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Model simplification and development via reuse, sensitivity analysis and composition: A case study in crop modelling

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A B S T R A C T

Crop models, like many representations of environmental processes, tend to be over-parameterised. A redesign of the SUCROS family of crop models, largely driven by sensitivity analysis, is presented here. In particular, two new versions of WOFOST, the most widespread model from this family, were developed. The first (WOFOST-GT) reduces model complexity through the definition of functions driven by few parameters with biological meaning. The other (WOFOST-GT2) improves canopy representation and senescence. Each version was evaluated for rice and winter wheat. Results highlighted a similar accuracy for the three versions: the original one achieved mean normalized RMSE of 13.75% and 10.75% for winter wheat and rice; corresponding values for the new versions were 14.42% and 10.79% (WOFOST-GT), and 14.38% and 10.85% (WOFOST-GT2). The new versions were considerably less complex, (60% less parameters). These improvements, increasing model usability without compromising its sophistication, can be transferred to other models from the same family.

Software availability

CropML.WOFOST-GT, CropML.WOFOST-GT2 are distributed free of charge for noncommercial purposes as .NET 4.5 components. The Software Development Kit is supplied on request (cassandra.lab@unimi.it) to interested users, and includes hypertext files documenting algorithms and code, as well as source codes of sample applications.

1. Introduction

The formalization of knowledge in agro-environmental models often leads to representations of the underlying systems characterized by a marked tendency towards over-parameterisation (Tremblay and Wallach, 2004). This might be due to different factors, like (i) the need to compose results from researches which targeted different subsystems, (ii) the partial understanding of key processes, that leads to models suitable for accommodating *flexible* calibrations against sets of observations, and (iii) technological bottlenecks partly preventing the adoption of advanced techniques for analysing and improving model design. To a certain extent, these considerations apply to the widespread crop models belonging to the SUCROS family (Bouman et al., 1996; van Ittersum et al., 2003). The worldwide spread of these models stems from the soundness of the approaches used to reproduce crop growth and by the high level of detail in describing the interactions between plants and environment. These features allowed the successful application of these models across a wide range of climatic (e.g., Supit et al., 2010) and management (e.g., Hengsdijk et al., 2005) conditions, and make them the first choice when a high level of adherence to real systems is needed, as in the case of, e.g., *in silico* phenotyping studies (Confalonieri et al., 2012), or for analyses in environments with a complex orography (Ferrara et al., 2010). On the other hand, this demands a huge amount of information for their parameterization, in turns increasing the effort for using them operationally (Donatelli and Confalonieri, 2011) and exposing users to risks because of the large number of freedom degrees during calibration. Indeed, the higher the number of parameters, the higher the risk of including site- and season-specific factors affecting observations in the values of parameters, which should instead describe only morphological and physiological plant traits. A portion of the large number of parameters present in SUCROS-type models is explained by the high level of detail used to represent biophysical processes, and should be considered as a positive, intrinsic feature of this family of models. Nevertheless, the main reason for the over-parameterization is the presence of AFGEN (Arbitrary Function GENerator) tables to describe the dependence of some parameters on air temperature or development stage.

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Especially when parameters are calibrated using observations related to just one state variable (e.g., aboveground biomass), AFGEN tables could allow the user to fit unrealistic functions for the description of plant processes. Therefore, although these functions could potentially lead to a better fit of the outputs during calibration because of their high flexibility, they increase the risks of losing adherence with actual biophysical phenomena. Another critical issue related to the presence of AFGEN tables refers to the difficulty of coupling the crop models to advanced tools for sensitivity analysis and automatic calibration. The reasons are that many of the algorithms implemented in such tools sample the parameters hyperspace by considering parameters as independent, and – for the sampling methods accounting for parameters correlation – it is often very difficult to define *a priori* the degree of correlation. In case of different parameters defining, e.g., specific leaf area (SLA) in two different development stages, these algorithms iterate sampling combinations of SLA values which could lead to a function without any physiological meaning. Some authors (e.g., Confalonieri, 2010; Ceglar et al., 2011) succeeded in performing Monte Carlo based sensitivity analyses on these models only at the cost of drastically reducing the number of couples defining the AFGEN tables with the aim of minimizing the risks of overlaps among the parameters distributions for different values of development stage code or average air temperature.

Another source of possible inconsistencies in the way SUCROS-type models reproduce the underlying system is represented by their peculiar representation of the canopy structure. They divide the canopy in a fixed number of layers, for which instantaneous gross assimilation rates are calculated. This number appears to be arbitrary, e.g., it is three for WOFOST (van Keulen and Wolf, 1986) and five for SUCROS (van Keulen et al., 1982), apparently with no justification in both cases. Moreover, this number is maintained constant from emergence to maturity, ignoring differences in canopy structure occurring during crop cycle. One of the most critical point in this representation is that the division of the canopy in different layers is explicitly considered only for some processes, e.g., gross photosynthesis. On the contrary, other processes, e.g., leaves death, do not take into account the position of leaf area index (LAI) units within the canopy, neither for ageing nor for self-shading. "Dead LAI" (representing leaves no more photosynthetically active) is thus evenly allocated along the canopy profile (i.e., to all the layers). This representation leads to situations where the last emitted LAI units, representing the youngest leaves, die exactly like the oldest ones, and where portions of dead leaves shade green ones (Confalonieri et al., 2012).

In light of the shortcomings highlighted above, two new versions of the WOFOST model were developed. WOFOST is considered as one of the most important representative of the SUCROS family: it is the main crop model used by the European Commission within the MARS Crop Yield Forecasting System (http://mars.jrc.it/mars/Bulletins-Publications), and it is widely used as a tool for analysing yield variability and the effects of climate change on crop productivity (Supit et al., 2012). The new versions and the original version were evaluated and compared using experimental data collected during rice and winter wheat field experiments, by considering their accuracy, robustness and complexity.

Therefore, the specific aims of this study were:

- to simplify WOFOST by substituting AFGEN tables with functions driven by few parameters with a clear biological meaning;
- to improve the usability and applicability of the model, by reducing the information needed to run simulations and increasing the possibility to couple the model with advanced tools for sensitivity analysis and automatic calibration;
- to investigate an alternative approach to describe the biophysical processes occurring within the canopy, via an explicit representation of the canopy vertical dimension.

2. Materials and methods

2.1. The WOFOST model

WOFOST is a generic crop simulator for annual field crops, based on a hierarchical distinction between potential and water-limited productions. Crop growth is simulated on the basis of its underlying eco-physiological processes. Among these, phenological development, light interception, gross photosynthesis, transpiration, growth and maintenance respiration, and partitioning of assimilates to the different plant organs play a major role. The appearance of vegetative and reproductive organs, which characterizes crop phenological development, is described as a function of average daily temperature, optionally corrected by a factor accounting for photoperiod. Thermal time accumulated is then normalized to a development stage code (DVS; unitless; 0: emergence; 1: anthesis; 2: maturity) by using two parameters describing the thermal time from emergence to anthesis and from anthesis to maturity. Instantaneous gross CO_2 assimilation is estimated in three moments during the day as a function of intercepted radiation and of a photosynthesis-light response curve of individual leaves. Light interception depends on total incoming radiation, on photosynthetic leaf area and on leaf angle distribution. Given that photosynthesis response to light intensity is non-linear, variations in the irradiance level are considered along the vertical profile. This is carried out by splitting the canopy into three horizontal layers and calculating the amount of radiation intercepted by each layer on the basis of the direct and diffuse light transmission through overlying layers. Daily increase in total LAI is estimated using a two-stage approach: using an exponential function driven by temperature during early stages, and from specific leaf area (SLA) and daily increase in leaves dry weight later. LAI is then allocated to the layers according to Gaussian Integration distances. Non-photosynthetically (dead) LAI units are computed daily as a function of self-shading and senescence. Part of the assimilates is consumed by maintenance respiration, depending on the dry weight of the different plant organs and on air temperature, assuming that the different organs have different respiration to dry weight ratios. Daily accumulated carbohydrates remaining after maintenance respiration are converted into plant organs components by considering development-dependent partitioning factors and the different efficiencies of conversion of assimilates into the components of the different plant organs (growth respiration). Potential evapotranspiration is estimated using the Penman approach (Frère and Popov, 1979), and water stress is derived by the actual to potential transpiration ratio.

For this study, the WOFOST version implemented in the Crop Models Library (CropML; http://agsys.cra-cin.it/tools/cropml/help/) was used. The library consists of a framework-independent MS .NET software component where different pure (e.g., WOFOST, CropSyst, WARM, STICS, CANEGRO), hybrid and new modelling solutions for crop growth and development are implemented following a fine level of granularity, according to the software architecture proposed by Donatelli and Rizzoli (2008). All the changes to the model presented and discussed in the following sections were implemented in the same component, as modelling solutions alternative to the original WOFOST.

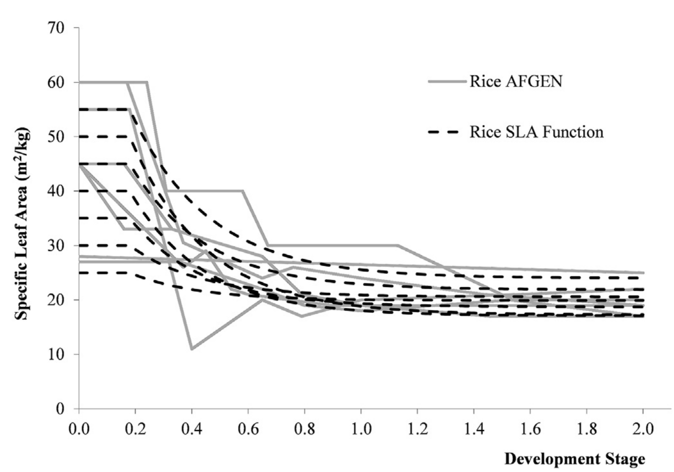

Fig. 1. Specific leaf area (SLA) as a function of development stage: grey continuous lines represent AFGEN parameterizations of eight rice cultivars available in the Wofost Control Centre release; black dashed lines show four possible parameterizations of the function that replace the SLA AFGEN table in the new versions of the model.

2.2. Decreasing model complexity

The methodology used to reduce the complexity of the original version of WOFOST is based on the substitution of the AFGEN tables (identified in the text by the suffix "TB") with functions (i) driven by few parameters with a clear biophysical meaning to simplify parameterization activities, and (ii) able to properly formalize the available knowledge on changes in parameter values according to crop development or air temperature. A concrete example of how we proceeded in replacing AFGEN tables is represented by the reduction of the number of pairs [SLA ($m^2\ kg^{-1}$)–DVS] needed to run a simulation. This parameter corresponds to the ratio between area ($m^2\ m^{-2}$) and the dry weight ($kg\ m^{-2}$) of a representative sample of leaves. Leaf dry weight can be easily measured after oven-drying the leaves until constant weight, whereas accurate LAI measurements – needed for SLA determination – are time-consuming (Negron Juàrez et al., 2009), since indirect methods (e.g., LAI2000) are not adequate in this case, and direct (i.e., planimetric) methods involving destructive sampling are normally used. Moreover, during crop development the effort required by planimetric methods for LAI determination progressively increases, because of the increasing number of leaves to be processed. In the original WOFOST version, up to ten couples of SLA values have to be provided by the user, together with the corresponding crop development stage starting from emergence to maturity. In this case, the objective of the work aimed at substituting the AFGEN table involved with SLA was to develop a function (Fig. 1) driven by SLA values (i) only in two clearly recognizable phenological stages and (ii) with the two stages characterized by a moderate number of leaves per plant, to increase the possibility of easily parameterizing the model for this aspect.

