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TECHNICAL ADVANCE

ORCHIDEE-STICS, a process-based model of sugarcane biomass production: calibration of model parameters governing phenology

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Abstract

Agro-Land Surface Models (agro-LSM) combine detailed crop models and large-scale vegetation models (DGVMs) to model the spatial and temporal distribution of energy, water, and carbon fluxes within the soil–vegetation–atmosphere continuum worldwide. In this study, we identify and optimize parameters controlling leaf area index (LAI) in the agro-LSM ORCHIDEE-STICS developed for sugarcane. Using the Morris method to identify the key parameters impacting LAI, at eight different sugarcane field trial sites, in Australia and La Reunion island, we determined that the three most important parameters for simulating LAI are (i) the maximum predefined rate of LAI increase during the early crop development phase, a parameter that defines a plant density threshold below which individual plants do not compete for growing their LAI, and a parameter defining a threshold for nitrogen stress on LAI. A multisite calibration of these three parameters is performed using three different scoring functions. The impact of the choice of a particular scoring function on the optimized parameter values is investigated by testing scoring functions defined from the model-data RMSE, the figure of merit and a Bayesian quadratic model-data misfit function. The robustness of the calibration is evaluated for each of the three scoring functions with a systematic cross-validation method to find the most satisfactory one. Our results show that the figure of merit scoring function is the most robust metric for establishing the best parameter values controlling the LAI. The multisite average figure of merit scoring function is improved from 67% of agreement to 79%. The residual error in LAI simulation after the calibration is discussed.

Keywords: agro-LSM, calibration, cross-validation, LAI, multisite, scoring functions, sensitivity analysis, sugarcane

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Introduction

Ethanol produced from crop biomass has emerged as a potential contributor to a more renewable transportation energy mix. Driven by policy mandates and global markets, the global production of ethanol has increased more than fourfold between 2000 and 2009 (Licht, 2007). Sugarcane has the highest energy ratio (energy delivered per energy spent) of the most commonly used biofuels and therefore has the best potential to date to produce ethanol for fossil fuel substitution (de Vries *et al.*, 2010). Of the 75 million liters of ethanol produced globally in 2009, 45–50% came from sugarcane while another 45% was produced from corn (Fischer *et al.*, 2008). The recent rise in sugarcane demand, as driven by biofuel production, resulted in an increase in sugarcane area from 19.4 million ha in 2000 to 23.9 million ha in 2010 (FAO, n.d.). This trend impacts the biosphere–atmosphere exchanges of water, carbon, and energy, and ultimately climate at local to continental scales. Fully grasping the consequences of the conversion of land to bioenergy crops therefore warrants a better knowledge and simulation of the interactions between sugarcane and its environment, and in particular the processes of crop growth and development which drive the biosphere-atmosphere fluxes (Smith *et al.*, 2010).

Agronomical plot-scale models generally simulate the growth and biomass yield of sugarcane (both from a quantitative and qualitative standpoint) with good accuracy under different types of conditions (Keating *et al.*, 1999; Singels & Bezuidenhout, 2002). They may also be used to study the interactions between crops and their environment, for instance soil carbon dynamics (Galdos

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et al., 2009) and water use (Inman-Bamber *et al.*, 1993). However, they require a high number of input parameters (soil texture, management practices, genotype-specific parameters) and their application is therefore restricted to small scales. On the other hand, the land surface modules of Earth System Models (ESM), which operate at larger scales, are based on a restricted set of generic vegetation types and are thus unable to take into account the specificities of any given crop. Efforts were made recently to alleviate this limitation and lead to the development of so-called agro-Land Surface Models (Agro-LSMs; Table 1). Wheat, maize, and soybean are the crops most often parameterized in agro-LSMs (Kucharik, 2003; Gervois *et al.*, 2004; Bondeau *et al.*, 2007; Lokupitiya *et al.*, 2009; Van den Hoof *et al.*, 2011), but sugarcane has recently gained interest in the modeling community as well. To our knowledge, three agro-LSMs include sugarcane (Table 1): Agro-IBIS, LPJml, JULES (Black *et al.*, 2012; Surendran Nair *et al.*, 2012). A highly simplified sugarcane new crop functional type was added in LPJml (Lapola *et al.*, 2009) and sugarcane has also been included to the Agro-IBIS and JULES models with a different approach, by adding a new module with specific parameters and allocation rules (Black *et al.*, 2012; Cuadra *et al.*, 2012). However, none of these studies included a thorough evaluation of the sensitivity of the models to the many parameters, or their calibration. Previous validations of sugarcane agro-LSMs were obtained with either country or state level yield data (Lapola *et al.*, 2009; Cuadra *et al.*, 2012), or site-level micrometeorological and yield measurements (Cuadra *et al.*, 2012). Here, we used the ORCHIDEE-STICS agro-LSM, which results from a coupling between the process-based LSM ORCHIDEE (Krinner *et al.*, 2005), and the generic crop model STICS (Brisson *et al.*, 1998). STICS drives ORCHIDEE mainly through its crop-specific phenology component (Gervois *et al.*, 2004), while other ecosystem state variables (biomass, fluxes) are produced by ORCHIDEE (Fig. 1).

Since agro-LSM models generally involve many more parameters than standard land-surface models, some calibration is required prior to running them on a large scale. This step raises two issues regarding computing time and application scale. Regarding the first point, the high number of parameters involved (several dozen) precludes the use of factorial runs (whereby each parameter is varied one at a time), which would be too computer intensive. Calibration may be facilitated by carrying out a preliminary sensitivity analysis (SA) with the aim of identifying the most important parameters of the model and restricting optimization to this limited subset of parameters. Several families of SA techniques have been developed, which may be categorized based on several features such as global or local, quantitative or qualitative, dependent on the model's structure. Here, we used the method of Morris (Morris, 1991) described in the next section which is common in crop model calibration (Monod *et al.*, 2006). It is simple and easy to implement and interpret. It is also computationally efficient and requires few constraints from the model. Depending on the number of key parameters identified, a method can be chosen for calibration, such as simulated annealing algorithms, genetic algorithms, or simple factorial minimization of an objective function, which will be used here.

The second problem faced when calibrating parameters of an agro-LSM has to do with the different scales of application. Site-level parameterization is a way of evaluating LSM models, which allows quantifying model uncertainties and prioritizing possible improvements (Calvet *et al.*, 1998; Harris *et al.*, 2004). However, calibrations done on a single site have the weakness of representing a unique situation, which hampers a generalization to larger areas (Xiong *et al.*, 2008). Multi-site studies involving both parameterization and independent 'cross-validation' sites provide more robust evidence that the model may be extrapolated from plot to regional scales. Here, we developed a

Table 1 Selected characteristics of current Agro-LSMs

Initial model	Agro-LSM	Reference	Crops included
IBIS	Agro-IBIS	Kucharik & Brye 2003	Corn, soybean, winter wheat, spring wheat, sugarcane (Cuadra *et al.*, 2012)
ORCHIDEE	ORCHIDEE-STICS	Gervois *et al.*, 2004;	Wheat, corn, soybean, sugarcane
LPJ	LPJml	Bondeau *et al.*, 2007;	Managed grass (grazing or harvested grass, C3), managed grass (grazing or harvested grass, C4), temperate cereals (wheat, barley, rye, oat), rice, maize, tropical cereals (millet, sorghum), pulses (lentils), temperate roots & tubers (sugarbeet), tropical roots & tubers (cassava), sunflower, groundnuts, soybean, rapeseed sugarcane (Lapola *et al.*, 2009)
SiB	SiBcrop	Lokupitiya *et al.*, 2009	Wheat, corn, soybean
JULES	JULES-SUCROS JULES-SC	Van den Hoof *et al.*, 2011; Black *et al.*, 2012	Winter wheat, sugarcane (Black *et al.*, 2012)

