative sizes of cc_o are: maize > wheat > tomato, the same ranking as the relative mass per seed for these crops. Another guiding principle is that crops of similar nature and similar seed size should have similar cc_o. Thus, the cc_o value for wheat should be a good starting point for cc_o of barley, and the cc_o value for cabbage should be a good starting point for cc_o of canola.

Maximum canopy cover (CC_x)

When the planting is sufficiently dense, the theoretical upper limit for CC_x is 1.0, but in practice CC_x seldom reaches 0.99 and often lies in the range of 0.95 to 0.99 even for unusually high plant densities. This range is referred to in this writing as full canopy cover and the time when this is reached is referred to as canopy closure. However, these terms are used rather loosely in the literature, and can be referred to CC substantially less than 0.95, as low as 0.9 or even lower in some writings. As a general guide, CC is 0.95 or higher when LAI exceeds about 4.5 or 5.0 (Figure 1), with some exceptions. One exception is species exhibiting strong sun-tracking behaviour, such as sunflower, which requires an LAI of 3.5 to achieve full canopy cover. Another exception is if the crop is planted in clumps, or very close to each other in rows that are spaced widely apart. In this case LAI significantly higher than 5.0 is necessary to achieve full canopy cover.

As plant density is reduced below a particular level, the density is insufficient for the canopy to close and CC falls substantially below 0.95. This point depends on the kind of crop, each with its particular limit of potential leaf area per plant. Ideally, for each kind of crop a curve of CC_x vs. plant density, based on experimental data, should be constructed for use in *AquaCrop* simulations. Unfortunately, for some species, the required experimental data are lacking. If the user has CC_x measurements of his/her crop at the plant density in question under optimal growth conditions, these CC_x values are obviously the best to use in the simulation. Otherwise CC_x needs to be estimated. One way is simply visual, judging the extent of CC by eye around the time when CC is maximum. A word of caution here, viewing the canopy from the side or even at a downward angle (or photograph taken from similar positions) tends to overestimate the CC because this view may include too many plant layers. Viewing the canopy from directly above, or viewing the proportion of the soil shaded by the canopy when full sun is directly overhead, is the better way to make the estimate. Estimates can also be made based on general knowledge of the crop or similar crops.

If the CC_x of a particular crop is known for a particular plant density (reference planting), to estimate CC_x of a planting of the same kind of crop but planted at a different density (d_p), one can start by estimating the maximum LAI of the planting of known CC_x (LAI_{ref}) from Figure 1 (or a similar relationship if more accurate), and calculating first the LAI of the planting assuming leaf area per plant is independent of plant density, then make a rough adjustment for the impact of change in plant density. This is summarized as an equation:

$$LAI = LAI_{ref}\left(\frac{d_p}{d_{ref}}\right)\left(\frac{1}{F_{adj}}\right) \tag{1}$$

where d_{ref} is the plant density of the reference, and F_{adj} is the adjustment factor.

F_{adj} is limited between the range of d/d_{ref} and 1.0, for cases where $d_p > d_{ref}$, as well as where $d < d_{ref}$. To illustrate, first take the case of $d_p > d_{ref}$. If the $d_p/d_{ref} = 1.3$, F_{adj} would be limited to the range of 1 to 1.3. At one extreme where $F_{adj} = 1$, the leaf area per plant would be independent of plant density. At the other extreme where $F_{adj} = 1.3$, the leaf area per plant is reduced by the increase in plant density so much that the LAI of the planting remains the same as LAI_{ref}. In the case of $d_p < d_{ref}$, if $d_p/d_{ref} = 0.7$, F_{adj} would be limited to the range of 1 to 0.7. Obviously, in most cases, the limit values of F_{adj} should not be used to estimate LAI. The extent the plant adjusts its leaf area in response to crowding is related to how determinate the crop is in growth habit. So the more indeterminate the crop is, the more F_{adj} should deviate from 1.0, either smaller or larger.

