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### Modeling sugar cane yield with a process-based model from site to continental scale: uncertainties arising from model structure and parameter values

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Discussion Paper

Full Screen / Esc Discussion Pape Printer-friendly Version

Interactive Discussion



**GMDD** 

### Modeling sugar cane vield

7, 1197-1244, 2014

A. Valade et al.

Title Page

Introduction **Abstract** 

Conclusions References

**Figures** 

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Agro-Land Surface Models (agro-LSM) have been developed from the integration of specific crop processes into large-scale generic land surface models that allow calculating the spatial distribution and variability of energy, water and carbon fluxes within the soil-vegetation-atmosphere continuum. When developing agro-LSM models, a particular attention must be given to the effects of crop phenology and management on the turbulent fluxes exchanged with the atmosphere, and the underlying water and carbon pools. A part of the uncertainty of Agro-LSM models is related to their usually large number of parameters. In this study, we quantify the parameter-values uncertainty in the simulation of sugar cane biomass production with the agro-LSM ORCHIDEE-STICS, using a multi-regional approach with data from sites in Australia, La Réunion and Brazil. In ORCHIDEE-STICS, two models are chained: STICS, an agronomy model that calculates phenology and management, and ORCHIDEE, a land surface model that calculates biomass and other ecosystem variables forced by STICS' phenology. First, the parameters that dominate the uncertainty of simulated biomass at harvest date are determined through a screening of 67 different parameters of both STICS and ORCHIDEE on a multi-site basis. Secondly, the uncertainty of harvested biomass attributable to those most sensitive parameters is quantified and specifically attributed to either STICS (phenology, management) or to ORCHIDEE (other ecosystem variables including biomass) through distinct Monte-Carlo runs. The uncertainty on parameter values is constrained using observations by calibrating the model independently at seven sites. In a third step, a sensitivity analysis is carried out by varying the most sensitive parameters to investigate their effects at continental scale. A Monte-Carlo sampling method associated with the calculation of Partial Ranked Correlation Coefficients is used to quantify the sensitivity of harvested biomass to input parameters on a continental scale across the large regions of intensive sugar cane cultivation in Australia and Brazil. Ten parameters driving most of the uncertainty in the ORCHIDEE-STICS modeled biomass at the 7 sites are identified by the screening procedure. We found

GMDD

Paper

Discussion Paper

Discussion Paper

Discussion Pape

7, 1197–1244, 2014

Modeling sugar cane vield

A. Valade et al.

Title Page

Abstract Introduction

Conclusions References

Tables Figures

I∢ ►I

- ◆

Back Close

Full Screen / Esc

**Printer-friendly Version** 



7, 1197–1244, 2014

## Modeling sugar cane vield

**GMDD** 

A. Valade et al.

Title Page

Abstract Introduction

Conclusions References

Tables Figures

I∢ ⊳I

- ◆

Back Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



that the 10 most sensitive parameters control phenology (maximum rate of increase of LAI) and root uptake of water and nitrogen (root profile and root growth rate, nitrogen stress threshold) in STICS, and photosynthesis (optimal temperature of photosynthesis, optimal carboxylation rate), radiation interception (extinction coefficient), and transpiration and respiration (stomatal conductance, growth and maintenance respiration coefficients) in ORCHIDEE. We find that the optimal carboxylation rate and photosynthesis temperature parameters contribute most to the uncertainty in harvested biomass simulations at site scale. The spatial variation of the ranked correlation between input parameters and modeled biomass at harvest is well explained by rain and temperature drivers, suggesting climate-mediated different sensitivities of modeled sugar cane yield to the model parameters, for Australia and Brazil. This study reveals the spatial and temporal patterns of uncertainty variability for a highly parameterized agro-LSM and calls for more systematic uncertainty analyses of such models.