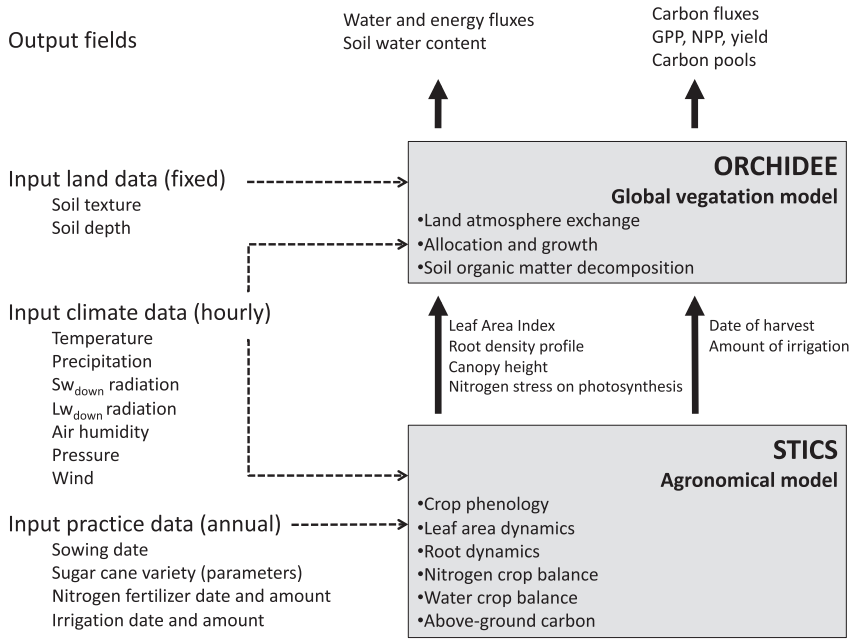

Fig. 1 Description of the ORCHIDEE-STICS coupling showing the input data, variables exchanged between the model's components and output variables. The two components of the model (shaded) are fed input data (dashed arrows) and communicate between each other through a few variables (solid arrows). Both models require meteorological forcing data at hourly time step (interpolated from 6-hourly forcing data files). STICS also requires data describing the crop management (sugarcane variety, sowing date, irrigation, and fertilization), and ORCHIDEE requires basic soil data (soil texture and depth).

multisite calibration procedure for sugarcane field trial sites across a range of contrasted climate conditions in Australia and La Reunion Island (southern Indian ocean), to ensure that the parameterization of the ORCHIDEE-STICS model remains valid over a range of climatic conditions.

The goal of this study is to calibrate and evaluate the capacity of ORCHIDEE-STICS to predict the dynamics of leaf area index (LAI) of sugarcane prior to regional simulations. We also investigated methodological issues such as the configuration of the sensitivity analysis and the scoring function used to define the best parameters values.

In the next section, we describe ORCHIDEE-STICS and the sugarcane field trial sites calibration and validation data as well as the sensitivity analysis and the calibration method (adjustment of the parameters). Then, we describe the results of the sensitivity analysis and calibration. Finally, the last section discusses the residual bias in the simulations after calibration.

Material and methods

ORCHIDEE-STICS Agro-LSM

ORCHIDEE-STICS simulates crop growth in a mechanistic and dynamic framework at regional to global scales (Gervois *et al.*, 2004). The approach is a partial coupling of the agronomical model STICS (Brisson *et al.*, 1998) with the generic model ORCHIDEE (Krinner *et al.*, 2005), where some variables are exchanged between the two models as illustrated in Fig. 1. ORCHIDEE is used for carbon fluxes and pools, as well as water and energy balance and STICS for phenology and LAI, the main focus of this study. Thus, STICS calculates the growth of sugarcane on a daily time step (phenology, leaf area dynamics, root dynamics, nitrogen status, water balance, biomass) based on meteorological data, crop management and soil parameters, and given generic and crop-specific parameters. As a generic model, the strength of STICS is its ability to simulate different crops with the same set of formalisms through the establishment of analogies. The concepts are therefore adjusted to some extent from one crop to another. Thus, for sugarcane, the filling of elements to be harvested refers to the accumulation of sucrose in the internodes of the cane but for another crop it could refer to the growth of the grains or the fruits. Another example, a specificity of sugarcane is that it is an indeterminate crop (Fauconnier & Bassereau, 1970), meaning that the leaves keep growing as the cane internodes start filling. In STICS, the 'indeterminate' feature of a crop is represented by a significant trophic stress to imitate the competition between cane internodes and leaves for assimilates (Brisson *et al.*, 2003). ORCHIDEE uses the LAI, nitrogen and irrigation requirements calculated by STICS on a daily basis to calculate photosynthesis, water and energy balances (with a hourly time step), and carbon dynamics (biomass, mortality, and soil organic matter decomposition). In this article, the focus is on the improvement of the parameterization of LAI simulated by STICS for minimizing the error transmitted to ORCHIDEE. Another study (A.

Valade, N. Vuichard, P. Ciais, N. Viovy, F. Marin, N. Huth, J-F. Martiné, in preparation) addresses the full uncertainty budget of the coupled ORCHIDEE-STICS model with crop biomass as a target variable.

Experimental sites

Eight data sets were collated from five field trial sites in Australia (Ayr, 3 years; Ingham, 2 years; Grafton, 1 year) and two sites on the island of La Réunion (Colimaçons, 1 year; Tirano, 1 year), providing a gradient of climatic conditions (Fig. 2). The Australian sites are located in the sugarcane cultivation belt on the East coast of the continent. The Grafton site has a temperate climate (Keating *et al.*, 1999) and the Ayr and Ingham sites have a tropical climate but with very different precipitation seasonality (Muchow *et al.*, 1994; Robertson *et al.*, 1996). The sites in La Reunion are located on the western coast, the driest part of the island, in mountainous areas where the weather is strongly influenced by topography. The Colimaçons site is located at an altitude of 800 m a.s.l., and the Tirano site is located south of the western coast at an altitude of 150 m.

The locations and management characteristics of the experimental sites are given in Table 2. All the sites received irrigation and fertilization inputs, so that the model could be parameterized under optimal growing conditions. For the rest of the study, each combination of site, year and treatment is called 'site' and named with a convention of 'site-year', for example, 'Ayr 92–93' for the Ayr field trial data during the 1992–1993 growing season. At each site, crop biomass and LAI were measured six to eleven times during the growing season. When replicate plots were available, we pooled the corresponding observations.

Soil characteristics

At regional scales, it is difficult to know and prescribe with accuracy the spatial distribution of soil properties with the level of detail required by the STICS crop model (water holding capacity, drainage class, rooting depth). We thus performed several test runs of STICS with different soil configurations and found that the model's predictions of LAI was only weakly impacted by the soil characteristics – in particular because the crops were irrigated and fertilized. We therefore used the same soil configuration for all sites (see Table 3 for soil characteristics).

Meteorological forcing data

ORCHIDEE-STICS requires hourly meteorological data that are usually interpolated from 6-hourly forcing files. We need to use the best possible meteorological forcing for the model at each site, to prevent the aliasing of climate forcing bias to parameter estimation bias. We thus gathered weather station measurements of precipitation, air temperature, and solar radiation (arguably, the best possible forcing) close to each site. For Australia, the data were downloaded from the website of the Australian Bureau of Meteorology (BOM), and for La Reunion, they were obtained from stations close to the field sites. However, these weather station data cannot be directly used to force ORCHIDEE-STICS, because (i) additional variables are required by the model (specific humidity, wind speed, pressure, and long wave downward radiation), and (ii) the station data were only available at a daily time step. We combined the local station measurements with numerical weather prediction globally gridded data from the ECMWF ERA-Interim