After LAI of the planting is estimated, the corresponding CC can be read off Figure 1 or similar relations, and used as CC_x for the simulation. As is obvious in Figure 1, for cases where the canopy is full or nearly full and the plant density is not widely different from that of the reference, the CC_x estimate made with the above procedure should be accurate within a few percentage points. The estimates become less and less reliable as the difference in density becomes greater, or if CC_x or reference CC_x is substantially less than full cover. On the other hand, for cases where there is little interplant competition for PAR because of a sparse canopy (e.g. $CC < 0.5$), Equation 1 can be used along with Figure 1 to obtain a reasonable estimate of CC_x by setting F_{adj} close to 1.0.

Canopy growth coefficient (CGC)

CGC is a measure of the intrinsic ability of the canopy to expand. A CGC of 0.11, for example, means that each day the CC is 11 percent greater than the CC of the day before during the first half of canopy development. CGC is virtually a constant when temperature effects are accounted for by using GDD as the driver and there is no stress. Because CGC is based on first order kinetics (Bradford and Hsiao, 1982), a good way to derive CGC is to plot the log of CC vs. time and take the slope of the linearly fitted curve to be CGC, provided that only CC data measured from shortly after seedling emergence to approximately 60 percent cover, that do not include periods of heavy fruit load on the crop, are used. If CC data are too limited for the period specified above, but additional data have been collected up to canopy closure or near full cover, CGC can be parameterized using the canopy growth components of *AquaCrop*. Instead of running the model, which is more time consuming, a simple Excel programme limited only to canopy growth is available on the FAO *AquaCrop* website for this purpose.

Commonly, both cc_o and CGC would be unknown, requiring trial-and-error iterations to find the best values for the two parameters. As general guiding principles for parameterizing CGC, the main considerations appear to be whether the crop is C_3 or C_4, and whether the crop is more efficient in the capture of PAR. For maize and sorghum, two important C_4 crops already parameterized for *AquaCrop*, the CGC is 0.17 per day on a calendar time basis and 0.013 on a GDD basis. For a number of C_3 species, the CGC is around 0.09 to 0.12 per day on a calendar time basis. There are exceptions. One is the C_3 crop sunflower, its CGC is in the order of 0.22 per day (calendar time), presumably because of its solar tracking ability to capture more PAR per unit of canopy. In the trial-and-error runs to parameterize cc_o and CGC, several scenarios of outcome are possible when the simulated CC over time are compared with the measured data. These are listed in the first column of Table 3. In the second column are given possible causes for the lack of agreement and adjustments to make.

If the comparison of simulated vs. measured data does not follow any of the scenarios in the table, it is possible that either the experimental data are questionable, or the weather data may be deficient. The weather data are particularly suspect if 10-day or monthly minimum and maximum temperature are used instead of daily values

AquaCrop has built in an alternative to estimate CGC, based on the time required for CC to reach CC_x. This feature is provided for users who want to simulate roughly the production and water use of a crop with some or many of the crop parameters not known. It should not be relied on to parameterize CGC, because in such cases cc_o and plant density or initial canopy cover (CC_o), which are equally important in determining the time to reach maximum cover, are most certainly not known.

TABLE 3 Comparison of simulated with measured canopy cover and possible adjustments in the model parameters to improve the match.

Agreement between simulated CC (CC_{sim}) and measured CC (CC_{meas})	Possible cause(s) of discrepancy and suggested remedial action
CC_{sim} is either lower or higher than CC_{meas} from time of emergence to CC_x. Same CC_x reached but at different times. Slopes of the two curves for the period of rapid canopy growth are similar	Either cc_o is too low or plant density is too low, or, respectively, cc_o is too high or plant density is too high. Check plant density data and try larger (or smaller) cc_o. CGC and CC_x probably OK
CC_{sim} coincides with CC_{meas} early in season but gradually becomes either lower or higher. Same CC_x reached but at different times	CGC is either too low or too high, respectively. Make the appropriate adjustment in CGC. CC_x and cc_o probably OK
CC_{sim} is either lower or higher than CC_{meas} early in season but the trend reverses gradually later and the same CC_x is reached but at different times	Either cc_o is too low or plant density is too low, or, respectively, cc_o is too high or plant density is too high. CGC is either too high or too low respectively. Check plant density data and try larger (or smaller) cc_o and lower (or higher) CGC. CC_x probably OK
CC_{sim} coincide well with CC_{meas} over the season	Values of cc_o, CGC, and CC_x are good for this set of experimental data

Canopy decline coefficient (CDC)