2.2.1. Replacement of AFGEN tables

Two approaches were used to replace AFGEN tables. The first approach involves AFGEN tables which highlighted negligible differences among available WOFOST parameterizations for a group of species (e.g., van Diepen et al., 1988; van Heemst, 1988). In these cases, the tables were substituted with non-editable functions, developed by interpolating the available WOFOST parameterizations for rice and wheat, without introducing any additional parameters. The AFGEN tables replaced according to this approach were those related to specific stem area (SSATB; function of DVS; $ha\ kg^{-1}$, replaced by Equation (1)), reduction factor of gross assimilation rate (TMNFTB; function of minimum temperature; $kg\ kg^{-1}$, Equation (2)), dry biomass partitioning to roots (FRTB; function of DVS; $kg\ kg^{-1}$, Equation (3)) and storage organs (FOTB; $kg\ kg^{-1}$, Equation (4)), and relative death rates of roots (RDRTB; function of DVS; $kg\ kg^{-1}\ d^{-1}$, Equation (5)) and stems (RDRSTB; $kg\ kg^{-1}\ d^{-1}$, Equation (5)).

$$SSA = \begin{cases} 0.0003 & DVS < 0.9 \\ -0.00027 \cdot DVS + 0.00054 & DVS \geq 0.9 \end{cases} \tag{1}$$

$$TMNF = \begin{cases} 0.333 \cdot T_{min} & T_{min} < 3 \\ 1 & T_{min} \geq 3 \end{cases} \tag{2}$$

$$FR = \begin{cases} 0.2 \cdot DVS^2 - 0.7 \cdot DVS + 0.5 & DVS < 1 \\ 0 & DVS \geq 1 \end{cases} \tag{3}$$

$$FO = \begin{cases} 0 & DVS < 0.7 \\ \dfrac{1}{1 + 0.5 \cdot \exp\left[\dfrac{-33.3 \cdot DVS + 33.3}{2}\right]} & 0.7 \leq DVS \leq 1.5 \\ 1 & DVS > 1.5 \end{cases} \tag{4}$$

$$RDR = \begin{cases} 0 & DVS \leq 1.5 \\ 0.02 & DVS > 1.5 \end{cases} \tag{5}$$

The second approach to replace AFGEN tables involves cases for which marked differences among parameterizations available in literature were observed. In these cases, the differences were in the values assumed by parameters, whereas the shapes (e.g., monotonic decreasing for partitioning to leaves) of the AFGEN functions proposed by different authors were coherent, since reflecting biological features of the plants. This led to the need of introducing functions driven by editable parameters to allow users to modulate the physiological crop responses to temperature and development stage. A set of functions was therefore developed to interpolate the available AFGEN parameterizations – mainly derived from measurements (e.g., Spitters et al., 1989) – with the aim of minimizing the number of parameters. These parameters were defined providing them with a clear morphological or physiological meaning, in order to ease the attribution of their values through field measurements and/or literature search. This allowed a consistent reduction of the number of parameters without undermining the degree of adherence of the model to real systems.

Temperature effect on thermal time accumulation rate (originally represented by the AFGEN DTSMTB; °C-d) was simulated by using the β function proposed by Yin et al. (1995, Equation 6)), driven by the parameters minimum, optimum and maximum temperature for development ($T_{base,dev}$, $T_{opt,dev}$ and $T_{max,dev}$, respectively; °C). The same temperature response function (Equation (6), editable through the parameters $T_{base,gro}$, $T_{opt,gro}$ and $T_{max,gro}$, representing cardinal temperatures for growth) was used for the temperature effects on CO_2 assimilation (AFGEN TMPFTB; unitless), where maximum rate is represented by the parameter A_{max} ($kg\ ha^{-1}\ h^{-1}$). Changes in A_{max} during the crop cycle are now simulated without the need of further parameters.

$$\beta = \begin{cases} 0 & T < T_{base} \\ \left[\left(\dfrac{T - (T_{base} - a)}{T_{opt} - (T_{base} - a)}\right) \cdot \left(\dfrac{(T_{max} - a) - T}{(T_{max} - a) - T_{opt}}\right)^{\dfrac{(T_{max} - a) - T_{opt}}{T_{opt} - (T_{base} - 2)}}\right]^b \cdot (T_{opt} - T_{base}) & T_{base} \leq T \leq T_{max} \\ 0 & T > T_{max} \end{cases} \tag{6}$$

where $a = 2$ and $b = 1.8$ for thermal time accumulation and $a = 0$ and $b = 1$ for the calculation of thermal limitation to gross photosynthesis.

The light use efficiency table (EFFTB; function of daily mean temperature; $kg\ ha^{-1}\ h^{-1}\ J^{-1}\ m^2\ s$) was replaced by a linear function between two parameters (EFF_{10} and EFF_{40}; $kg\ ha^{-1}\ h^{-1}\ J^{-1}\ m^2\ s$), representing light use efficiency of single leaves at 10 °C and 40 °C. The original table describing the evolution of the extinction coefficient for diffuse visible light (KDIFTB; function of DVS; unitless) was substituted by Equation (7), driven by the parameter $KDIF_{max}$ (unitless), representing the maximum value of KDIF; changes in this parameter simulate the extinction of light along canopies of different cereal species or cultivars.

$$KDIF = \begin{cases} 0.4 & DVS < 0.65 \\ (KDIF_{max} - 0.4) \cdot \dfrac{1}{1 + \exp\left[\dfrac{-(57.14 \cdot DVS - 47.14)}{3.3}\right]} & 0.65 \leq DVS \leq 1 \\ KDIF_{max} & DVS > 1 \end{cases} \tag{7}$$

The AFGEN table describing the changes in specific leaf area (SLA) during crop cycle (SLATB; function of DVS; $ha\ kg^{-1}$) was replaced by a function returning SLA values which are constant during early stages and decrease exponentially later (Equation (8)). Two parameters are required to adapt this function to different cereal species or varieties: SLA at emergence (SLA_{em}; $ha\ kg^{-1}$) and at mid-tillering (SLA_{035}; $ha\ kg^{-1}$).

$$SLA = \begin{cases} SLA_{em} & DVS < 0.18 \\ (SLA_{em} - SLA_{035} \cdot f) \cdot SLA_{em}^{[0.7(DVS - 0.18)]} + SLA_{035} \cdot f & DVS \geq 0.18 \end{cases} \tag{8}$$

where f (estimating the ratio between minimum SLA reached by the crop and SLA at mid-tillering) is derived using Equation (9):

$$f = 15,936 \cdot SLA_{em}^2 - 251.22 \cdot SLA_{em} + 1.43 \tag{9}$$

This formulation allows model users to specify the value of SLA at tillering instead of the value reached by the variable at the end of the crop cycle (minimum SLA), the former being easier to measure within field experiments.

Since the changes discussed above led to a non-editable FOTB function and FSTB (the fraction of aboveground photosynthates partitioned to stems; $kg\ kg^{-1}$) is – for each DVS – the complement to one of the sum of FOTB and FLTB (the fraction partitioned to leaves), partitioning to the aboveground organs is now completely dependent on the partitioning to leaves (FL, $kg\ kg^{-1}$). FL is derived by using a function driven by a single editable parameter: partitioning to leaves at emergence (RIP_{L0}; $kg\ kg^{-1}$) (Equations (10) and (11)). The same concepts behind this type of representation of allocation patterns to the different plant organs are used in the rice-specific WARM model (Confalonieri et al., 2009b).

$$FL = \begin{cases} -0.3 \cdot \dfrac{1 - 1.7 \cdot \exp[-(16.67 \cdot DVS - 10)]}{1 + n \cdot \exp[-(16.67 \cdot DVS - 10)]} + 0.3 & DVS \leq 1.1 \\ 0 & DVS > 1.1 \end{cases} \quad (10)$$

with:

$$n = \left[0.043 \cdot 0.051^{2.7 \cdot (RIP_{L0} - 0.4)} + 0.008\right] \cdot 1000 \quad (11)$$

The version of the model with functions replacing AFGEN tables – aimed at reducing model complexity – was named WOFOST-GT.

2.3. Improving the representation of canopy architecture

The methodology adopted to improve the representation of senescence dynamics within the canopy was based on the use of phenological development (via DVS) for deriving indirect information on the main variables involved, i.e., LAI and plant height. DVS identifies critical phases closely related to (i) photosynthetic area evolution, e.g., tillering ($0.3 < DVS < 0.6$) and flag leaf emission ($DVS = 0.9$), and (ii) stem elongation ($0.6 < DVS < 0.9$). In the same way, DVS – via its role in modulating the patterns of assimilates partitioning to the different plant organs – is indirectly related to plant height, since this variable is strictly related to the fraction of photosynthates daily allocated to stems (Confalonieri et al., 2011).

Starting from WOFOST-GT, a further version of the model (named WOFOST-GT2) was developed, aimed at explicitly considering the vertical canopy profile, via the implementation of a model for plant height (Confalonieri et al., 2011) coupled to a function for deriving the number of canopy layers from DVS (Equations (12) and (13)).

$$\text{Number of Canopy Layers} = \begin{cases} 2 & l < 2 \\ \lfloor l \rfloor & l \geq 2 \end{cases} \quad (12)$$

where the second equation is the floor function of

$$l = \begin{cases} \dfrac{20}{1 + \exp\left(-\dfrac{15 \cdot DVS - 6}{1.5}\right)} & DVS \leq 0.9 \\ 20 & DVS > 0.9 \end{cases} \quad (13)$$

This dynamic simulation of the emission of canopy layers assumes that during early stages ($DVS < 0.2$) the canopy can be adequately described as composed by two layers; as long as the crop is growing, the number of photosynthetic layers increases according to a logistic function, with the maximum rate of emission of new layers set during tillering ($DVS \approx 0.25$–0.35). The emission rate of new layers decreases during stem elongation, and ends with the emission of the flag leaf ($DVS = 0.9$). Leaf senescence is then computed allocating dead LAI units starting from the lowest canopy layer until the dead LAI of the layer is equal to its total LAI. Then, this layer is considered no longer photosynthetically active, and dead LAI units start to be allocated to the layer above. Simulating leaf senescence with such a bottom-up dynamic is coherent with both the drivers for leaves senescence reproduced by WOFOST: the ageing of leaves (the bottom layers contains the first emitted leaves) and self-shading (the bottom layers are those which are shaded).