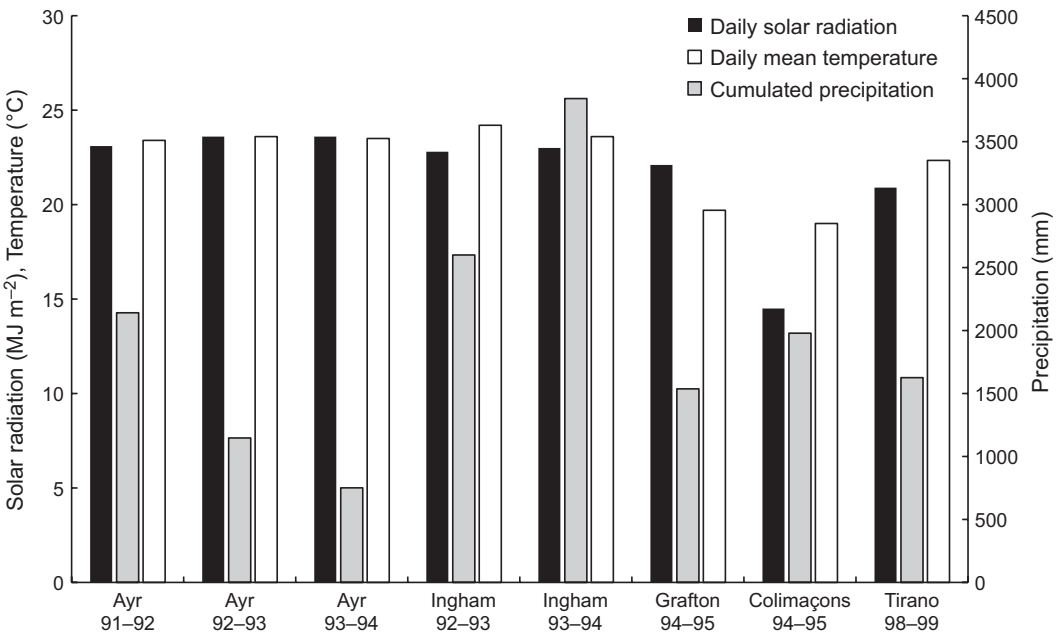

Fig. 2 Climate characteristics of the sites. Each group of columns refers to one site and each color to one variable: 2-years averaged daily solar radiation (MJ m^{-2}) in black, 2-years averaged daily mean temperature (°C) in gray, 2-years cumulated precipitation (mm) in white.

Table 2 Description of the experimental sites in Australia and La Reunion used for the sensitivity analysis and calibration

Site name	Year	Latitude/ Longitude	Altitude (m)	Crop class, variety	Start day (julian)	Irrigation	Fertilization (kg N ha^{-1})	Reference
Ingham, Qld, Australia	1992–1993	18.7S/146.2E	10	Plant, Q117	239	Irrigated	257	Robertson *et al.*, 1996;
	1993–1994			Plant, Q117	230	Irrigated	774	Muchow *et al.* 1996
Ayr, Qld, Australia	1991–1992	19.5S/147.3E	15	Plant, Q96	109	Irrigated	250	Muchow *et al.*, 1994;
	1992–1993			Plant, Q117	112	Irrigated	257	Keating *et al.*, 1999;
	1993–1994			Ratoon, Q117	254	Irrigated	350	Keating *et al.*, 1999;
Grafton, NSW, Australia	1994–1995	29.5S/152.9E	9	Plant, Q117	271	Irrigated	590	Keating *et al.*, 1999
Colimaçons, La Réunion	1994–1995	21.1S/55.3E	786	Ratoon, R570	215	Irrigated	210	JF Martiné (unpublished)
Tirano, La Réunion	1997–1998	21.3S/55.5E	150	Ratoon, R570	330	Irrigated	242	JF Martiné (unpublished)

Table 3 Selected properties of the soil used in all field sites

	Layer depth (cm)	Field capacity water content (g g^{-1})	Permanent wilting point (mass %)	Bulk density (g cm^{-3})
Layer 1	30	41	30	1.2
Layer 2	40	42	35	1.14
Layer 3	90	42	35	1.14

reanalysis product (Dee *et al.*, 2011). For the missing weather variables, we used directly the ERA-Interim fields sample at the grid point containing each site, and when weather station measurements were available, we corrected the 6-hourly ERA-Interim data to match the observed daily data with the method of (Berg *et al.*, 2003) (section S1 of Supplementary Material). The correction of the bias between the ERA-Interim and station data was based on a ratio-based algorithm for precipitation and solar radiation fields, and upon a difference-based algorithm for temperature, to conserve the diurnal amplitude cycle. The bias correction led to an important reduction in the root mean squared error (RMSE), of 1.8 °C for daily air temperature, 422.6 mm for cumulative precipitation, 17.4 MJ m^{-2} for daily solar radiation (Table S1).

The Morris method to identify sensitive parameters

The Morris method (Morris, 1991) is a one-at-a-time approach. First, each parameter is assigned a range of variation divided regularly to provide p levels, or possible values, for each parameter. Then, from a random starting point in the parameters space, each of the k parameters of the model is varied one after the other to the previous or next level, generating as many new points in the parameters space as there are parameters and thus building a 'trajectory'. Once one trajectory has been built by varying all parameters once, the sampling procedure is repeated r times by selecting different starting points in the parameters space, resulting in $r^*(k + 1)$ different samples of the parameter space. For each of the r trajectories, the elementary effect $ee_i(Y)$ for the output variable Y associated with each input factor i (parameter P_i) is calculated by Eqn (1) (Saltelli *et al.*, 2004) that gives the elementary effect, *ee*, based on the gradient of the output variable Y generated by a normalized change Δ in the ith input parameter P_i

$$ee_i(Y) = \frac{Y(\ldots, P_i + \Delta, \ldots) - Y(\ldots, P_i, \ldots)}{\Delta} \quad (1)$$

The Morris method defines two sensitivity indices: μ^*, the average of elementary effects' absolute values, and σ, their standard deviation. The value of μ^* provides information about the importance of each parameter (the larger the value of μ^*, the more important the parameter) which defines a ranking for multiple parameters. The larger the value of σ, the more non-linearities are involved.

To calculate the Morris indices, all the elementary effects are calculated at different points in the space of the parameters. The settings of the parameter screening (the number of levels, p, and the number of trajectories, r) are left to the user's choice. A requirement is that r must be large enough compared to p, so that all levels are sufficiently explored. According to (Saltelli *et al.*, 2004), values of $p = 4$ and $r = 10$ give good results in the Morris method, and this combination has been used by (Cariboni *et al.*, 2007) for 103 parameters in a best practice study for sensitivity analyses for ecological models. Previous studies (Francos *et al.*, 2003; Confalonieri *et al.*, 2010; Richter *et al.*, 2010) compared the results obtained with different p and r values for crop models, and found that there was little effect of the number of r and p on the ranking of parameters.

We performed two sensitivity analyses using the Morris method based on the variable of the maximum seasonal value of LAI during one growing season.

Not all the parameters in STICS need to be included in the SA, because some parameters are either not used for the sugarcane application of the model or because they are known to have little or no effect on LAI (Ruget *et al.*, 2002). Therefore, from the ca. 200 parameters used to describe sugarcane growth in STICS, and based on expert knowledge from the model developers, we selected a subset of 50 parameters that could govern LAI (Table 4). Of these 50 parameters, twelve are soil-related (8) or general (4) generic plant parameters (applying to all species), while the others are specific to sugarcane, yield (10), biomass growth (5), phenological stages (10), nitrogen (1),

water (2), radiation interception (1), foliage development (5), and root growth (4). The selection of a range of variation allowed for each parameter is of importance because it impacts the results of the SA. We selected upper and lower bound values based on previous work with STICS for sugarcane (Smith, 2001), on a survey of scientific publication results on sugarcane modeling (Teruel *et al.*, 1997; Zhou *et al.*, 2003; Singels *et al.*, 2008), and on the expert opinion of developers (F. Ruget, INRA Avignon, DATEN) when no information was available.

A preliminary analysis, described in Supplementary Material (section S2), was carried out to test the influence of the number of repetitions of the Morris algorithm on the results of the SA. We found that for the most sensitive parameters, a number of repetitions between 20 and 30 had negligible influence on parameter ranking (Figure S2). Thus, we set the value of r to 20 repetitions to limit computational costs. Four of the sites were randomly selected among the eight available. The SA was carried out for each of the four sites separately with Morris settings of $p = 6$ levels and $r = 20$ iterations, therefore requiring (50+1)*20 = 1020 runs per site.