After the canopy begins to senesce, CC is reduced progressively by applying an empirical canopy decline coefficient (CDC) (*Raes et al., 2011*). If there are LAI data spanning the senescence phase, they should be converted to CC using Equation 1 and a value for CDC selected to match the simulated CC decline with the measured values. Regrettably, in many studies detailed LAI data are lacking for this phase. In this case, CDC may be set initially according to observations of the canopy's speed of yellowing, and then refined by trial-and-error simulations to find the CDC that gives the best fit of the measured biomass data during the senescence phase. In terms of predicting biomass and yield, *AquaCrop* is not very sensitive to the extent of CC decline near maturity, because the model assumes a continuous decrease in the efficiency of converting normalized Tr to biomass for that period.

Normalized water productivity (WP*)

The water productivity (WP) of concern here is the ratio of biomass produced to the amount of water transpired ($WP_{B/Tr}$), and the normalized water productivity (WP*) is the ratio of biomass produced to water transpired, normalized for the evaporative demand and CO_2 concentration of the atmosphere.

WP normalized for evaporative demand

Transpiration, the denominator of WP, is extremely difficult to measure and separate from soil evaporation in the field. Fortunately, there are numerous sets of data on biomass production vs. consumptive water use, which can be used to derive $WP_{B/Tr}$, and hence WP* if the required weather data are available. Plots of biomass vs. normalized ET, based on sequential sampling over the season, should exhibit a portion of rising slope at the beginning followed by a straightline portion of near constant slope, and then ending with the slope being reduced for one to several data points sampled near the end of the crop life-cycle. The slope at any given point, of course, is the water productivity at that point in terms of normalized ET, not just normalized transpiration. The early rising slopes represent a period of low water productivity, when CC is small and much of the soil is exposed, and soil evaporation accounts for much of the ET. The middle portion of the plot, encompassing the data points collected from the time when the crop canopy covered more than about 70 percent of the ground to the time when about one-fourth of the maximum LAI has senesced as maturity is approached, are to be fitted with a linear equation. The slope of this linear regression is the WP normalized for evaporative demand, but only after a correction is made for soil evaporation. Once the canopy is nearly full, even when the soil surface is wet, evaporation may constitute only 12 to 18 percent of the total ET (Villalobos and Fereres, 1990). So, depending on how frequently the soil is wetted by rain or irrigation during the period spanning the middle portion of the plot, its slope should be reduced by 5 to 15 percent to obtain normalized WP.

For the plotting of biomass vs. normalized ET, ET_o is used to normalize for each time interval encompassing a biomass sample (Steduto *et al.*, 2007) according to the equation:

$$\text{Normalized ET} = \sum_{i=1}^{n} \left(\frac{Tr}{\overline{ET_o}} \right)_i \tag{2}$$

where i is a running number designating the sequential time interval between two adjacent biomass samples, Tr is the cumulative transpiration within that interval, and $\overline{ET_o}$ is the mean of daily ET_o within that interval, and n is the number of the biomass sample in question. The interval may not be fixed in duration and represents the time preceding the biomass sampling to the previous sampling time, e.g. for i = 5, the relevant time interval is the time between sample No. 4 and No. 5. For each biomass sample (n), the summation starts at the beginning (i = 1) and ends when i = n. If there are no ET and weather data for the time preceding the first biomass sample (i = 1), they can be assumed to be zero.

The reason for using Equation 2 to normalize is to account for any variation in ET_o among the different time intervals. If daily weather data are lacking and the weather is relatively stable, plots of biomass vs. ET instead of normalized ET can be used to obtain WP in a way analogous to the procedure above. Then the WP can be divided by a mean ET_o calculated from less detailed weather data to estimate normalized WP. However, this clearly is a rough approximation.