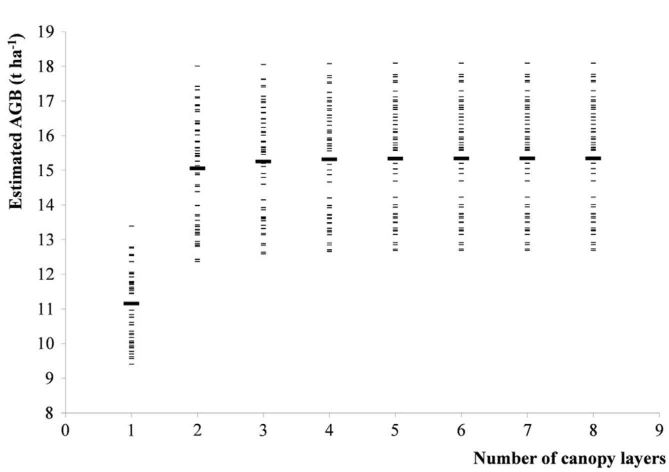

Fig. 2. Aboveground dry biomass values simulated with WOFOST by changing the number of canopy layers. Results of 400 simulations (10 nations × five years × eight layers). Thicker points indicate the mean values of the outputs calculated with the number of canopy layers reported on the *X*-axis.

The maximum number of canopy layers is set to 20 and is reached at anthesis. This value represents a compromise between the need to increase the vertical resolution to allow a fine description of leaf senescence dynamics and the need to limit the increase in the computational cost of the simulation, given the frequent adoption of WOFOST in projects requiring simulations against large-area databases. The adoption of two canopy layers at emergence is justified by (i) the pronounced worsening of the performance of the original WOFOST version run with a single canopy layer (data not shown) and (ii) by simulation experiments that revealed that the original WOFOST version markedly changes its behaviour only while increasing the number of canopy layers from one to two (Fig. 2). Moreover, coupling the approach for dynamic emission of canopy layers and bottom-up leaves senescence with a model for estimating plant height allows to assign an explicit thickness to each canopy layer and to identify the height above which LAI is photosynthetically active and below which it is represented by senescent tissues. This gives the opportunity to improve the simulation of micrometeorological aspects within the canopy (e.g., dead LAI units do not transpire, thus their temperature is higher), which, in turns, could lead to a more realistic simulation of biophysical processes involved with biotic (e.g., fungal pathogens) and abiotic stressors affecting the crop.

2.4. Testing the WOFOST versions

2.4.1. Sensitivity analysis experiments

Sensitivity analysis experiments were carried out for all the three versions of the model. For the original WOFOST version, the sensitivity analysis was carried out twice, with the second run performed by adding the number of canopy layers to the set of parameters investigated. For this parameter, a discrete uniform distribution (values ranging from one to eight) was used. For all sensitivity analysis experiments, aboveground dry biomass at maturity (AGB, kg ha^{-1}) was selected as the output variable, as it is best at synthetizing all the processes involved with crop growth. A two-step sensitivity analysis procedure was carried out: the Morris (1991) screening method (as improved by Campolongo et al., 2007) was first applied to identify a sub-set of relevant parameters, on which the computationally expensive Sobol' variance-based method (Sobol', 1993; Saltelli, 2002) was then applied to better discriminate among their relevance. The Morris method calculates a set of incremental ratios ($\Delta_{output}/\Delta_{parameter}$) when moving across different points of the parameter hyperspace and derives average (μ^*) and standard deviation (σ) of the ratios distribution. The higher the μ^* value, the higher the overall parameter importance, whereas the lower the σ value, the lower the interactions with other parameters. According to Morris method, the most relevant parameters are therefore those achieving high values for both these sensitivity indices. The Sobol' method identifies the relevance of each parameter or group of parameters via the quantification of their contribution to the variance of the model output, providing statistical estimators of partial variances. This method explores the parameters hyperspace via Monte Carlo sampling. In this study, the Sobol' total sensitivity index (S_t) of each parameter was considered, which quantifies the overall effect of the parameter on the output, thus including all the possible interactions with others.

In order to carry out sensitivity analysis while exploring both temporal and spatial variability, 5-year simulations (2005–2009) were performed on different European countries where the crops are intensively cultivated. France, Italy and Spain were chosen for rice, whereas England, Germany and Italy were selected to run the sensitivity analysis experiments for wheat. Within each country × crop combination, the percentage of crop presence within each of the 25 km × 25 km grid cells of the MARS database of the European Commission (Micale and Genovese, 2004) was analysed, and the cell with the highest crop presence was selected for the sensitivity analysis experiments (Table 1).

The statistical distributions of the parameters of the original WOFOST version were taken from Confalonieri (2010) and Confalonieri et al. (2012) for rice and wheat, respectively (Table 2). For the new versions of the model, distribution parameters were derived from literature and unpublished data (Table 2); in case available data were not enough to reliably test distribution hypotheses, normality was assumed and standard deviations was set to 5% of the mean of available data (Richter et al., 2010).

In order to gain an in-depth understanding of the impact of changes in the number of canopy layers on AGB variability, 400 one-season rice simulations were

Table 1
Locations for which sensitivity analysis experiments were performed. Latitude and longitude refer to the centroids of the 25 × 25 km grid cells of the European Commission MARS database (Micale and Genovese, 2004).

		Latitude (°)	Longitude (°)
Rice	France	43.71 N	4.63 E
	Italy	45.42 N	8.52 E
	Spain	37.04 N	6.11 W
Winter wheat	Italy	41.43 N	15.56 E
	United Kingdom	53.31 N	0.29 W
	Germany	51.94 N	10.97 E

Table 2
Statistical settings used to define the distributions of the parameters involved in sensitivity analyses for WOFOST, WOFOST-GT and WOFOST-GT2. Mean values are derived from literature and unpublished data. Standard deviations of the parameters were set to 5% of the mean in case available data were not enough to test distribution (assumed as normal) and to reliably estimate standard deviation.

WOFOST	Unit	Rice			Winter wheat		
		Mean	St.Dev	Source	Mean	St.Dev	Source
CVL	–	0.5	0.025	f; l; p	0.685	0.03425	a; p
CVR	–	0.5	0.025	f; l; p	0.694	0.0347	a; p
CVS	–	0.5	0.025	f; l; p	0.662	0.0331	a; p
CVO	–	0.5	0.025	f; l; p	0.709	0.03545	a; p
KDIFTB000	–	0.436	0.1	d; f; j; k	0.6	0.03	m; p
KDIFTB100	–	0.625	0.02	d; f	0.6	0.03	m; p
FLTB000	kg kg^{-1}	0.7	0.083	f; l; p	0.65	0.0325	m; n; p
FLTB050	kg kg^{-1}	0.45	0.16	f; l; p	0.5	0.025	m; n; p
FOTB082	kg kg^{-1}	0.2	0.043	f; l; p	0.0001	0.0000001	m; n; p
FOTB100	kg kg^{-1}	0.65	0.083	f; l; p	1	0.05	m; n; p
FRTB000	kg kg^{-1}	0.45	0.058	f; l; p	0.5	0.025	m; n; p
FRTB100	kg kg^{-1}	0.25	0.042	f; l; p	0.02	0.001	m; n; p
LAIEM	m^2 m^{-2}	0.01	0.005	e	0.1365	0.006825	m; p
SPAN	days	35	3.5	l	35	1.75	a; p
EFFTB10	kg ha^{-1} h^{-1} J^{-1} m^2 s	0.55	0.04	l; p	0.45	0.0225	c; p
EFFTB30	kg ha^{-1} h^{-1} J^{-1} m^2 s	0.35	0.04	l; p	0.45	0.0225	c; p
TBASE	°C	9	1.5	l	0	0.05	m
AMAXTB000	kg ha^{-1} h^{-1}	40.24	5	g; i; q	35.83	4.4785	m
AMAXTB200	kg ha^{-1} h^{-1}	40.24	5	f; l; p	4.48	0.224	m; p
RGRLAI	m^2 m^{-2} day^{-1}	0.00855	0.000482	f	0.00817	0.0004085	m; p
TMPFTB14	–	0.2	0.08	f; l; p	0.92	0.046	m
TMPFTB23	–	0.8	0.02	f; l; p	1	0.05	m
Q10	–	1.8	0.1	f; l; p	2	0.1	a; m; p
RML	kg kg^{-1} day^{-1}	0.028	0.0004	f; l; p	0.03	0.0015	a; p
RMR	kg kg^{-1} day^{-1}	0.012	0.0011	f; l; p	0.015	0.00075	a; p
RMS	kg kg^{-1} day–1	0.018	0.001	f; l; p	0.015	0.00075	a; p
RMO	kg kg^{-1} day^{-1}	0.01	0.0005	f; l; p	0.01	0.0005	a; p
SLATB035	ha kg^{-1}	0.0035	0.000525	j	0.00212	0.000106	m; p
SLATB045	ha kg^{-1}	0.00262	0.0002128	j	0.00212	0.000106	m; p
SLATB065	ha kg^{-1}	0.0023	0.000276	j	0.00212	0.000106	m; p
SSATB030	ha kg^{-1}	0.000919	0.000269	f	0	0	p
SSATB120	ha kg^{-1}	0.000216	0.00003	f	0	0	p
SSATB150	ha kg^{-1}	0.000335	0.000009	f	0	0	p
NumberOfCanopyLayers	Discrete (from 1 to 8)						
WOFOST-GT/-GT2	Unit	Mean	St.Dev	Source	Mean	St.Dev	Source
$T_{base,gro}$	°C	12	0.6	h	0	0.05	s
CVL	–	0.5	0.025	f; l; p	0.685	0.03425	a; p
CVR	–	0.5	0.025	f; l; p	0.694	0.0347	a; p
CVS	–	0.5	0.025	f; l; p	0.662	0.0331	a; p
CVO	–	0.5	0.025	f; l; p	0.709	0.03545	a; p
$KDIF_{max}$	–	0.55	0.04	j	0.48	0.022	m; p
LAIEM	m^2 m^{-2}	0.01	0.005	e	0.1365	0.006825	m; p
SPAN	days	35	3.5	l	35	1.75	a; p
BASE	°C	9	1.5	l	0	0.05	m
RGRLAI	m^2 m^{-2} day^{-1}	0.00855	0.000482	f	0.00817	0.0004085	m; p
$T_{max,gro}$	°C	42	2	j	35	1.75	p
$T_{opt,gro}$	°C	28	2	h	19	1	b; o
Q10	–	1.8	0.1	f; l; p	2	0.1	a; m; p
RML	kg kg^{-1} day^{-1}	0.028	0.0005	f; l; p	0.03	0.0015	a; p
RMR	kg kg^{-1} day^{-1}	0.012	0.0011	f; l; p	0.015	0.00075	a; p
RMS	kg kg^{-1} day^{-1}	0.018	0.001	f; l; p	0.015	0.00075	a; p
RMO	kg kg^{-1} day^{-1}	0.01	0.0005	f; l; p	0.01	0.0005	a; p
RIP_{L0}	kg kg^{-1}	0.6	0.1	r	0.65	0.0325	m; n; p
SLA_{em}	ha kg^{-1}	0.0045	0.0003	r	21.2	1.06	m; p
SLA_{035}	ha kg^{-1}	0.0030	0.0002	r	21.2	1.06	m; p
A_{max}	kg ha^{-1} h^{-1}	40.24	5	g; i; q	20.155	1.00775	p
H^{*}_{max}	cm	100	5	r	100	5	r

a: Arora and Gajri (1998); b: Bechini et al. (2006); c: Biernath et al. (2011); d: Boschetti et al. (2006); e: Boschetti (unpublished data); f: Casanova et al. (2000); g: Choudhury (2001); h: Confalonieri and Bocchi (2005); i: Da Matta et al. (2001); j: Dingkuhn et al. (1999); k: Kiniry et al. (2001); l: Kropff et al. (1994); m: Richter et al. (2010); n: Rötter et al. (2011); o: Slafer and Rawson (1995); p: van Diepen et al. (1988); q: Ziska and Teramura (1992); r: unpublished data, collected in northern Italy under the same management conditions of the experiments described in Bechini et al. (2006) for wheat and Confalonieri and Bocchi (2005) for rice. *Only for WOFOST-GT2.

also run with 50 meteorological datasets (ten sites × five years, including those used for sensitivity analysis experiments) by changing the number of canopy layers from one to eight.