Design of the calibration experiment

The number of parameters chosen for the calibration results from a trade-off between computation costs and improved fit to the data. Because the goal of this study is to obtain a multi-site calibration, our selection of the most important parameters retained for calibration from the Morris sensitivity analysis is constrained by two criteria: the importance of a parameter at all the sites, and the limited amount of nonlinearities and/or interactions associated with this parameter. The calibration of STICS for the LAI was therefore performed on the three most sensitive parameters only, with a simple factorial method, whereby the model was run for all possible combinations of the three parameters within predefined ranges. Consistent with our approach (White *et al.*, 2000) used for vegetation models only a small number of parameters that had a significant impact on plant growth. For the parameters with little nonlinearities, the calibration was done by exploring extensively the parameters ranges. For parameters associated with nonlinearities, only few key values were explored. Modeled LAI values were then compared to observations through a scoring function. The minimization of the objective scoring function over all the simulations gave an optimal set of parameters.

The choice of the scoring function to select the best estimate of the most important parameters is not straightforward (Evans, 2003). Our goal here is the best possible match between the observed and modeled LAI at several sites, given uncertainties of measured LAI. Three different scoring functions are tested for the calibration: the Root Mean Squared Error (RMSE), the Figure of Merit (FM), and a Bayesian quadratic misfit function, here referred to as the J function. Each function is a multi-objective function as it aims at scoring the parameter sets at several sites simultaneously. The multi-objective configuration of the problem was tackled by aggregating the scores of all sites into a single score (Madsen, 2000). The functions are defined by Eqns (2–4) where n is the number of observations; *obs* and *run* stand for the observed and simulated LAI, respectively, at site s and time t_j; P_1, P_2, P_3 are the values of the 3 most sensitive parameters identified from the sensitivity analysis, and P_{1prior}, P_{2prior}, P_{3prior} are the prior estimates. σ_{obs}, σ_{P1}, σ_{P2}, σ_{P3}, respectively, refer to the errors on observation and on the prior estimates of the parameters.

We define below all three objective functions for site s, at times t_j. Observed and simulated LAI are, respectively, referred to as 'obs' and 'run'. n is the number of observations, for the observed LAI (respectively, simulated LAI).

$$\mathrm{RMSE}\ (s) = \sqrt{\frac{\sum_{j=1}^{n}\left(\mathrm{obs}(s,t_j) - \mathrm{run}\right)^2}{n}} \tag{2}$$

is defined as follows

$$\mathrm{FM}\ (s) = 1 - \mathrm{FMT}\ (s) = 1 - \frac{\sum_{j=1}^{n}\min\{\mathrm{obs}(s,t_j),\mathrm{run}(s,t_j)\}}{\sum_{j=1}^{n}\max\{\mathrm{obs}(s,t_j),\mathrm{run}(s,t_j)\}} \tag{3}$$

$$J(s,P_1,P_2,P_3) = \frac{(P_1 - P_{1prior})^2}{\sigma_{p_1}^2} + \frac{(P_2 - P_{2prior})^2}{\sigma_{p_2}^2} + \frac{(P_3 - P_{3prior})^2}{\sigma_{p_3}^2} + \frac{1}{n}\sum_{j=1}^{n}\frac{(run(s,t_j) - obs(s,t_j))^2}{\sigma_{obs}^2} \tag{4}$$

The figure of merit in time (FMT) is usually defined as the ratio of overlapping between the observed and simulated LAI curves, that is, the area defined by the union below the two curves divided by the area defined by their intersection [Eqn (3)]. Here we use, FM = 1 − FMT, to more easily compare the three scoring functions. A value of FM close to 0 means a perfect agreement between model and observations (i.e., optimal parameter value) as opposed to a value of FM close to 1 meaning no match between both data sets.

The RMSE and the J function are quadratic error functions [Eqns (2) and (4)]. They quantify the distance between modeled and observed LAI, but with an extra term in the Bayesian function J to represent the quadratic distance between optimum and prior parameter value. By adding a prior term in the J scoring function, we put weight to a specific location in the parameters space based on the most likely value of the parameter (i.e., the prior). The intent of the calibration is to minimize each of the FM, RMSE, and J functions, to determine a set of parameters that minimizes a distance between observed and modeled LAI.

Cross-validation

Cross-validation is performed to evaluate the dependence of the calibration to the choice of sites. For this, we use a leave-one-out method where the same calibration is performed using different combinations of sites, each with one site being removed and therefore used for validation purposes.

Table 4 List of parameters included in the sensitivity analysis

Processes involved	Parameters descriptions	Parameters notations and names	Lower values	Upper values	References
Soil	Thickness of 3rd layer of soil (cm)	epc3	5	60	Smith, 2001
	Organic nitrogen content in moisture soil horizon (from the soil surface to profhum) as a weighted %	Norg	0.05	0.2	Smith, 2001
	Initial profile of amount of mineral nitrogen in Kg N ha^{-1}	Ninitf1	0	30	Smith, 2001
		Ninitf2	0	30	Smith, 2001
		Ninitf3	0	30	Smith, 2001
	Initial profile of water content in weighted % for fine soil	Hinitf1	11	22	Smith, 2001
		Hinitf2	11	22	Smith, 2001
		Hinitf3	10	21	Smith, 2001
General	Links storage organs' n demand to N status of the crop (unitless)	absodrp	0.02	0.078	Smith, 2001
	Threshold to calculate trophic stress on LAI: minimum value for source/sink ratio for leaf growth (unitless)	splaimin	0	0.3	Smith, 2001
	Reference temperature for soil mineralization parameters (°C)	TREF	15	27	Smith, 2001
	Radiative effect on conversion efficiency (unitless)	coefb	0.0015	0.0815	Smith, 2001
Yield components	Maximum number of set cane internodes per cane and by degree per day	afruitpot	0.0015	0.2	Smith, 2001
	Speed for increase in N harvest index g grain. g $plant^{-1}$. day^{-1}	vitirazo	0.0085	0.0115	Smith, 2001
	Cane internode's relative age when growing speed is maximum (unitless)	afpf	0.15	0.5	Smith, 2001
	Maximum growing speed relative to cane internode's maximum weight (unitless)	bfpf	1	10	Smith, 2001
	Maximum daily allocation of assimilates to cane internodes (unitless)	allocamx	0.63	0.86	Smith, 2001
	Biomass remobilized each day ($g.m^{-2}.d^{-1}$)	remobil	0.68	0.92	Smith, 2001
	Number of 'age classes' for growth of cane internodes for indeterminate plants	nboite	12	25	Smith, 2001
	Time during which cane internodes are set (degree.day)	sdrpnou	552.5	747.5	Smith, 2001
	Growing period for cane internodes, from setting to maturity (degree.day)	dureefruit	2850	3000	Smith, 2001
	Maximum grain weight (0% water) (g)	pgrainmaxi	1200	2000	Smith, 2001
Biomass	Maximum growing efficiency between LEV and AMF ($g.MJ^{-1}$)	efcroijuv	1.7	2.3	Smith, 2001
	Maximum growing efficiency between DRP and MAT ($g.MJ^{-1}$)	efcroirepro	2	6	Smith, 2001
	Maximum growing efficiency between AMF and DRP ($g.MJ^{-1}$)	efcroiveg	3.2	6	Smith, 2001
	Optimum temperature for growth in biomass (if plateau between teopt and teoptbis) (°C)	teoptbis	0	15	Smith, 2001
	Optimum temperature for growth in biomass (°C)	teopt	15	34.4	Smith, 2001
Development & Phenological stages	Minimum threshold temperature for development (°C)	tdmin	10	14	Smith, 2001
	Maximum threshold temperature for growth in biomass (°C)	tdmax	28	40	Smith, 2001
	Parameter to compensate between the number of stems and the density of plants (unitless)	adens	−1	−0.2	Smith, 2001
	Cumulated development units allowing germination (degree.day)	stpltger	50	200	Teruel *et al.*, 1997
	Stress threshold from which there is an effect on the LAI (supplementary senescence compared with natural senescence) (unitless)	tustressmin	0	1	Smith, 2001
	Time between emergence and senescence (degree.day)	stevsenms	400	800	Smith, 2001
	Cumulated development units between the LEV and AMF stages (degree.day)	stlevamf	50	400	Smith, 2001