#### 1 Introduction

In the recent years, many governments have set targets in terms of biofuels consumption for transportation fuel (Sorda et al., 2010), resulting in a large increase in bioenergy cropping area around the world. Concerns about energy shortage, policy to reduce  $CO_2$  emissions, and the search for new income for farmers can explain why energy policies have considered biofuels as a serious alternative to fossil fuel in many countries (Demirbas, 2008). Yet, the claimed benefits of biofuels for fossil fuel substitution have been questioned in terms of their net effect on atmospheric  $CO_2$  and climate, and even of their economic return (Doornbosch and Steenblik, 2008; Naylor et al., 2007). In particular, the conditions of biofuel cultivation, such as the type of crop, practice, previous land use, and local climate, have emerged as key factors that determine the effectiveness of their carbon emissions reduction (Fargione et al., 2008; Hill et al., 2006; Searchinger et al., 2008). At the heart of biofuel cultivation is ethanol that represents today 74% of the energy content of the world production of liquid biofuels (Howarth

**GMDD** 

7, 1197–1244, 2014

Modeling sugar cane vield

A. Valade et al.

Title Page **Abstract** Introduction

Conclusions References

**Figures** 

Back

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



et al., 2008) and whose production is expected to double between 2011 and 2021 (OECD, 2012), hence the urgency to better quantify and understand regional potentials of bioethanol crops. Based on recent life cycle analysis studies (de Vries et al., 2010; Schubert, 2006; von Blottnitz and Curran, 2007), ethanol from sugar cane is the 5 most competitive in terms of energy use and net carbon balance and the energy use projections from the International Energy Agency foresee that by 2050, sugar cane is the only 1st generation biofuel that that will keep expanding (IEA, 2011).

The impact of sugar cane expansion on climate and carbon balance is under scrutiny with different approaches. Satellite observation data have been used to study biophysical effects of sugar cane expansion on local temperature in the Brazilian Cerrado (Loarie et al., 2011). Survey for agricultural and industrial performances from sugar cane mills have allowed Macedo et al. (2008) to establish the carbon balance of sugar cane ethanol production in the Center-South of Brazil. Georgescu et al. (2013) simulate the hydroclimatic impacts of sugar cane expansion by forcing sugar cane land cover characteristics into a regional climate model. All approaches provide useful information on impacts and potentials but are impractical to apply outside of the regions and conditions (climate, management) where they have been conducted.

In parallel with empirical approaches, significant progress has been made towards mechanistic modeling of sugar cane yields using models. Crop models are generally used to simulate sugar cane production at site scale, with specific parameters (Cheeroo-Nayamuth et al., 2000). Land surface models (LSM) are rather used to estimate the spatial distribution of crop productivity under different soil and climatic conditions, over a region or even over the globe but with a simpler and generic description of sugar cane plants (Black et al., 2012; Cuadra et al., 2012; Lapola et al., 2009). Agro-LSM models stand at the interface between plot-scale crop models and global LSMs. Yet, as highlighted by Surendran Nair et al. (2012) if the development of agro-LSM models for biofuels has been the subject of much interest recently, detailed parameterization, validation and uncertainty quantification is still very limited in regional and global applications, and efforts must be made in that direction. The importance of evaluating

**GMDD** 

7, 1197–1244, 2014

Modeling sugar cane vield

A. Valade et al.

Title Page

**Abstract** Introduction

Conclusions References

**Figures** 

Back

Full Screen / Esc

**Printer-friendly Version** 

Interactive Discussion



and communicating about global models uncertainty was as well emphasized within the framework of the model inter-comparison project AgMIP – providing insights for IPCC AR5 report – in which crop models uncertainty is identified as a key theme of interest that was only little explored so far (Rosenzweig et al., 2013). ORCHIDEE-STICS (Gervois et al., 2004) is an agro-LSM model that has been developed from the coupling of the agronomical model STICS (Brisson et al., 1998) and the Land Surface Model ORCHIDEE (Krinner et al., 2005), that has been applied for studies from site to continent mainly for temperate crops in Europe (Gervois et al., 2008) and has been recently adapted to sugar cane simulation (Valade et al., 2013).