2.4.2. Experimental data

Experimental data used to evaluate the performances of the original and of the new versions of WOFOST come from 20 datasets collected in Italy (rice and winter wheat) and in the United Kingdom (winter wheat) (Table 3). Experiments 1–6, carried out in the Po Valley (Northern Italy), are described in detail by Confalonieri and Bocchi (2005) and Confalonieri et al. (2006). Experiments 1 and 2 were aimed at evaluating the production of two japonica-type rice varieties differing in the length of the crop cycle under non-limiting conditions for water and nutrients. During experiments 3–6, different rice varieties were grown under flooded conditions and different levels of nitrogen fertilization. For experiment 3, three levels of nitrogen (60, 120, 180 kg N ha^{-1}) were applied as urea in two or three events, in a split-plot design with three replicates. In experiment 4, four nitrogen levels (0, 40, 80, 120 kg N ha^{-1}) were applied in one or two events as urea or calcium cyanamide. Three levels of nitrogen were applied as urea during the experiment 5: 0–70–150 kg N ha^{-1} and 0–50–110 kg N ha^{-1} levels were used in two different sites. In experiment 6, two levels of nitrogen (0 and 140 kg N ha^{-1}), split in two events, were tested. Experiments 7–9 were aimed at investigating growth dynamics of winter wheat and other grass species (Bechini et al., 2006). During experiment 7, three levels of nitrogen fertilization were used (0–140–210 kg N ha^{-1}). Experiment 8 was aimed at studying the dynamics of biomass accumulation of five species, including winter wheat, under non-limiting conditions for water and nitrogen. In experiment 9, nine nitrogen treatments were evaluated (0, 50, 100 kg N ha^{-1} in pre-sowing combined with 0, 40, 80 kg N ha^{-1} top-dressed). Experiments 10 and 11 were conducted by ADAS (former Agricultural Development and Advisory Service, Nottinghamshire, UK) with the aim of measuring – under different irrigation managements (fully irrigated and rainfed) – green area expansion, radiation interception, water uptake and AGB accumulation of six winter wheat cultivars (Foulkes et al., 2001). 180 kg N ha^{-1} as ammonium nitrate were distributed in two events.

In this study, the three WOFOST versions were run under potential conditions, i.e., with solar radiation and air temperature as the only factors driving crop growth and development. Therefore, in case different water or nitrogen levels were tested during the experiments, only data coming from the non-limiting treatments were used for model calibration and evaluation. For the experiments where fertilization and irrigation were not experimental factors, water and nutrient availability was always adequate in fully satisfying crop needs. All the datasets refer to experimental plots which were kept weed, pest and disease free.

Available data were split in calibration and validation datasets as shown in Table 3.

The weather data used to run the models (daily air maximum and minimum temperature and global solar radiation) came from different sources: a floating micrometeorological weather station placed inside the field for experiments 5–6, automatic weather stations near the fields for experiments 1–4 and 7–9, and ECMWF (European Centre for Medium-Range Weather Forecast; www.ecmwf.int/) ERA-Interim data, with a resolution of one degree latitude × one degree longitude, for experiments 10–11.

2.4.3. Calibration of the models

The parameters of WOFOST-GT identified as the most relevant during the sensitivity analysis experiments were calibrated to obtain the best agreement between measured and simulated AGB values for rice and winter wheat. Phenology parameters (i.e., growing degree days to reach a certain phase and cardinal temperatures for development) were adjusted to reproduce observed flowering and maturity dates. For processes formalized in the same way in the three versions of the model, the same parameterization was used to increase the comparability among the three WOFOST versions (see, e.g., base temperature for emergence); the same was done for parameters with a clear biological meaning, although included in processes formalized in different ways in the three versions (see, e.g., base temperature for development) (Appendices A–C).

The absence of AFGEN tables allowed the calibration of WOFOST-GT parameters using the downhill simplex method (Nelder and Mead, 1965) and root mean square error (RMSE; Fox, 1981; optimum and minimum value = 0, maximum = +∞) as the objective function. A single simplex is a geometrical entity characterized by $n + 1$ vertices moving through the n-dimensional space of the model parameters to calibrate. Each vertex represents a combination of model parameters that leads to a certain value of the objective function. The simplex moves in the parameters hyperspace following a gradient of the objective function until the minimum (or the maximum, according to the objective function selected) is reached. In this study, the evolutionary shuffled simplex method described by Acutis and Confalonieri (2006) was adopted as it (i) lowers the risk of finding local minima and (ii) forces the simplex to explore a region of the hyperspace defined by realistic values of the parameters, since boundaries are defined according to the parameters biophysical range. The calibrations were performed running simultaneously 10 simplexes, with the tolerance for the objective function set to 10^{-5} and the maximum number of iterations for each of the simplexes fixed at 150.

After calibration, the models were evaluated against independent datasets (Table 3) adopting a multi-metric procedure. The metrics were chosen among those proposed by Bennett et al. (2013), focussing on the ones suitable to test the model ability to reproduce time- and space-dependent data. They are root mean square error (RMSE, optimum and minimum = 0, maximum = +∞, t ha^{-1}), normalized RMSE (NRMSE, corresponding to RMSE divided by the range of variation of measured data, optimum and minimum = 0 and maximum = 100%), modelling efficiency (NSE, Nash and Sutcliffe, 1970, optimum and maximum = 1, minimum −∞) and the coefficient of determination (R^2, optimum and maximum = 1 and minimum = 0).

3. Results and discussion

3.1. Sensitivity analyses

The results of the sensitivity analysis carried out on the original WOFOST version pointed out the relevance of the parameter "number of canopy layers" according to both the Morris and Sobol' methods. Regardless of the combination location × year, this parameter is the most relevant in explaining the variability of simulated AGB. Indeed, Morris μ^* and σ indices for the number of canopy layers are, respectively, three and five times larger than those of the second ranked parameter (CVS, efficiency of conversion into stems; kg kg^{-1}), and – according to Sobol' – 67% of total AGB variance is explained by the number of canopy layers. However, this high sensitivity of the model to the

Table 3
Datasets used for model calibration and validation. Exp.: experiment number; DOY: day of the year; J: japonica rice; I: indica rice; WW: winter wheat; C: calibration datasets; V: validation datasets.

Exp.	Country	Location	Latitude, longitude	Years	Crop/variety cultivar	Sowing DOY	Flowering DOY	Maturity DOY	Dataset
1	Italy	Vercelli	45°19′ N, 8°25′ E	1989	J Cripto	128	224	249	C
1	Italy	Vercelli	45°19′ N, 8°25′ E	1990	J Cripto	130	209	254	V
1	Italy	Gudo Visconti	45°22′ N, 9°00′ E	1990	J Cripto	104	218	264	V
2	Italy	Castello d'Agogna	45°14′ N, 8°41′ E	1995	J Ariete	130	217	245	C
3	Italy	Castello d'Agogna	45°14′ N, 8°41′ E	1996	J Drago	128	229	273	C
3	Italy	Mortara	45°14′ N, 8°41′ E	1996	J Drago	129	230	273	V
4	Italy	Velezzo Lomellina	45°09′ N, 8°44′ E	1999	I Thaibonnet	91	204	237	V
5	Italy	Vignate	45°29′ N, 9°22′ E	2002	I Sillaro	119	218	279	C
5	Italy	Opera	45°22′ N, 9°12′ E	2002	I Thaibonnet	119	213	264	V
6	Italy	Opera	45°22′ N, 9°12′ E	2004	I Gladio	145	230	262	C
7	Italy	S. Angelo Lodigiano	45°15' N, 9°22' E	1986–1987	WW Gemini	294	145	186	V
7	Italy	S. Angelo Lodigiano	45°15' N, 9°22' E	1987–1988	WW Gemini	298	133	174	V
8	Italy	S. Angelo Lodigiano	45°15' N, 9°22' E	1989–1990	WW Pandas	306	130	191	C
8	Italy	S. Angelo Lodigiano	45°15' N, 9°22' E	1990–1991	WW Centauro	320	141	176	C
9	Italy	S. Angelo Lodigiano	45°15' N, 9°22' E	2001–2002	WW Guadalupe	320	130	184	C
10	UK	Gleadthorpe	55°13' N, 1°6' W	1993–1994	WW Haven	307	175	213	C
10	UK	Gleadthorpe	55°13' N, 1°6' W	1993–1994	WW Soisson	307	168	210	C
10	UK	Gleadthorpe	55°13' N, 1°6' W	1993–1994	WW Rialto	307	175	215	V
11	UK	Gleadthorpe	55°13' N, 1°6' W	1994–1995	WW Mercia	287	165	215	C
11	UK	Gleadthorpe	55°13' N, 1°6' W	1994–1995	WW Riband	287	168	215	V