Table 4 (continued)

Processes involved	Parameters descriptions	Parameters notations and names		Lower values	Upper values	References
	Cumulated development units between AMF and LAX stages (degree.day)		stamflax	1000	2100	Smith, 2001
	Cumulated development units between the LEV and DRP stages (degree.day)		stlevdrp	1000	1740	Smith, 2001
	Fraction of senescent biomass (with relation to the total biomass)		ratiosen	0	1	Smith, 2001
Nitrogen	Minimum INN value possible for the crop	INN_{min}	innmin	0	1	Smith, 2001
Water	Absolute value for start of reduction in cell expansion (unitless)		psiturg	1	5	Smith, 2001
	Absolute value for stomatic closure potential (bars)		psisto	5	15	Smith, 2001
Radiation interception	Coefficient of extinction (unitless)		extin	0.424	0.7	Zhou *et al.*, 2003 Muchow *et al.*, 1994
LAI	Maximum rate of production of net leaf surface area m^2 leaf . $plant^{-1}$. $degree.day^{-1}$	δ_{LAI}^{max}	dlaimax	0.0002	0.0015	Smith, 2001
	Minimum density as from which there is competition between plants for leaf growth $plants.m^{-2}$	β_{dens}	bdens	2	10	Smith, 2001
	Minimum temperature for growth (°C)		tcmin	10	14	Singels *et al.*, 2008
	Maximum temperature for growth (°C)		tcmax	35	42	Smith, 2001
	Coefficient of sink strength of vegetative organs $cm^2.g^{-1}$		sbv	127.5	172.5	Smith, 2001
Roots	Shape of root profile depth of tillage (m)		zlabour	17	23	Fauconnier & Bassereau, 1970
	Shape of root profile: depth at which root density is half of surface density for reference root profile (m)		zpente	24	110	Fauconnier & Bassereau, 1970
	Shape of root profile: maximum depth for reference root profile (m)		zprlim	111	140	Fauconnier & Bassereau, 1970
	Growing rate of root front (cm.degree-day^{-1})		croirac	0.05	0.2	Smith, 2001

Development stages are LEV: emergence, AMF: end of juvenile phase, DRP: beginning of harvested elements filling, MAT: physiological maturity, LAX: maximum leaf area index (Brisson *et al.*, 2003).

Results

Sensitivity analysis and selection of sensitive parameters

Here, we used maximum LAI during the annual growth cycle as a target variable to define the most sensitive parameters. Figure 3a–d shows the results of the Morris sensitivity analysis at the four sites with μ^* (elementary effects mean of absolute values) as x-axis and σ (elementary effects standard deviation) as y-axis. Figure 3e displays the ranking of all parameters by decreasing order of importance (at the four sites) for their influence on μ^*. The important parameters stand out from the Morris sensitivity analysis based on their μ^* with little variability from site to site, especially for the three most important parameters whose roles and related equations are explained in Fig. 4 (Brisson *et al.*, 2009). The parameter δ_{LAI}^{max} comes out consistently as the most sensitive one controlling LAI across the four sites (Fig. 3a–d: highest μ^* and a relatively low σ revealing a first order effect on maximum LAI). This parameter intervenes in the calculation of LAI to limit the maximum daily increment of foliage per degree-day (number of degrees that separate actual temperature from a minimum temperature threshold; see Fig. 4). A higher value of δ_{LAI}^{max} allows a faster growth of LAI during the first stage of the crop development.

Following δ_{LAI}^{max} in importance, two other parameters, β_{dens} and INN_{min} have a high impact on μ^*. The β_{dens} parameter corresponds to a critical plant density below which there is no competition between individual plants to form LAI (Fig. 4). The parameter INN_{min} is a threshold for the nitrogen nutrition index (INN) of the crop, which controls the sensitivity of the crop to nitrogen stress and impacts LAI in an indirect way. This parameter is associated with nonlinearities in the response of LAI to parameters as shown by the high σ values. Because of the nonlinearity of the response of LAI to

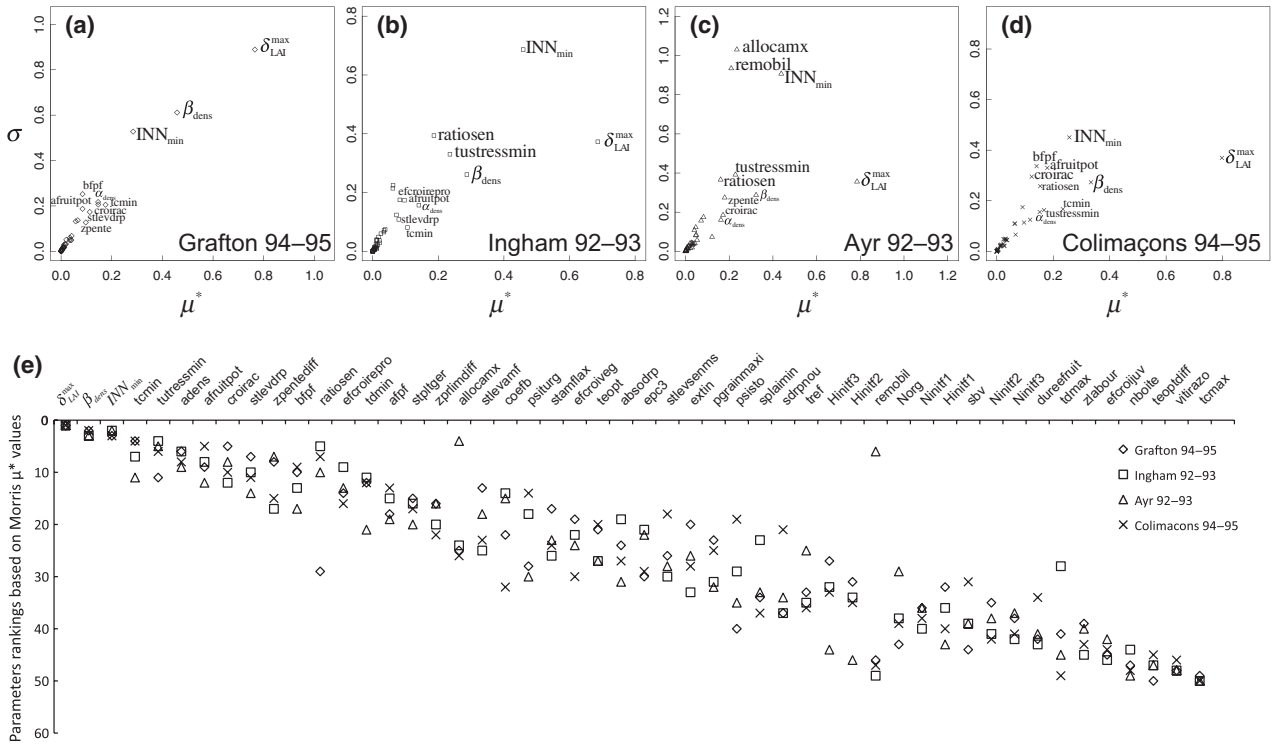

Fig. 3 Morris indices and ranking of the parameters for the four sites included in the Morris sensitivity analysis. (a–d) Morris indices μ^* and σ for each site, respectively. A large value of μ^* indicates a large impact on the maximum LAI simulated, a large σ indicates the involvement of nonlinearities or interactions between parameters. (e) Ranking of the parameters based on their μ^* comparing the rankings at the four sites. The first three parameters show a very good consistency between the sites, after the third parameter a large dispersion of the rankings appears.

this parameter, only a few key values of INN_{min} are included in the calibration procedure, like in White *et al.* (2000).