Four uncertainty sources affect the simulation of sugar cane biomass with ORCHIDEE-STICS: (1) input uncertainty, on boundary conditions used for climate drivers and soil properties, (2) structure uncertainty, related to model equations and parameterizations, (3) parameters value uncertainty, and (4) uncertainty associated with the measurements used for model evaluation or calibration. Here we focus on structure and parameters uncertainty (2) and (3) and try to estimate how these two sources of uncertainties affect the simulations of sugar cane harvest biomass. We want to determine which parameters are responsible for most of the uncertainty in harvest biomass simulations (screening analysis) and to what extent this is related to the model's structure (uncertainty analysis). In addition, we want to quantify this uncertainty and examine its temporal and spatial variability (sensitivity analysis).

In the following, we first present the sites and regions considered in this study (Sect. 2.1) and the main features of the ORCHIDEE-STICS model (Sect. 2.2). We then describe the screening algorithm used to sort the most important parameters (Sect. 2.3), and the methodology used for the uncertainty and the sensitivity analyses (Sects. 2.4 and 2.5). Then we discuss the results of the screening analysis, in terms of the parameters identified by the screening as the most important for controlling harvested sugar cane biomass (Sect. 3.1). We describe the results for the measure of the uncertainty calculated for 7 sites in Sects. 3.2 to 3.4 and present maps of the sensitivity of the model to its main parameters in Sect. 3.5.

In this study, we aim to quantify the uncertainty related to the parameter values of a chain of two process-based models (STICS-ORCHIDEE) used to simulate sugar cane yield (biomass at harvest date). This is a difficult task because this model is a detailed and complex model that contains over 100 plant specific parameters within the primitive equations of phenology, energy and water balance, photosynthesis and allocation. We perform the uncertainty analysis in three steps, illustrated in Fig. 1 and consisting of screening, uncertainty and sensitivity analyses, all described in more details in Sect. 2. These three steps are sequential and complementary. The first step is a screening to sort the most important parameters controlling yield, and to reduce the dimension of the parameter space from a large number of parameters to a few key parameters, allowing a moderate number of sensitivity simulations. The screening thus allows the restriction of the two further steps to a smaller parameter subset. The second step is an uncertainty analysis that considers all retained parameters together with their probability distributions and determines the probability distribution for the output variable (biomass). The third step is an analysis of the sensitivity of the modeled spatial distribution of sugar cane yield to the model parameters for two large regions, in Brazil and Australia, at a spatial resolution of 0.5°. The sensitivity is established from the spatial distribution of ranked correlations between each parameter and simulated yield in each grid point. Along the study steps, we address several problems inherent to uncertainty and sensitivity evaluation such as the determination of the uncertainty on the input parameters and the spatial (regional) differences of the sensitivity of the model to its key parameters.

### 2.1 Sites and study areas

This study is based on sugar cane field trials in three regions (Fig. 2) where sugar cane is of economical importance, Brazil (1 site), Australia (4 sites), and La Réunion Island (2 sites). These sites, already used by Valade et al. (2013) span different climatic

iscussion

Paper

### GMDD

7, 1197-1244, 2014

# Modeling sugar cane vield

A. Valade et al.

Title Page

Discussion Paper

Discussion Paper

Discussion

Paper

Abstract

Introduction

Conclusions

References

Tables

Figures

I₫

►I

- ■

•

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



conditions and agricultural practices, as shown in Table 1, which makes them useful for our purpose to provide continental-scale sugar cane yield uncertainty estimates. More details about the four sites from Australia and La Réunion can be found respectively in Keating et al. (1999); Muchow et al. (1994); Robertson et al. (1996) and in Martiné (unpublished). The site from Brazil is described in Marin et al. (2011). The sensitivity analysis of the yield spatial distribution to the model parameters is carried out for two continental-scale areas where sugar cane is cultivated at large scale. In Brazil, we consider the region encompassing partly the Sáo Paulo and Mato Grosso states, and in Australia the sugar cane cultivation belt of the northeastern coast (Fig. 2).