Normalization for atmospheric CO_2

The concentration of CO_2 in the atmosphere increases each year with time and impacts WP of crops. *AquaCrop* accounts for this effect by normalizing WP for CO_2 in a general way based on conceptual understanding and empirical data (Steduto *et al.*, 2007). The WP already normalized for evaporative demand is multiplied by a factor, f_{CO_2}, defined by Equation 3 below, to obtain WP*.

$$f_{CO_2} = \frac{(C_a/C_{a,o})}{1+0.000138\ (C_a - C_{a,o})} \tag{3}$$

In Equation 3 C_a is the mean air CO_2 concentration for the year of the experimental data, and $C_{a,o}$ is the mean CO_2 concentration for the year 2000 (equals 369.77 μLL^{-1}), both measured at the observatory at Mauna Loa, Hawaii. The C_a measured for the years 1980 up to present, are listed in *AquaCrop* in the climate file under the atmospheric CO_2 *tab*. The numerical values of the measured data can be found in the Mauna Loa CO_2 file in the SIMUL subdirectory of *AquaCrop*. The C_a of future years varies with the selected greenhouse gas-emission scenario (e.g. A2, A1B, B2 and B1 storylines). Users can enter their own projections or select one of the CO_2 files available in the DATA subdirectory of *AquaCrop*.

Reference harvest index (HI_o)

The value of reference harvest index is chosen as the middle high end of HI values reported for the majority of the given crop species or class. This value should be carefully chosen and not altered without good reason, because a change in reference HI would require the recalibration of the parameters modulating water stress effects on HI. In terms of guiding principles, reference HI can be 0.50 or even slightly higher for modern high-yielding cultivars of grain crops, but considerably lower for earlier cultivars and land races. Over the last century plant breeders selected for high HI by selecting for higher-yielding ability (Evans, 1993). For example, HI for wheat and rice were in the range of 0.33 at the beginning of the twentieth century and rose to as high as 0.53 in the 1980s (Evans, 1993). Since the 1980s only marginal improvements have been made in the HI of the major crops (Evans and Fischer, 1999). The reason could be that the limits for stems strong enough to support the grain weight and for the amount of leaves needed to support photosynthesis have been reached (Hsiao *et al., 2007*). It should be noted that HI considerably higher than 0.50 for grain crops have been reported from time to time in the literature. These values should be viewed with caution, to see if there is any indication of substantial loss of biomass such as the old and dead leaves to the wind just before harvest.

HI for oil seed crops and root crops differ from those of grains. Because it takes approximately 2.5 times as much assimilate to make a gram of oil as compared to sugar or starch, HI for oil seed crops are substantially lower than for grain crops, between 0.25 to 0.4. HI for root crops, on the other hand, are usually much higher, with the range of 0.7 to 0.8 being common for high-yielding cultivars of potato, sweet potato, and sugar beet, presumably because strong stems are not required to support the harvestable product.

WATER STRESS RESPONSE FUNCTIONS (K_S)

Water stress effects on leaf growth, stomata conductance, and accelerated canopy senescence are mediated through the stress response function (K_s) for these processes, with their characteristic thresholds expressed in terms of the fractional depletion (p) of the potential total available water in the root zone (TAW). As elaborated in Steduto *et al.* (2009), of the three processes leaf growth is the most sensitive to water stress; hence, its upper threshold (p_{upper}) should not be much below field capacity of the root zone soil (very small depletion) for virtually all the crops. Leaf growth is stopped completely at the lower threshold (p_{lower}), a point where water content in the root zone is still considerably above PWP, i.e. depletion is considerably smaller than complete. For stomatal conductance and accelerated senescence, p_{upper} should be considerably larger than that for leaf growth, and p_{lower} is fixed as 1 (complete depletion) in *AquaCrop*. Depending on the tendency to senesce of the kind of crop, p_{upper} for conductance may be the same, slightly or substantially smaller than that for senescence. Senescence is presumably much less sensitive to water stress in 'stay green' cultivars. A guiding principle is that crops possessing strong osmotic adjustment capability should have larger p_{upper} for conductance and senescence than those that do not. But p_{upper} for leaf growth may not be that different, although p_{lower} could also be larger. In setting the thresholds, it is not necessary to base the values too literally on results reported in short-term physiological studies, because *AquaCrop* runs in daily time steps and the thresholds represent integrated values over a diurnal cycle.

The shape of each stress response function (K_s vs. p) also needs to be parameterized. In most cases the shape should be convex. The convex shape may be interpreted as a reflection of crop acclimation to water stress, with earlier responses under milder water stresses being modulated by acclimation, and the limits of acclimation as stress becomes more and more severe.