Parameter calibration results

The factorial calibration of the values of the three top ranked parameters was repeated with three scoring functions [Eqns (2–4)]. The optimal value of the nitrogen stress threshold parameter INN_{min}, was rapidly determined since all best scores are reached for the same value of $INN_{min} = 0.2$, below which no change is observed in the LAI simulations. The bivariate response of each scoring function to variations of parameters δ_{LAI}^{max} and β_{dens} (axes of the horizontal plane) is shown in Fig. 5, with INN_{min} fixed at a value of 0.2.

All three scoring functions reached a local minimum in the (δ_{LAI}^{max}, β_{dens}) two-dimensional parameter space that corresponds to the best parameter values, but the location of this minimum (i.e., the optimum parameter sets) and the shape of the 2-D response surfaces (δ_{LAI}^{max}, β_{dens}) around the minimum differs between the functions. The three optimum parameter sets resulting from the different scoring functions are shown in Fig. 6. The corresponding simulations of LAI are shown in Fig. 7(a–h).

The optimum parameter sets obtained with the three scoring functions are hereafter called p-RMSE, p-FM, and p-J. Overall, the date of LAI emergence was generally well reproduced by STICS (Fig. 7). Later during the crop foliar development, different growth trajectories and onsets of senescence were obtained from the different parameter couples, leading to different trajectories of LAI. None of the three couples of optimal parameters led to a better simulation at all sites simultaneously. As an example, the p-FM couple of parameters favored a LAI growth with a very late LAI senescence, whereas the p-RMSE couple resulted in an earlier than observed decrease in LAI. For this reason, the choice of a best (i.e., most robust) scoring function is not trivial. We introduce an additional criterion for the selection of a robust scoring function that the parameter calibration should be as independent as possible from the set of sites used for calibration. The selection of a robust scoring function is done through a cross-site validation, as explained below.

Parameter	Variable impacted	Equation	Impact on LAI
$\delta_{\mathrm{LAI}}^{max}$	$\Delta_{\mathrm{LAI}}^{dev}$: Crop development based increment of LAI	$\Delta_{\mathrm{LAI}}^{dev} = \dfrac{\delta_{\mathrm{LAI}}^{\max}}{1+e^{f(k_{\mathrm{LAI}})}}$ $\delta_{\mathrm{LAI}}^{\max}$: Maximum daily increment of foliage per degree.day (m^2 leaf. $plant^{-1}$.degree.day^{-1}) k_{LAI} : LAI development stage (dimensionless)	$\mathrm{LAI} = \int_0^T \Delta_{\mathrm{LAI}}^{dev} \cdot \Delta_{\mathrm{LAI}}^{T} \cdot \Delta_{\mathrm{LAI}}^{\mathrm{dens}} \cdot \Delta_{\mathrm{LAI}}^{stress} .splai.dt$ $\Delta_{\mathrm{LAI}}^{T}$: Temperature effect on increment of LAI (°C) $splai$: Trophic stress index for competition between leaves and harvested components (dimensionless)
β_{dens}	$\Delta_{\mathrm{LAI}}^{\mathrm{dens}}$: Plant density effect on increment of LAI	$\Delta_{\mathrm{LAI}}^{\mathrm{dens}} = e^{\alpha_{\mathrm{dens}} \log\left(\frac{d}{\beta_{\mathrm{dens}}}\right)} \cdot d$ β_{dens} : Minimum density as from which there is competition between plants for leaf growth (plants.m^{-2}) α_{dens} : Ability of a plant to endure increasing densities (dimensionless) d : Plant density (plants.m^{-2})	
$\mathrm{INN}_{\min}$	$\Delta_{\mathrm{LAI}}^{stress}$: Nitrogen and water stress effect on increment of LAI	$\Delta_{\mathrm{LAI}}^{stress} = \min\begin{cases} \mathrm{INN} = \max\left(\dfrac{C_N^{plant}}{C_N^{crit}}, \mathrm{INN}_{\min}\right) \\ W_s \end{cases}$ $\mathrm{INN}_{\min}$: Minimum Nitrogen nutrition index value possible (dimensionless) C_N^{crit}, C_N^{plant} : Critical and actual Nitrogen concentration in the plant (gN. g dry matter $^{-1}$) W_s : Water stress index (dimensionless)	

Fig. 4 Impacts of the parameters $\delta_{\mathrm{LAI}}^{\max}$, β_{dens} and $\mathrm{INN}_{\min}$ on the calculation of LAI in the STICS model. The parameters $\delta_{\mathrm{LAI}}^{\max}$, β_{dens} and $\mathrm{INN}_{\min}$, respectively, impact on the calculation of intermediary variables, daily increment of LAI, competition effect from planting density, and threshold for nitrogen nutrition index.

Cross-validation

We performed a leave-one-out cross-validation to assess the robustness of the calibration for the three scoring functions (Fig. 8). In Fig. 8, each group of adjacent bars represents the model-data misfit at one site for nine possible combinations of sites used for calibration (all of the eight sites used, or one site removed at a time being used as cross-validation). The misfits shown in Fig. 8 are very different between the scoring functions. For example, the RMSE at site Ayr 92–93 is 25% higher when this site is left out for calibration.

The calibration based on J is found to be the most site-dependent (Fig. 8c), with a large variation in the misfit depending on which sites are excluded from the calibration. With the J scoring function (Fig. 8c) for instance, the use of Colimaçons 94–95 as a calibration site impacts most of the misfits of optimized LAI at other sites. When Colimaçons 94–95 is removed from the calibration, seven sites out of eight had a much lower score (higher J), whereas the Ayr 92–93 site had a much better score (lower J). With the RMSE function, the Ayr 92–93 site has the largest impact on the calibration, with its own score being severely degraded (higher RMSE) where it is excluded, whereas five sites out of eight have a lower RMSE when Ayr 92–93 was removed. With the FM function (Fig. 8b), excluding the two Ingham sites from the calibration has a large influence on the misfit at those sites but only a slight impact at the other sites. The RMSE and FM functions have similar results as far as cross-validation is concerned with a relative good stability of the calibration regardless of the sites combinations used. However, because of the large impact of the exclusion of Ayr 92–93 at this site, we conclude that the use of the FM as a scoring function is more robust than the two other functions, and therefore, parameters determined from this approach will be chosen for future applications of the ORCHIDEE-STICS model to sugarcane. With the calibration performed using the FM scoring function, we obtain a multisite average figure of merit score (average of the FM-scores at each site) of 79% of agreement instead of 67% before calibration.