### 2.2 Model and parameters considered

We use the agro-Land Surface Model ORCHIDEE-STICS (Gervois et al., 2004) in a version that has been calibrated for sugar cane for Leaf Area Index at the same sites than used here (Valade et al., 2013). This model chains the crop model STICS with sugar cane specific phenology and management with the generic process-based land surface model ORCHIDEE that can be applied either at a site, or on a grid for regional runs.

STICS (Brisson et al., 1998) is an agronomical model designed for site-scale operational applications, which describes in details the soil and crop processes associated with specific crop varieties and with management practices, such as aboveground biomass, biomass nitrogen content, water and nitrogen content in the soil, yield, root density. Yet, STICS is a generic crop model, because from a set of common equations it can describe a large number of crop species through specific parameterizations. Similarly, specific vectors of parameters define crop cultivars. STICS has been validated for a variety of cropping situations (Brisson et al., 2003)

ORCHIDEE (Krinner et al., 2005) is a land surface model developed for global applications, standing now as the land surface model of the IPSL Earth System Model. It has been developed from the association of a surface energy and water balance scheme (SECHIBA) with a biogeochemistry module (STOMATE) and as such simulates the

**GMDD** 

7, 1197–1244, 2014

Modeling sugar cane yield

A. Valade et al.

Title Page

Abstract Introduction

Conclusions References

Tables Figures

l∢ ⊳l

■ •

Back Close

Full Screen / Esc

Printer-friendly Version



Discussion



short time scale exchanges of water and energy between the land surface and the atmosphere, as well as the processes of the carbon cycle including photosynthesis, respiration, carbon allocation, soil decomposition. The vegetation is represented in OR-CHIDEE with the Plant Functional Type (PFT) concept, by grouping species into a few categories based on the similarities of their traits and resulting in an average plant. For example, sugar cane would fall in the generic "C4 crop" PFT in the standard version of ORCHIDEE, and this un-calibrated version of the model fails to reproduce site-level phenology, as shown by Valade et al. (2013).

The chaining of STICS with ORCHIDEE was performed to improve the ability of ORCHIDEE to simulate specific crops, for which the PFT concept was not appropriate, as it lacks representation of crop phenology and crop management practices (Gervois et al., 2004). In the chain-like structure (Fig. 3), STICS calculates phenology, water and nitrogen requirements, and passes the key variables of Leaf Area Index (LAI), root profile and nitrogen stress as well as the input data concerning irrigation requirements to ORCHIDEE that uses them to calculate carbon assimilation and allocation, water balance, and energy-related variables.

ORCHIDEE and STICS each have a large number of parameters involved at every step of a simulation over the course of a growing season. The values of these parameters - often empirically prescribed - are not easy to measure or are not measurable at all, calling in many cases for expert judgment to set their values, when it is impractical to find reference values. The uncertainty of these parameters is propagated onto the output variables of ORCHIDEE-STICS and has impacts on the output variables which strength depends on the structure of both STICS and ORCHIDEE. Because of the chain-type structure of ORCHIDEE-STICS (Fig. 3), the parameters from STICS that control LAI and nitrogen stress are expected to have a weaker and more indirect effect on downstream variables such as biomass compared with parameters from OR-CHIDEE that directly control carbon assimilation processes and the development of biomass to produce yield at the date of harvest.

**GMDD** 

7, 1197–1244, 2014

Modeling sugar cane vield

A. Valade et al.

Title Page

**Abstract** Introduction

Conclusions References

**Figures** 

Full Screen / Esc

Back

Printer-friendly Version

The advantage of the Morris method is that it is computationally efficient and easy to implement and interpret. It is based on a one-at-a-time approach, in which only one parameter is changed between two runs, allowing for the calculation of a local partial derivative of the output variable with respect to the input parameter, called an elementary effect. The Morris method is considered to be a "global" screening method, because the algorithm is repeated several times to calculate the elementary effects of each parameter in several locations of the parameters space so that the average and standard deviation of all elementary effects associated with each parameter are representative of the behavior of this parameter in its whole range of variation. The results of the Morris screening algorithm can be represented by a 2-D plot of standard deviation vs. mean value of the elementary effects on the output variable (here harvested biomass) of each parameter. A parameter with a high mean elementary effect (called  $\mu$ , or  $\mu^*$  for mean of absolute values) is interpreted as a parameter with high influence on the output harvested biomass variable. A parameter with a high standard deviation of