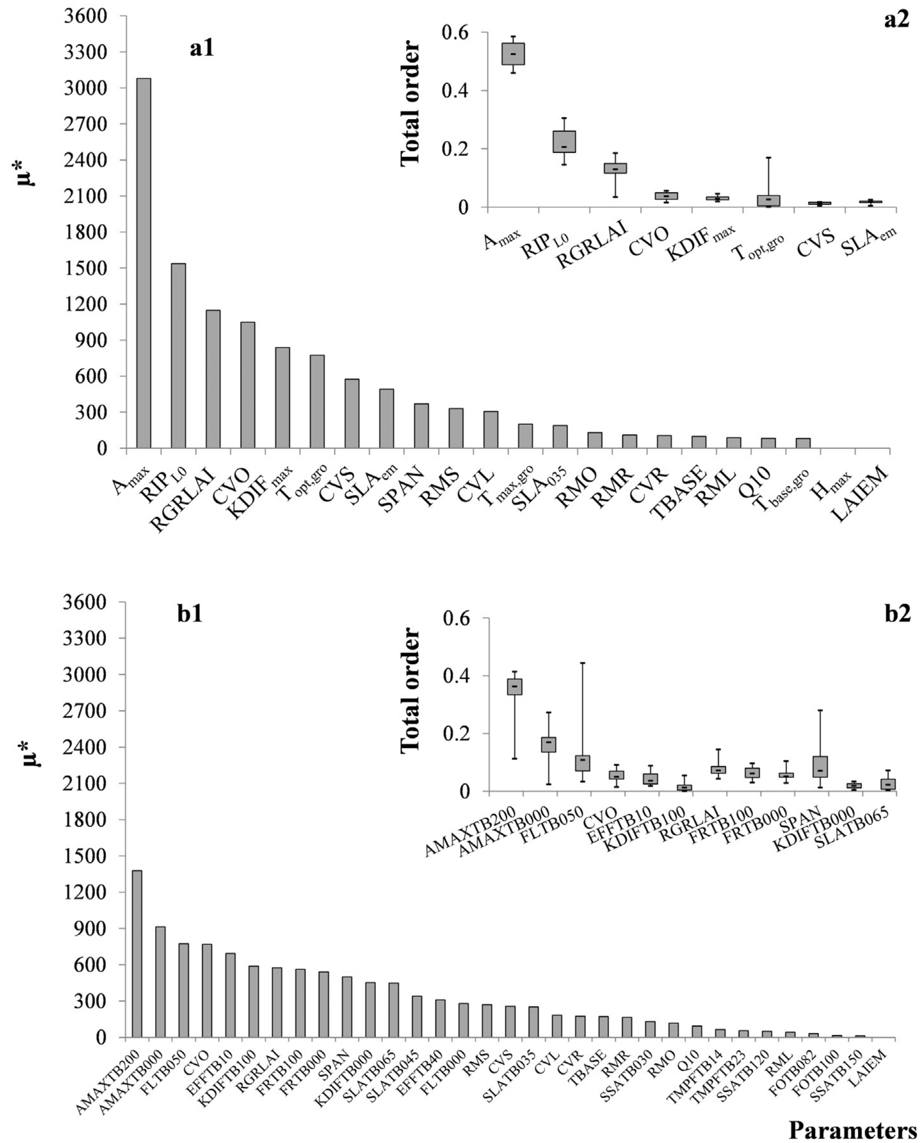

Fig. 3. Results of the sensitivity analysis experiments performed for rice. a: WOFOST-GT2; b: WOFOST; 1: Morris Method; 2: Sobol' method. The suffix "TB" identifies a parameter listed in an AFGEN table. The code following "TB" is the value of the independent variable of the AFGEN table. Two digit code: average air temperature (°C); three digit code: development stage (unitless; decimal point after the first digit).

number of canopy layers is almost completely explained by the marked increase in simulated AGB while shifting from one to two layers, as outlined by the results of the simulations presented in Fig. 2.

Sensitivity analysis experiments performed on WOFOST without considering the number of canopy layers as a parameter, i.e., by fixing three layers like in the original version, highlighted a different behaviour of the model in terms of parameters relevance between rice and wheat simulations (Figs. 3 and 4). These differences were analysed in terms of concordance between the rankings of parameters sorted according to Morris μ^* for the two crops and were significant, with a value of the top-down concordance coefficient TDCC (Iman and Conover, 1987) equal to 0.71. The differences were particularly marked for some parameters, like AMAXTB200 and RGRLAI, whose variations explained a large part of rice AGB variability, but were found to be rather irrelevant for wheat. This was both due to the different meteorological conditions characterizing the growing period of the two crops (rice is a summer crop, whereas wheat is a winter one) and to the different parameter distributions used for the sensitivity analysis experiments.

WOFOST-GT and -GT2 achieved practically the same values for the sensitivity analysis metrics and presented smaller differences in the parameter rankings obtained for rice and wheat (TDCC = 0.87). In fact, top-ranked parameters according to Morris μ^* always included – for both rice and wheat – A_{max}, RIP_{L0}, at least one parameter related to specific leaf area (SLA_{em} and/or SLA_{035}), optimum temperature for growth ($T_{opt,gro}$) and conversion efficiencies into different organs (CVO, CVS and CVL). For parameterization purposes, the higher concordance between sensitivity analysis results achieved by WOFOST-GT and -GT2 for rice and wheat could allow the identification of a single subset of parameters to calibrate, regardless of the crop simulated. This would increase model usability in case, e.g., parameter sets should be

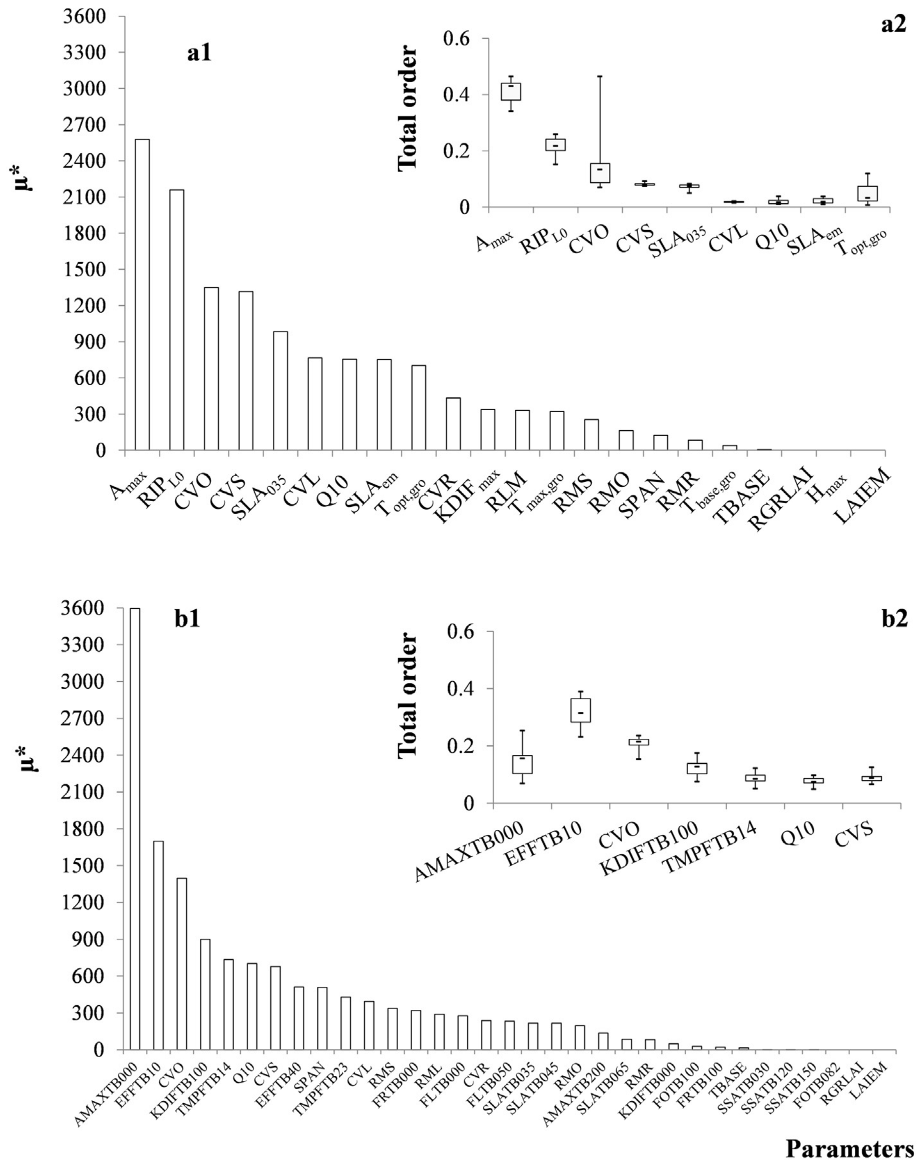

Fig. 4. Results of the sensitivity analysis experiments performed for wheat. a: WOFOST-GT2; b: WOFOST; 1: Morris Method; 2: Sobol' method. The suffix "TB" identifies a parameter listed in an AFGEN table. The code following "TB" is the value of the independent variable of the AFGEN table. Two digit code: average air temperature (°C); three digit code: development stage (unitless; decimal point after the first digit).

defined for more crops within a modelling study. Apart from conversion efficiencies, all the parameters that achieved the highest Morris μ^* values are among those introduced in the new versions of WOFOST to replace AFGEN functions. This confirms that the new formalizations included in the new versions of the model are focused on core processes.

The Sobol' method allowed deeper insight on the relevance of the parameters screened by Morris. For WOFOST-GT and -GT2, the values of Sobol' S_t confirmed the results of the analyses performed with the Morris method, whereas for the original version of the model the two sensitivity analysis methods led to substantial disagreement in the rankings of the most relevant parameters, especially for wheat. In this case, Sobol' method did not recognize AMAXTB000 as the most important parameter, with the variations of EFFTB10 and CVO achieving the highest S_t values (Fig. 4). The distributions of Sobol' S_t indexes (Fig. 3.a2, 2.b2, 3a2, 3.b2) highlighted a marked variability according to the conditions explored: for each version of WOFOST, only few parameters showed a small range of S_t values (e.g., the WOFOST-GT2 CVS for both rice and wheat, and the WOFOST parameters Q10 and KDIFTB000 for wheat and rice, respectively).