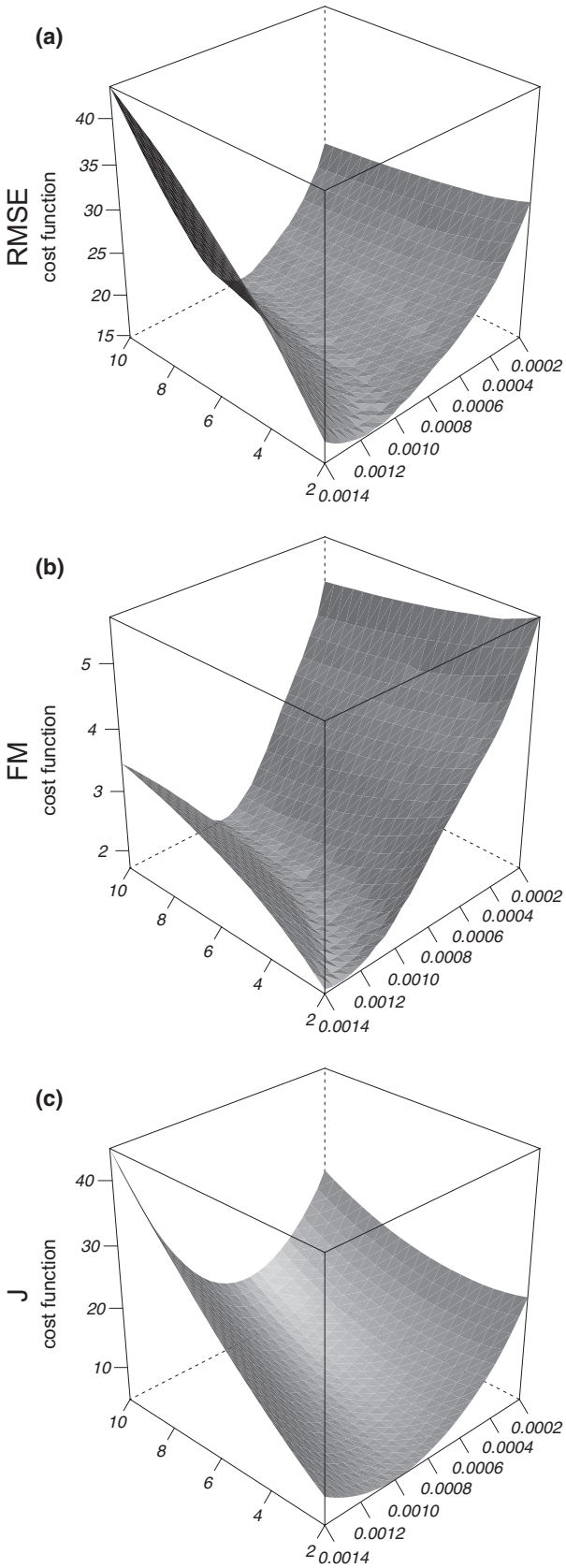

Fig. 5 Surface representations of cost functions (a) RMSE, (b) FM, (c) J for all combinations of the values of δ_{LAI}^{max} and β_{dens} parameters within their ranges of variation shown on the horizontal axes, for $INN_{min} = 0.2$ (optimal value). The optimal parameter set is the point for which the objective functions are the smallest.

Discussion and conclusion

A successful and robust multisite calibration relies on the assumption that the same model can be improved (i.e., systematic errors reduced) at different sites through the adjustment of few parameters only. For our purposes of regional applications of the model, for instance to estimate regional sugarcane yields, we need to avoid local fine-tuning of a large number of parameters.

Parameters δ_{LAI}^{max}, β_{dens} and INN_{min} were the top most influential parameters for LAI simulations at the eight sites in ORCHIDEE-STICS, with δ_{LAI}^{max} being far more important. These three parameters were already among those identified as critical for STICS applied to maize and wheat (Guillaume *et al.*, 2011; Ruget *et al.*, 2002; Tremblay and Wallach, 2004). Parameter δ_{LAI}^{max} in particu-

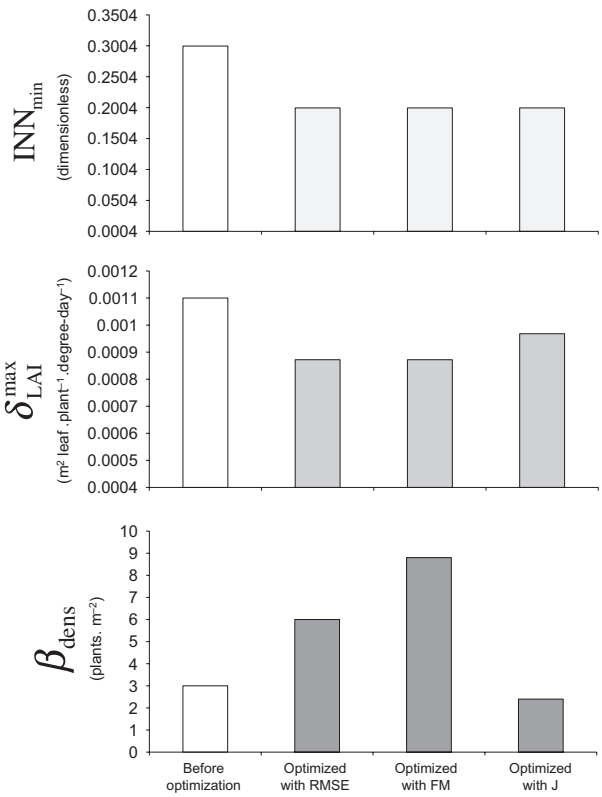

Fig. 6 Values obtained for the parameters and after optimization of the three scoring functions Root Mean Squared Error (RMSE), Figure of merit (FM), Bayesian function (J).

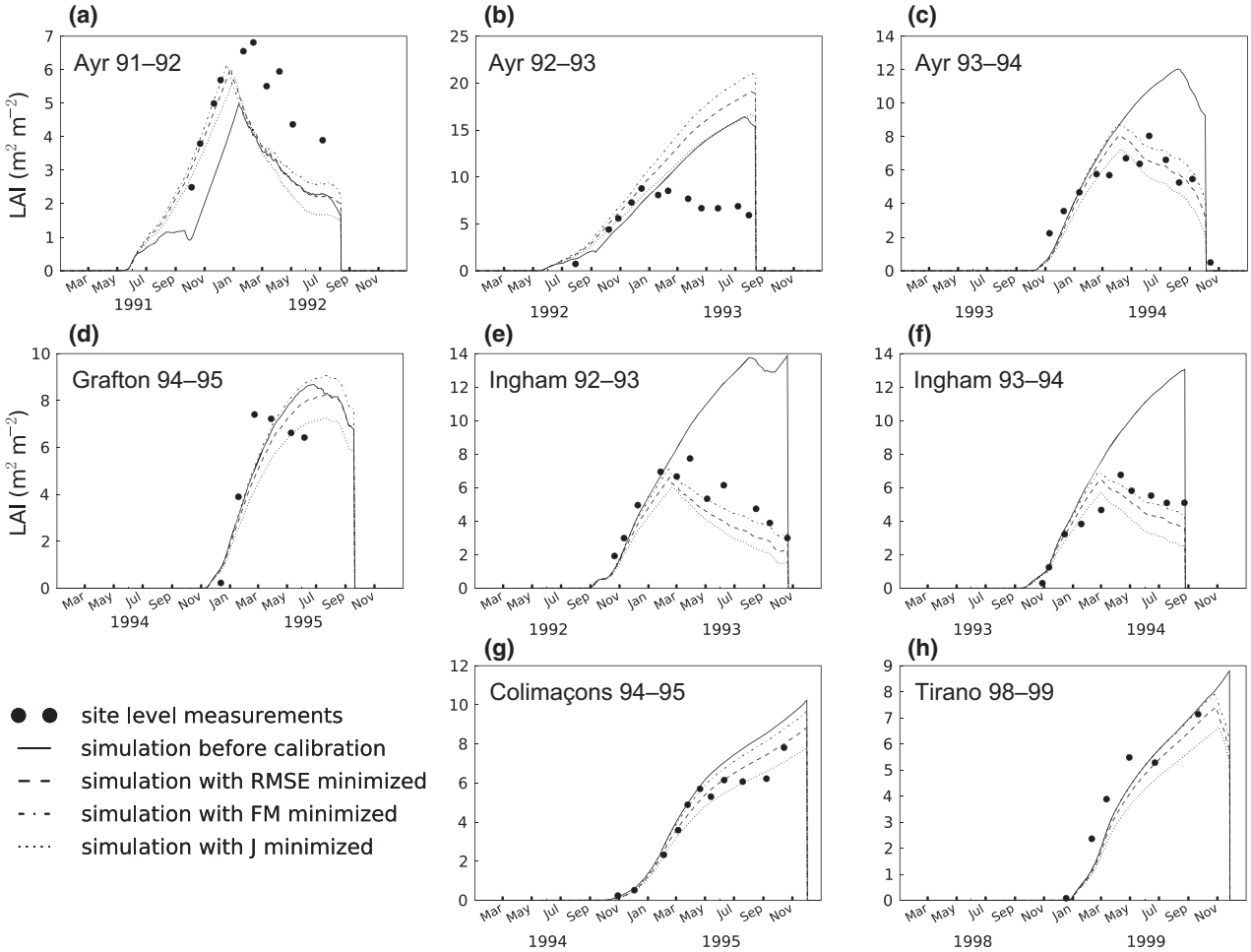

Fig. 7 LAI simulated at each site after multisite parameters calibration based on the optimization of the RMSE (dashed), Figure of merit (dash-dotted), J (dotted).

lar was shown to have a much stronger influence on the maximum rate of LAI increase in the beginning of the growing season which is crucial to the simulation of harvested biomass (A. Valade, N. Vuichard, P. Ciais, N. Viovy, F. Marin, N. Huth, J-F. Martiné, in preparation). Parameter β_{dens} indicates the importance of the initial planting density as a management factor influencing the seasonal trajectory of LAI through competition between individuals. The identification of the threshold for nitrogen nutrition index as the second most important parameter on sugarcane LAI illustrates the connection between below-ground nutrient availability and green leaves development.