GMDD

Paper

Discussion Paper

Discussion Paper

Discussion Pape

7, 1197-1244, 2014

Modeling sugar cane vield

A. Valade et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

la l

N.

4

**•** 

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



ut,

its elementary effects ( $\sigma$ ) is interpreted as inducing non-linearities in the model output, and/or as having interactions with other parameters.

Here, we apply the Morris method as implemented in the R "sensitivity" package (Pujol et al., 2013) using site-scale simulations of ORCHIDEE STICS across the 7 field trial sites listed in Table 1. For each site, we identify the most influential parameters for the output variable harvested biomass. The parameters identified as important at least at two sites are selected for the rest of the study.

### 2.4 Uncertainty analysis (UA)

The goal of the UA is to quantify the overall uncertainty in the harvested biomass output variable that results from uncertain input parameter values. Firstly, based on the a priori probability of each parameter's value, a Probability Density Function is assigned to each parameter in order to generate sample parameter sets according to the Latin Hypercube Sampling (LHS) method. Secondly, an ensemble of model runs is performed using those samples. Thirdly, the uncertainty on the output variables is obtained from the statistical properties of the distribution of simulated harvested biomass from the ensemble runs by defining the uncertainty as the 1- $\sigma$  standard deviation of the distribution.

The first step is thus to generate parameters samples constrained with prior parameters ranges and statistical distributions that are then used as inputs for ensemble simulations.

The parameters considered for the uncertainty (UA) for both STICS and ORCHIDEE are those selected by the screening analysis, allowing a reduction in the parameters space hypercube dimensionality and therefore in the required computing resources. Starting from the initial set of 17 and 50 parameters respectively for the screening of ORCHIDEE and STICS parameters, the Morris algorithm result (see Sect. 3.1) allows us to reduce the parameter numbers to 8 and 3 parameters for ORCHIDEE and STICS, respectively.

**GMDD** 

7, 1197–1244, 2014

Modeling sugar cane vield

A. Valade et al.

Title Page

Abstract Introduction

Conclusions References

Tables Figures

l∢ ⊳l

→

Back Close

Full Screen / Esc

Printer-friendly Version



Discussion



For the UA, we use Monte-Carlo methods, which are less computationally expensive than variance-based approaches (Marino et al., 2008), making them a frequent choice in environmental sciences (Poulter et al., 2010; Verbeeck et al., 2006; Zaehle et al., 2005). The Monte-Carlo sampling scheme used here is the stratified Latin Hypercube Sampling (LHS), which is an efficient scheme for generation of multivariate samples of statistical distributions (McKay et al., 1979). In LHS, the range of each of the k parameters  $X_1, X_2, \dots X_k$  included in the study is divided into N intervals of equal probability. One value is randomly selected from each interval. The N values obtained for the  $X_1$  parameter are then paired at random, without replacement, with the N values obtained for the  $X_2$  parameter, then to the N values obtained for the  $X_3$  parameter and so on until the kth parameter. The procedure results in N sets of k parameters, or samples, that can be used for input to the model. In this study, from the 11 parameters identified by the screening, N is set to 250 resulting in 250 simulations for exploring the uncertainty around modeled biomass for each site.

In order to get insights on the part of the uncertainty attributable to each of the two models chained together, STICS and ORCHIDEE (Fig. 1), first, only the uncertainty coming from ORCHIDEE parameters is evaluated (Fig. 1), secondly, only the uncertainty propagated from STICS parameters (Fig. 1), and last, uncertainties propagated from both ORCHIDEE and STICS parameters are considered together through the chained model ORCHIDEE-STICS.