3.2. Calibration and evaluation

For all the versions of the model and for both the crops, calibrated parameters are presented in Appendices A and B (WOFOST) and C (WOFOST-GT and -GT2). Fig. 5 shows the growth dynamics of aboveground, leaves, stems and storage organs dry biomass simulated by WOFOST and WOFOST-GT. No sizable differences between the two versions of the model were observed for AGB, leaves and stems dry mass, whereas storage organs biomass simulated by the original version of WOFOST was slightly larger than for WOFOST-GT. The pronounced agreement between WOFOST and WOFOST-GT outputs is explained (i) by the fact that the functions used to

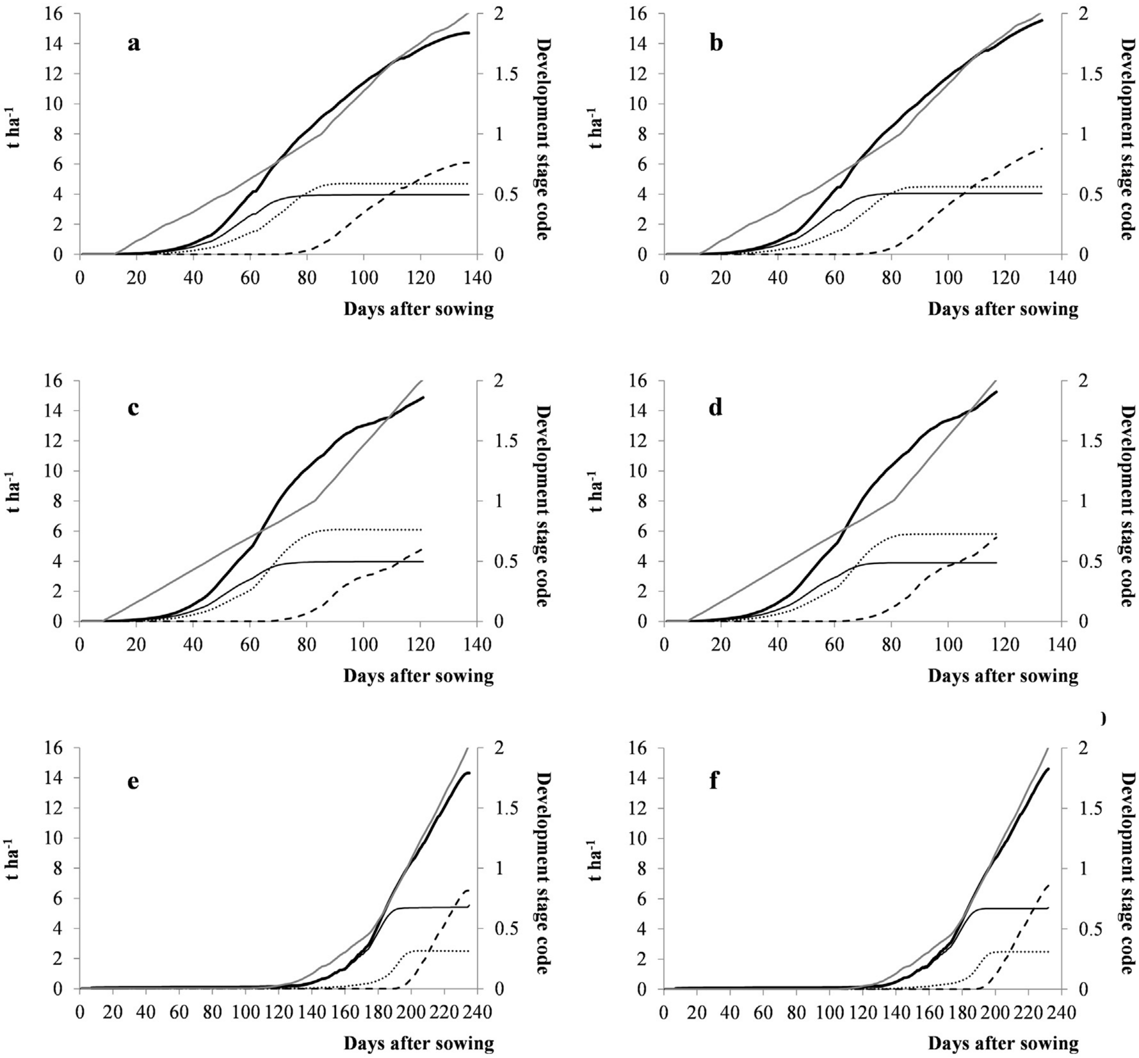

Fig. 5. Comparison between WOFOST and WOFOST-GT for the simulation of aboveground biomass (black continuous thick line), leaves biomass (black continuous line), stems biomass (black dotted line), storage organs (black dashed line) and development stage (grey continuous line) for Indica-type rice (a, b), Japonica-type rice (c, d) and winter wheat (e, f). The main *y*-axis refers to dry biomass values (t ha^{-1}), the secondary one-axis to the development stage code. The *x*-axis indicates the days after sowing. a) WOFOST, Opera 2004; b) WOFOST-GT, Opera 2004; c) WOFOST, Vercelli 1990; d) WOFOST-GT, Vercelli 1990; e) WOFOST, Sant'Angelo 1989–1990; f) WOFOST-GT, Sant'Angelo 1989–1990.

replace AFGEN tables were developed with aim of preserving to the full extent the behaviour of WOFOST, and (ii) by the coherence between the parameterization of the two versions of the model. These considerations provide guarantees on the suitability of the partitioning functions implemented in the new versions of the model.

Fig. 6 presents the results of the comparison between measured AGB values and corresponding outputs of WOFOST (circles) and WOFOST-GT (triangles), whereas agreement metrics are shown in Table 4; results for WOFOST-GT2 are not shown in the figure since very close to those simulated by the -GT version of the model. Under the explored conditions, the three versions of the model achieved similar values for RMSE, NRMSE, NSE and R^2 for both rice and winter wheat (Table 4). In particular, the performances of WOFOST-GT and -GT2 are almost identical to those of the original version of the model for rice, with average RMSE equal to 1.59 t ha^{-1} for WOFOST and WOFOST-GT, and 1.60 t ha^{-1} for the -GT2 version of the model. Although the original version of the model achieved the best values for all the accuracy metrics for wheat, differences were also in this case acceptable (average RMSE = 1.80 t ha^{-1} for WOFOST and 1.94 t ha^{-1} for the -GT and -GT2 versions). The analysis of NSE, NRMSE and R^2 (the latter higher than 0.90 in 59 out of 62 cases) values confirmed the closeness of the performances of the three WOFOST versions, and the slightly better performances of WOFOST for wheat, although differences were always negligible. These differences are due to small discrepancies between the linear interpolation of the AFGEN tables and the non-linear functions used to replace them.

In general, the reduction of the number of parameters led to a decided improvement of the new versions of WOFOST in terms of complexity, quantified using the Akaike index (Akaike Information Criterion, Akaike, 1974, optimum = 0). The values of the Akaike index of the new versions of the model (Table 5) are in fact 35% and 50% lower – for wheat and rice, respectively – than those calculated for the original version of the model. Besides the obvious advantages deriving from the reduction of the number of parameters, the elimination of the AFGEN tables increases the model usability by lowering the risk of developing incoherent parameter sets while changing parameter values

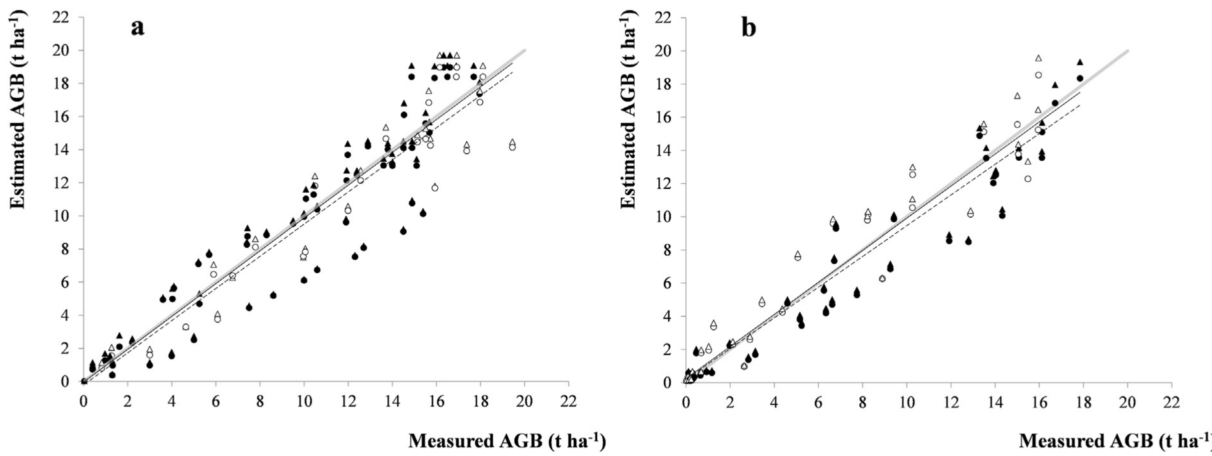

Fig. 6. Comparison between measured and simulated aboveground dry biomass values for wheat (a) and rice (b); WOFOST: calibration datasets (black circles), validation datasets (white circles); WOFOST-GT: calibration datasets (black triangles), validation datasets (white triangles). The grey lines are the 1:1 line. Dotted lines are the regression $y = 0.9704x - 0.2016$ ($R^2 = 0.8747$) and $y = 0.9263x + 0.1974$ ($R^2 = 0.926$) of WOFOST values for wheat and rice, respectively. Continuous lines are the regression $y = 0.9899x - 0.0249$ ($R^2 = 0.863$) and $y = 0.9673x + 0.2414$ ($R^2 = 0.925$) of WOFOST-GT values for wheat and rice, respectively.

during calibration. The tuning of AFGEN points requires a higher degree of knowledge on plant physiology, since more degrees of freedom are left to the user. On the contrary, the functions used to replace AFGEN tables are forced to reproduce realistic dynamics during the crop cycle. The adherence of these functions to actual physiological processes is enhanced – with our implementation – by smaller biophysical ranges for the parameters (derived from literature). As an example, photosynthates partitioning to leaves in the corresponding WOFOST AFGEN table must range between 0 and values around 0.90, and

Table 4
Indices of agreement between aboveground dry biomass observations and corresponding values simulated by WOFOST, WOFOST-GT and WOFOST-GT2. RMSE: root mean square error; NRMSE: normalized root mean square error (equal to RMSE divided by the range of variation of measured data); NSE: modelling efficiency (Nash and Sutcliffe, 1970); R^2: coefficient of determination.