After calibration of the three most important parameters determined from the Morris sensitivity analysis, the overall simulation of LAI is improved, but a residual error remains mainly in the late LAI development cycle, which may arise either from parameter values (discussed in this article), but also from forcing data and model structure (e.g., other factors that influence the LAI during the late development phase not included in STICS).

Part of the model error due to internal parameters has been addressed in this article. Here, only three parameters were calibrated based on the intersite consistency of model sensitivity to these parameters. Another issue related to the internal model parameters setting is that by searching a common set of parameter values to apply to all sites, we assume that all crops are of the same variety and type (all crops are considered to be planted each year, as opposed to real-field conditions where sugarcane is often ratooned, i.e., cut and left in the soil to grow again the following year), which in reality may differ from one field to another and one region to another. For example, in this study, all Australian sites are planted with variety Q117 (or R570 in La Reunion), except Ayr 91–92, which could partly explain the poor results after calibration at that site along with other factors such as an over-detected water stress (Table 2).

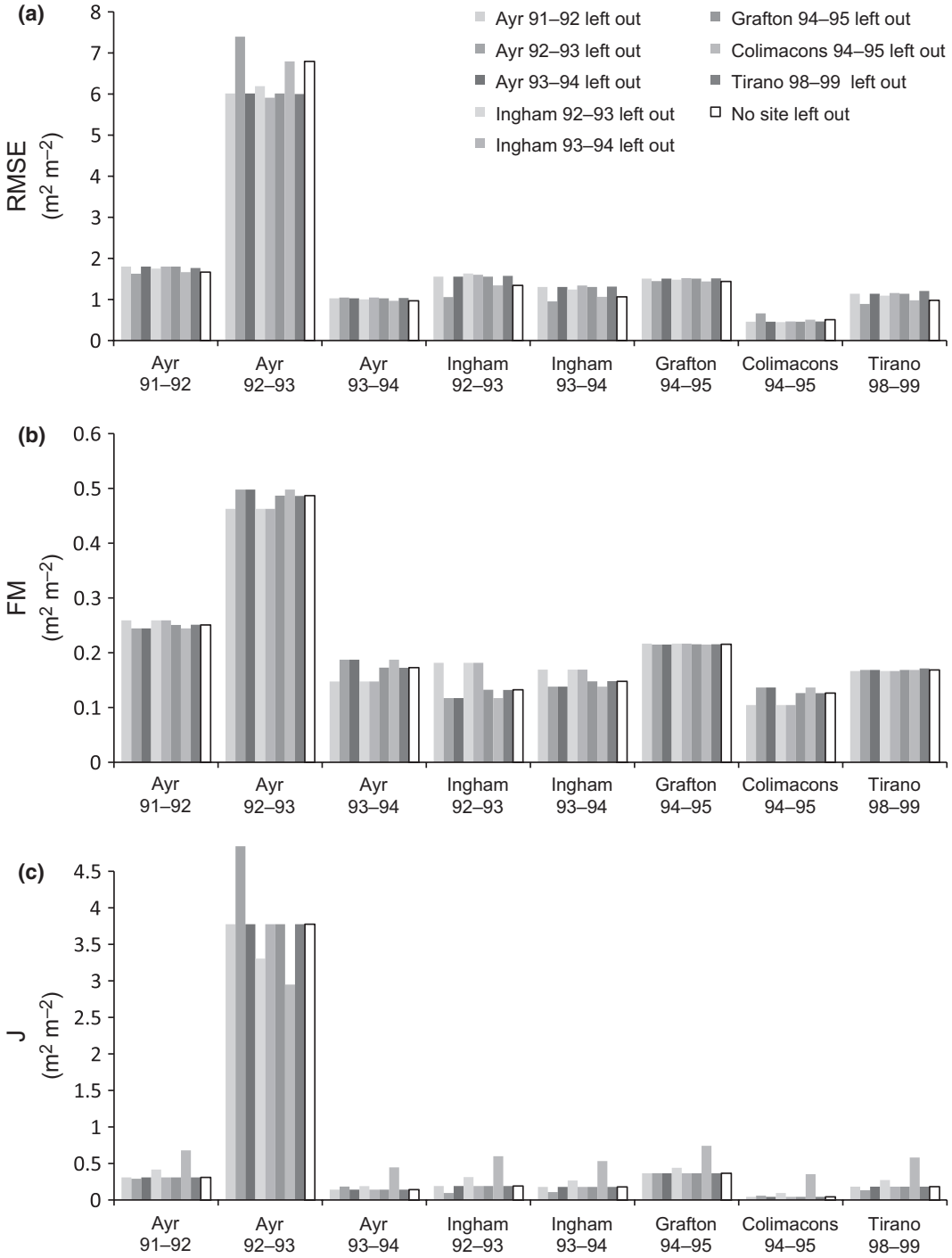

Fig. 8 Cross-validation scores for the calibration with the three scoring functions. (a) RMSE, (b) FM, (c) J. The horizontal axis indicates the site that is evaluated. The shades of the bars refer to the site that is left out of the calibration and therefore considered a validation site (the white bar refers to the reference calibration based on all eight sites).

Just like variety differences, environmental conditions and accuracy of forcing data add uncertainty to the simulation and are responsible for a fraction of the residual error. In particular, using a generic soil physics parameterization (depth, texture, water holding parameters) ignores local specificities that are determinant for describing accurately soil water content, water availability to plants, and therefore root growth and water stress. The identification of the limitation of the nitrogen nutrition index as the second parameter

exerting the most influence on LAI simulation also highlights the need for a more detailed and thorough description of soil conditions. However, the type of data needed, such as soil carbon content, organic nitrogen content, or minimum soil humidity exploitable by the plant, is not easily retrievable during crop growth experiments and is therefore not often available to constrain models, even for site-level simulations. A complete account of the soil's characteristics however requires data about the nature of the land at this site but also about the previous years' management practices, that are difficult to gather at regional level.

Leaf area index is an indicator of crop development and was considered the only output variable in this study. However, at the ecosystem level, other variables driven by crop development are also of interest, such as biomass or net primary productivity, which are controlled by different parameters and processes than LAI. The calibration of LAI alone is not sufficient for a good simulation of other variables by the model, but it is a necessary pre-requisite for the model to provide good estimates of plant growth and interactions with its local environment and climate.

Acknowledgements

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Supporting Information

Additional Supporting Information may be found in the online version of this article:

Table S1 RMSE of the reanalysis data versus the weather-station data before and after correction.
Figure S1 Meteorological data from weather station measurements (grey solid), globally gridded product ERA-Interim (dotted), combination of the two datasets (black solid). (a) cumulated and daily precipitation (mm), (b) daily mean air temperature (K), (c) daily solar radiation (W m^{-2}).
Figure S2 Ranking of the parameters for three configurations of the Morris sensitivity analysis applied at the site Grafton. Each of the three shades of grey refers to one of the three configurations (r = 20, 30 and 40). Groups of bars refer to each parameter combined with the different Morris configurations. The rank of importance of each parameter is represented by a bar which length is inversely proportional to its rank (the largest bar corresponds to the parameter ranked first, the smallest bar to the parameter ranked last).