During trial-and-error runs of *AquaCrop* to calibrate the stress response functions, the choices are to adjust either the thresholds or shape of the curve, or both. Obviously, if the time of the start of the stress effect is either clearly ahead or behind the effect shown by the measured data, the first adjustment should be in p_{upper}, by making it larger and smaller, respectively. After the starting times of the effect are matched between the simulated and measured, the degree of convex curvature can then be adjusted to match the progression of the stress effects between the simulated and measured. The more convex the curve is, the more gradually the stress effect intensifies initially as soil water depletes (p increases), but the stress effect intensifies more readily as p approaches the lower threshold. In the case of the stress function for leaf growth, p_{lower} may also need to be adjusted.

Because at the same soil water status plants experience more severe stress on days of high transpiration and less stress on days of low transpiration, *AquaCrop* automatically adjusts the various stress thresholds according to the evaporative demand of the atmosphere, represented by the daily ET_o. In most cases the default setting for this adjustment should suffice. Only in the rarest cases, where good data indicate a clear need, should this setting be changed under the Programme Setting *tab sheet*.

WATER STRESS EFFECTS ON HARVEST INDEX (HI)

AquaCrop accounts for three different effects of water stress on HI. The first is the effect related to accelerated senescence of canopy, shortening the life-cycle of the crop. In *AquaCrop* HI increases linearly with time shortly after the start of flowering to the time of maturity, when the reference HI value is reached (provided there is no modulation due to stress along the way). This increase is stopped automatically when CC drops to a threshold value (default value is 5 percent of the maximum CC reached). Early senescence of the canopy reduces HI by shortening the time available for HI to increase, because of the shortened life-span of the crop. If the resultant final HI simulated by the model does not match the measured HI, the match may be improved by altering the parameters that affect the timing and acceleration of canopy senescence, or by changing the threshold of percent CC remaining for stopping HI increase. The latter, however, should not be done unless there are good data supporting the change. Before making either alteration, it is prudent to first examine the impact of the other two stress effects on HI, discussed next, to see if their parameter values and simulated impact on HI are reasonable.

The next stress effect on HI to discuss is apparently the result of the competition for assimilates between vegetative and reproductive growth. A part of this effect is what accounts for higher HI under the right water-stress conditions. This beneficial water-stress effect is well known for cotton, and somewhat less well known for tomato and other vegetable fruit crops such as pepper and eggplant. The increase of HI over time would be accelerated for this situation as long as stress is not severe enough to inhibit photosynthesis. When stress is severe enough to markedly reduce photosynthesis, the increase of HI would be reduced. Three parameters in *AquaCrop* determine the sensitivity and extent of the changes in HI caused by the vegetative/reproductive competitions. The first parameter (*Before flowering* tab sheet under *Water stresses*) determines the increase in HI as the result of a minor reduction in biomass (reduction in leaf growth) caused by water stress for a short period before the start of flowering. This is based on empirical data, but may possibly be the result of flower bud formation and development being stimulated by accumulated assimilates. In many cases, this enhancement should be only a couple of percent. The next two parameters are in the During yield formation tab sheet. On *View corresponding HI adjustment* the values of the two parameters, ‘a’ and ‘b’, can be changed. Increase ‘a’ to reduce the enhancing effect on HI of leaf growth inhibition, and decrease ’b’ to enhance the reduction of HI caused by stomatal closure.

The third effect of stress on HI is because of failures of pollination and fruit set. The literature often state that pollination is sensitive to water stress. It turns out, however, that in detailed studies pollination and fruit set were found to be resistant to water stress, requiring stress levels much stronger than those inhibiting stomatal opening. Accordingly, in *AquaCrop* the threshold for pollination failure should be set close to the PWP (e.g. 85 percent depletion of TAW).

Most crops have an excess of potential fruits for the available assimilates to fill, so a portion of the embryos is aborted after pollination. For a stress to diminish HI by inhibiting pollination, it must be sufficiently severe to reduce the number of potential fruits below the number that can be filled by the available assimilates. Hence, the impact of stress on HI depends on the proportion of excessive potential fruits. The default proportion of excessive potential fruits is given in the model for a given crop, but is adjustable by the user on the *Water stress/Harvest index/During flowering* tab sheet.

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