Dataset	RMSE (t ha^{-1})			NRMSE (%)			NSE			R^2		
	W	W-GT	W-GT2	W	W-GT	W-GT2	W	W-GT	W-GT2	W	W-GT	W-GT2
Winter wheat – calibration												
Sant'Angelo 89–90	3.56	3.45	3.42	30.7	29.8	29.5	0.376	0.412	0.422	0.841	0.833	0.833
Sant'Angelo 90–91	0.92	1.01	1.04	6.4	7.0	7.1	0.960	0.952	0.950	0.975	0.978	0.978
Sant'Angelo 01–02	1.41	1.20	1.17	10.4	8.9	8.6	0.951	0.965	0.967	0.988	0.987	0.987
Haven 93–94	0.99	1.41	1.46	6.7	9.5	9.8	0.970	0.939	0.934	0.977	0.978	0.978
Soisson 93–94	1.71	2.10	2.16	11.8	14.5	14.9	0.905	0.856	0.848	0.952	0.953	0.954
Mercia 94–95	1.67	2.29	2.35	10.7	14.6	15.0	0.912	0.835	0.826	0.997	0.997	0.997
Mean	*1.71*	*1.91*	*1.93*	*12.8*	*14.0*	*14.2*	*0.846*	*0.826*	*0.824*	*0.955*	*0.954*	*0.954*
Winter wheat – validation												
Sant'Angelo 86–87	3.01	2.88	2.77	18.0	18.8	18.7	0.673	0.701	0.724	0.907	0.904	0.904
Sant'Angelo 87–88	2.20	1.90	1.87	23.7	22.7	21.8	0.809	0.859	0.862	0.983	0.983	0.983
Rialto 93–94	0.81	0.98	1.01	13.7	11.8	11.6	0.981	0.973	0.971	0.982	0.982	0.983
Riband 94–95	1.53	2.14	2.20	5.4	6.6	6.8	0.922	0.847	0.839	0.993	0.994	0.994
Mean	*1.89*	*1.98*	*1.96*	*15.2*	*15.0*	*14.7*	*0.846*	*0.845*	*0.849*	*0.966*	*0.966*	*0.966*
Rice – calibration												
Vercelli 1989	2.01	1.83	1.78	12.5	11.4	11.1	0.899	0.917	0.921	0.961	0.959	0.958
Castello d'Agogna 1995	0.78	0.72	0.71	5.7	5.3	5.2	0.971	0.975	0.976	0.976	0.977	0.978
Castello d'Agogna 1996	1.47	1.83	1.89	8.3	10.3	10.7	0.956	0.932	0.927	0.986	0.989	0.989
Vignate 2002	2.38	2.16	2.13	14.3	13.0	12.8	0.858	0.883	0.886	0.934	0.926	0.927
Opera 2004	1.43	1.24	1.24	10.7	9.3	9.2	0.881	0.910	0.911	0.951	0.952	0.951
Mean	*1.61*	*1.55*	*1.55*	*10.3*	*9.8*	*9.8*	*0.913*	*0.923*	*0.924*	*0.962*	*0.961*	*0.961*
Rice – validation												
Mortara 1996	1.94	2.42	2.50	12.3	15.3	15.8	0.907	0.856	0.846	0.989	0.990	0.990
Gudo Visconti 1990	1.49	1.71	1.75	14.6	16.7	17.1	0.827	0.772	0.762	0.978	0.979	0.979
Vercelli 1990	0.90	0.86	0.88	5.7	5.4	5.6	0.978	0.980	0.979	0.979	0.984	0.984
Velezzo Lomellina 1999	1.63	1.45	1.43	10.7	9.5	9.4	0.925	0.942	0.943	0.956	0.963	0.964
Opera 2002	1.87	1.73	1.71	12.7	11.7	11.6	0.893	0.908	0.910	0.947	0.941	0.942
Mean	*1.57*	*1.63*	*1.66*	*11.2*	*11.7*	*11.9*	*0.906*	*0.892*	*0.888*	*0.970*	*0.971*	*0.972*

Table 5
Robustness indicator (Confalonieri et al., 2010) and Akaike Information Criterion (Akaike, 1974) calculated for WOFOST, WOFOST-GT and WOFOST-GT2.

Crop	WOFOST	WOFOST-GT	WOFOST-GT2
Robustness indicator			
Winter wheat	1.16	1.03	1.00
Rice	0.30	0.30	0.33
Akaike information criterion			
Winter wheat	330.9	211.3	213.3
Rice	281.2	144.8	150.1
Number of parameters for crop growth and development under potential conditions			
Winter wheat	104	40	41
Rice	104	38	39

it is very difficult – in this case – to define bounds to check user-specified values. In the new versions of the model, partitioning to leaves is driven by a single parameter, corresponding to the values at emergence. In this case, bounds can be restricted to 0.40 and 0.90, increasing possibility of performing pre-simulation quality checks of the information provided. All these features increase the model usability even for scientists and technicians not necessarily specialized in crop physiology but interested in analysing agroecosystems (e.g., hydrologists, soil scientists), because the lower the degree of freedom during calibration, the lower the risk of inconsistencies in the parameter sets. Of course, the drawback for crop physiologists or experienced crop modellers is a certain decrease in model flexibility.

Compared to what achieved for WOFOST, the robustness of the new versions of the model decreased for winter wheat, whereas it remained practically unchanged for rice (Table 5). This was partly unexpected, since decreasing the number of parameters should reduce the risk of including season- or site-specific factors in model parameters values. In general, the values calculated for the robustness indicator (Confalonieri et al., 2010, optimum and minimum = 0, maximum = $+\infty$) are more satisfactory for rice (Robustness Indicator = 0.31) than for winter wheat (Robustness Indicator = 1.06). However, a general worsening of the performances of the three WOFOST versions for wheat was, to a certain extent, expected. The reason is that a single parameter set was calibrated here for wheat, despite the large number (nine) of varieties and thus potential differences in the plant traits to be codified in parameter values. This was done because of the absence of objective criteria to cluster the available varieties in groups with similar morphological and physiological features. For rice, the six varieties available were instead equally split into japonica- and indica-type, and two parameter sets were developed for each model. In practice, the impact of simulating different genotypes with the same parameter set was larger for wheat than for rice.

Even if the performances of the three versions of WOFOST were comparable in terms of agreement between measured and simulated AGB values, this study suggests the adoption of the new versions for both wheat and rice because of the substantial reduction of complexity which – however – does not undermine neither model accuracy nor its adherence to plant processes. Concerning WOFOST-GT and WOFOST-GT2, the choice between the two versions should be instead driven by the specific objectives of the modelling study, given that the -GT2 version is more suitable for being coupled with models for processes requiring a fine representation of micrometeorological aspects within the canopy.

4. Conclusions

Although the approaches implemented in the SUCROS family of models are recognized worldwide as conceptually sound and effective in reproducing dynamics related with crop growth, a main constraint to their operational use is represented by the huge effort needed for their parameterization. This is mainly due to the large number of parameters used to reproduce the effect of crop development or air temperature in modulating morphological and physiological plant features (AFGEN tables). Apart from the parameterization effort, this strongly limits the compatibility of SUCROS-type models with advanced tools for sensitivity analysis or automatic calibration. Moreover, the theoretical formalization behind the models belonging to this family remained – to a large extent – identical to what it was in the 80s, and reveals some inconsistencies with the underlying system, e.g., for the representation of canopy structure and senescence dynamics.

We propose here two new formalizations of WOFOST, which is one of the most widespread model from this family. The first (WOFOST-GT) enhances the usability of the model by markedly reducing the number of parameters of the model, via the substitution of AFGEN tables with functions driven by few parameters with a clear biological meaning. These changes increased the usability of the original version of the model, without compromising the high level of detail in the way biophysical processes are reproduced and without lowering its performances in terms of accuracy. The second version we propose (WOFOST-GT2; extending -GT) is based on an improved representation of the canopy structure, with an explicit consideration of the vertical dimension of the canopy and of the bottom-up dynamic of leaves senescence. This improvement would likely increase the capability of the model to interact with models for the simulation of micrometeorological aspects within the canopy, and with models for the simulation of biotic (e.g., diseases) and abiotic (e.g., frost, pre-flowering thermal shocks) factors affecting crop productions.

The development of the new versions of the model was greatly supported by the software architecture followed to implement the original version of the model in the software component CropML (Crop Models Library; http://agsys.cra-cin.it/tools/cropml/help/). This architecture enhances the extensibility of modelling approaches via the high level of granularity in the way sub-processes are isolated and composed. The redesign of the model also benefited from the use of advanced sensitivity analysis technique, that – despite their pervasive use for understanding model limitations (e.g., Petropoulos et al., 2013; Moreau et al., 2013) – are still rarely used for model redesign. Further developments include the definition of other functions to replace AFGEN tables for other types of crops. This because the functions presented in this study, e.g., assimilates partitioning, are specific for rice and winter cereals, and cannot be considered suitable for other crops. The need for developing specific functions for groups of crops with similar behaviour can be considered as a drawback of the elimination of AFGEN tables. Indeed, the AFGEN solution obviously guarantees the highest flexibility during parameterization, since such tables can be customized to draw whatever trend. However, we consider that the benefits deriving from the reduction of model complexity represent an advantage for model users that decidedly overcomes this drawback.

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Appendices

Appendix A

WOFOST parameters involved with development and growth of winter wheat and rice (Indica and Japonica type). *: calibrated values; parameters excluded from calibration come from Spitters et al. (1989).

Parameter	Units	Value			Description
		Rice Japonica	Rice Indica	Wheat	
Development					
TBASEM	°C	11*	11*	0*	Lower threshold of temperature for emergence
TEFFMX	°C	35*	35*	30*	Maximum effective T for emergence
TSUMEM	°C-days	80*	90*	60*	Temperature sum from sowing to emergence
IDSL	–	–	–	2	Pre-anthesis development based on temperature (=0), daylength (=1), both (=2)
DLO	h	–	–	14*	Optimum daylength for development
DLC	h	–	–	10*	Minimum daylength for development
TSUM1	°C-days	1050*	1055*	800*	Temperature sum from emergence to anthesis
TSUM2	°C-days	520*	595*	750*	Temperature sum from anthesis to maturity
DTSMTB	°C; °C-days	0.0; 0.0 9.0; 0.0* 15; 8.0* 20; 13 24; 15 29; 12 38; 0.0 40; 0.0	0.0; 0.0 9.0; 0.0* 15; 5.0* 22; 14* 26; 17* 29; 14* 31; 0.0* 40; 0.0*	0.0; 0.0 10.0; 10.0* 18.0; 20.0* 24.0; 24.0* 28.0; 21.0* 30.0; 13.0* 31.0; 0.0* 40.0; 0.0*	Daily increase in temperature sum as a function of average temperature
DVSI	–	0	0	0	Development stage start simulation
DVSEND	–	2	2	2	Development stage at harvest
Growth					
TDWI	kg ha^{-1}	100	100	210	Initial total crop dry weight
LAIEM	ha ha^{-1}	0.15	0.15	0.1365	Leaf area index at emergence
RGRLAI	ha ha^{-1}	0.009	0.009	0.00817	Maximum relative increase in LAI
SLATB	–; ha kg^{-1}	0.0; 0.0023* 0.18; 0.0023* 0.42; 0.0018* 0.7; 0.00175* 2.0; 0.0017*	0.0; 0.0021* 0.18; 0.0021* 0.37; 0.0018* 0.7; 0.00178 2.0; 0.00175*	0.0; 0.00231* 0.18; 0.00231* 0.42; 0.00215* 0.70; 0.00208* 2.0; 0.00206*	Specific leaf area as a function of development stage
SPA	ha kg^{-1}	0	0	0.0	Specific pod area
SSATB	ha kg^{-1}	0.0; 0.0 2.0; 0.0	0.0; 0.0 2.0; 0.0	0.0; 0.0 2.0; 0.0	Specific stem area as a function of development stage
SPAN	days	35*	35*	29.5*	Life span of leaves growing at 35 °C
TBASE	°C	8	8	0.0	Lower threshold temperature for ageing of leaves
KDIFTB	–	0.0; 0.4* 0.65; 0.4* 1.0; 0.6* 2.0; 0.6*	0.0; 0.4* 0.65; 0.4* 1.0; 0.6* 2.0; 0.6*	0.0; 0.4* 0.65; 0.4* 1.0; 0.65* 2.0; 0.65*	Extinction coefficient for diffuse visible light as a function of development stage
EFFTB	kg ha^{-1} h^{-1} J^{-1} m^2 s	0.0; 0.6* 40; 0.36	0.0; 0.6* 40; 0.36	0.0; 0.6* 40.0; 0.36	Light-use efficiency single leaf as function of daily mean temperature
AMAXTB	–; kg ha^{-1} h^{-1}	0.0; 26* 2.0; 26*	0.0; 24* 2.0; 24*	0.0; 20* 2.00; 20*	Maximum leaf CO_2 assimilation rate as function of development stage
TMPFTB	°C; –	0.0; 0.0* 12; 0.0* 14; 0.4* 17; 0.8* 22; 1.0* 26; 0.9* 28; 0.0*	0.0; 0.0* 12; 0.0* 14; 0.4* 18; 0.8* 23; 1.0* 27; 0.9* 38; 0.0*	0.0; 0.0* 12.0; 0.7* 17.0; 0.9* 23.0; 1.0* 28.0; 0.9* 31.5; 0.6* 33.0; 0.0*	Reduction factor of AMAX as function of average temperature
TMNFTB	°C; –	0.0; 0.0 3.0; 1.0*	0.0; 0.0 3.0; 1.0*	0.0; 0.0 3.0; 1.0*	Reduction factor of gross assimilation rate as function of low minimum temperature

Appendix B

WOFOST parameters involved with respiration, partitioning, organs death and rooting of winter wheat and rice (Indica and Japonica type). *: calibrated values; parameters excluded from calibration come from Spitters et al. (1989).

Parameter	Units	Value			Description
		Rice Japonica	Rice Indica	Wheat	
Respiration					
CVL	kg kg^{-1}	0.754	0.754	0.685	Efficiency of conversion into leaves
CVO	kg kg^{-1}	0.684	0.684	0.709	Efficiency of conversion into storage organs
CVR	kg kg^{-1}	0.754	0.754	0.694	Efficiency of conversion into roots
CVS	kg kg^{-1}	0.754	0.754	0.662	Efficiency of conversion into stems
Q10	–	2	2	1.5*	Relative increase in respiration rate per 10 °C
RML	kg CH_2O kg^{-1} day^{-1}	0.02	0.02	0.03	Relative maintenance respiration rate for leaves
RMO	kg CH_2O kg^{-1} day^{-1}	0.003	0.003	0.01	Relative maintenance respiration rate for storage organs
RMR	kg CH_2O kg^{-1} day^{-1}	0.01	0.01	0.015	Relative maintenance respiration rate for roots
RMS	kg CH_2O kg^{-1} day^{-1}	0.015	0.015	0.015	Relative maintenance respiration rate for stems
RFSETB	–; –	0.0; 1 2.0; 1.0	0.0; 1 2.0; 1.0	0.0; 1.0 2.0; 1.0	Reduction factor for senescence as function of development stage
Partitioning					
FRTB	–; kg kg^{-1}	0.0; 0.5 0.1; 0.5 0.2; 0.4 0.35; 0.22 0.4; 0.17 0.5; 0.13 0.7; 0.07 0.9; 0.03 1.2; 0.0 2.0; 0.0	0.0; 0.5 0.1; 0.5 0.2; 0.4 0.35; 0.22 0.4; 0.17 0.5; 0.13 0.7; 0.07 0.9; 0.03 1.2; 0.0 2.0; 0.0	0.0; 0.5 0.1; 0.5 0.2; 0.4 0.35; 0.22 0.4; 0.17 0.5; 0.13 0.7; 0.07 0.9; 0.03 1.2; 0.0 2.0; 0.0	Fraction of total dry matter to roots as a function of development stage
FLTB	–; kg kg^{-1}	0.0; 0.6* 0.5; 0.6* 0.65; 0.54* 0.85; 0.1* 1.0; 0.01* 2.0; 0.0*	0.0; 0.65* 0.5; 0.65* 0.65; 0.58* 0.85; 0.1* 1.0; 0.01* 2.0; 0.0*	0.0; 0.9* 0.5; 0.86* 0.65; 0.73* 0.85; 0.1* 1.0; 0.01* 2.0; 0.0*	Fraction of aboveground biomass to leaves as a function of development stage
FSTB	–; kg kg^{-1}	0.0; 0.4* 0.0; 0.4* 0.65; 0.46* 0.75; 0.65* 0.85; 0.78* 0.9; 0.68* 1.0; 0.25* 1.1; 0.08* 1.22; 0.02* 2.0; 1.0*	0.0; 0.35* 0.5; 0.42* 0.65; 0.42* 0.75; 0.65* 0.85; 0.78* 0.9; 0.68* 1.0; 0.25* 1.1; 0.08* 1.22; 0.02* 2.0; 1.0*	0.0; 0.1* 0.5; 0.14* 0.65; 0.3* 0.75; 0.65* 0.85; 0.78* 0.9; 0.68* 1.0; 0.25* 1.1; 0.08* 1.22; 0.02* 2.0; 0.0*	Fraction of aboveground biomass to stems as a function of development stage
FOTB	–; kg kg^{-1}	0.0; 0.0* 0.75; 0.0* 0.9; 0.2* 1.0; 0.67* 1.1; 0.9* 1.22; 1.0* 2.0; 1.0*	0.0; 0.0* 0.75; 0.0* 0.9; 0.2* 1.0; 0.67* 1.1; 0.9* 1.22; 1.0* 2.0; 1.0*	0.0; 0.0* 0.75; 0.0* 0.9; 0.2* 1.0; 0.67* 1.1; 0.9* 1.22; 1.0* 2.0; 1.0*	Fraction of aboveground biomass to storage organs as a function of development stage
Death rates					
PERDL	–	0.01	0.01	0.01	Maximum relative death rate of leaves due to water stress
RDRRTB	–; kg kg^{-1} day^{-1}	0.0; 0.0 1.5; 0.0 1.5001; 0.02 2.0; 0.2	0.0; 0.0 1.5; 0.0 1.5001; 0.02 2.0; 0.2	0.0; 0.0 1.5; 0.0 1.5001; 0.02 2.0; 0.2	Relative death rate of roots as a function of development stage
RDRSTB	–; kg kg^{-1} day^{-1}	0.0; 0.0 1.5; 0.0 1.5001; 0.02 2.0; 0.2	0.0; 0.0 1.5; 0.0 1.5001; 0.02 2.0; 0.2	0.0; 0.0 1.5; 0.0 1.5001; 0.02 2.0; 0.2	Relative death rate of stems as a function of development stage
Rooting					
RDI	cm	10	10	10	Initial rooting depth
RRI	cm day^{-1}	1.2	1.2	1.2	Maximum daily increase in rooting depth
RDMCR	cm	80	80	125	Maximum rooting depth

Appendix C

WOFOST-GT and WOFOST-GT2 parameters. *calibrated values; [a]parameter only for WOFOST-GT. Parameters excluded from calibration come from Confalonieri et al. (2009a) and from Spitters et al. (1989) for rice and winter wheat, respectively.

Parameter	Units	Value			Description
		Rice Japonica	Rice Indica	Wheat	
Development					
$T_{base,em}$	°C	11*	11*	0	Lower threshold of temperature for emergence
$TEFF_{max}$	°C	35	35*	30	Maximum effective temperature for emergence
$T_{sum,em}$	°C-days	80*	90*	60	Temperature sum from sowing to emergence
IDSL	–	0	0	2	Pre-anthesis development based on temperature (=0), daylength (=1), both (=2)
DLO	h	–	–	14	Optimum daylength for development
DLC	h	–	–	10	Minimum daylength for development
T_{sum1}	°C-days	1050*	1055*	800	Temperature sum from emergence to anthesis
T_{sum2}	°C-days	520*	595*	750	Temperature sum from anthesis to maturity
$T_{base,dev}$	°C	9*	9*	0	Lower threshold of temperature for development
$T_{opt,dev}$	°C	24*	26*	24	Optimum temperature for development
$T_{max,dev}$	°C	38*	31*	33	Maximum threshold of temperature for development
DVS_{end}	–	2	2	2	Development stage at harvest
Growth					
TDWI	kg ha^{-1}	100	100	210	Initial total crop dry weight
LAIEM	ha ha^{-1}	0.15	0.15	0.1365	Leaf area index at emergence
RGRLAI	ha ha^{-1}	0.009	0.009	0.00817	Maximum relative increase in LAI
SLA_{em}	m^2 kg^{-1}	23*	21*	23.1*	Specific leaf area at emergence
SLA_{035}	m^2 kg^{-1}	17*	18*	22*	Specific leaf area at tillering
SPA	ha kg^{-1}	0.0	0.0	0.0	Specific pod area
SPAN	days	35	35	29.5	Life span of leaves growing at 35 °C
TBASE	°C	8	8	0	Lower threshold temperature for ageing of leaves
$KDIF_{max}$	–	0.6*	0.6*	0.65*	Maximum extinction coefficient for diffuse visible light
EFF_{10}	kg ha^{-1} h^{-1} J^{-1} m^2 s	0.54	0.54	0.54	Light-use efficiency single leaf as function of daily mean temperature
EFF_{40}	kg ha^{-1} h^{-1} J^{-1} m^2 s	0.36	0.36	0.36	Light-use efficiency single leaf as function of daily mean temperature
A_{max}	kg ha^{-1} h^{-1}	26*	24*	20*	Maximum leaf CO_2 assimilation rate
NDGP	–	3	3	3	Number of instants in a day for which gross photosynthesis is estimated
$T_{base,gro}$	°C	12	12	0	Lower threshold of temperature effects on CO_2 assimilation
$T_{opt,gro}$	°C	22*	23*	23*	Optimum temperature effects on CO_2 assimilation
$T_{max,gro}$	°C	38	38	33	Maximum threshold of temperature effects on CO_2 assimilation
H^{a}_{max}	M	100	100	100	Maximum plant height
Respiration					
CVL	kg kg^{-1}	0.754	0.754	0.685	Efficiency of conversion into leaves
CVO	kg kg^{-1}	0.684	0.684	0.709	Efficiency of conversion into storage organs
CVR	kg kg^{-1}	0.754	0.754	0.694	Efficiency of conversion into roots
CVS	kg kg^{-1}	0.754	0.754	0.662	Efficiency of conversion into stems
Q10	–	2	2	1.5*	Relative increase in respiration rate per 10 °C
RML	kg CH_2O kg^{-1} day^{-1}	0.02	0.02	0.03	Relative maintenance respiration rate for leaves
RMO	kg CH_2O kg^{-1} day^{-1}	0.003	0.003	0.01	Relative maintenance respiration rate for storage organs
RMR	kg CH_2O kg^{-1} day^{-1}	0.01	0.01	0.015	Relative maintenance respiration rate for roots
RMS	kg CH_2O kg^{-1} day^{-1}	0.015	0.015	0.015	Relative maintenance respiration rate for stems
Partitioning					
RIP_{L0}	–	0.6*	0.65*	0.9*	Partitioning of assimilates to leaves at emergence
Rooting					
RDI	Cm	0	0	10	Initial rooting depth
RRI	cm day^{-1}	1.2	1.2	1.2	Maximum daily increase in rooting depth
RDM	Cm	80	80	125	Maximum rooting depth

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