An important difficulty in the utilization of sampling-based UA methods is the lack of literature about a priori probability distribution of most parameters, given the dependency of output upon a priori assigned values (Marino et al., 2008). If most studies rely on a thorough literature search and expert judgment (Medlyn et al., 2005; Verbeeck et al., 2006; Wang et al., 2005), this approach might result in an overestimation of the model output uncertainty due to combinations of extreme parameters values that are not realistic and therefore excessively decrease the estimated reliability of the models. Some studies have addressed this issue by trying to rationalize the parameters ranges through benchmarking outputs (removing parameter sets resulting in values for

**GMDD** 

7, 1197–1244, 2014

Modeling sugar cane vield

A. Valade et al.

Title Page Introduction **Abstract** 

Conclusions References

**Figures** 

Back Full Screen / Esc

A. Valade et al.

Title Page **Abstract** Introduction

**GMDD** 

7, 1197–1244, 2014

Modeling sugar cane

vield

Conclusions References

**Figures** 

Back

Full Screen / Esc

**Printer-friendly Version** 

Interactive Discussion



output variables outside of a given benchmark range) or by prescribing hypothesized correlations between parameters (Poulter et al., 2010; Zaehle et al., 2005). Here, after a first estimation of uncertainty based on expert opinion for the a priori parameters range (overestimation of uncertainty), we propose a second approach to overcome the scarcity of information about parameters reference distributions by reducing the parameters a priori range based on site-optimized values, thus providing narrower and more realistic a priori ranges that are constrained by observations (likely underestimation of uncertainty).

For the first a priori estimation of parameters range, ranges and distributions are assigned to parameters based on expert knowledge and previous parameterization studies (Kuppel et al., 2012) and centered on their a priori values. The a priori ranges prescribed using this approach are considered as overestimations of the likely ranges for parameters' values for sugar cane because they are adapted from studies in which parameters' ranges were assigned for plant functional types instead of a single crop as is the case here and sometimes used for optimization studies therefore requiring wide enough ranges within the model's domain of applicability (Groenendijk et al., 2011; Kuppel et al., 2012). By using overestimated ranges for input parameters, we estimate an upper bound for the value of the uncertainty on output variables.

The second (site-constrained) a priori estimation is a refinement of the uncertainty estimation based on the idea that the "real" probability distribution of the parameters can be approached by the distribution of optimal parameters over all the possible case studies (sites, weather, management). It is of course not possible to determine the model's optimal parameters for an infinite number of eco-climatic and land-management conditions, but a sample of representative case studies can provide a rough estimate of the parameters plausible range. Building on this hypothesis, the model is calibrated independently at 7 sites using an iterative method, seeking to constrain the uncertainty analysis with observation-based parameters ranges. For this, we performed a Bayesian calibration of the model parameters, using a standard variationnal method based on the iterative minimization of a cost function that measures both

the model data misfit as well as the parameters' deviations from a prior knowledge. The iterative scheme is described in (Tarantola, 1987) with the hypothesis of Gaussian error on the observations and the parameters. At each site, parameter values are varied iteratively until the best match between simulation and observation is found. More details on the calibration results can be found in the Supporting Information. We are aware that the optimization of the parameters at 7 sites only to obtain a representative a priori range of the parameters distributions likely results into an optimistic estimate of this range even though the sites chosen cover different climatic, edaphic and management conditions making them well suited for applying our method.

For both a priori parameters range estimations (expert judgment vs. site constrained), when no parameter value appears to be more likely than another, a uniform a priori uncertainty distribution is prescribed. When there is some level of confidence that the a priori value is more likely, we use a beta distribution. This type of distribution is often used for uncertainty analyses, because of its adjustable shape (parameterized equation) yet having the advantage of bounded tails (Monod et al., 2006; Wyss and Jorgensen, 1998). The successive analysis of both techniques provides an improvement in the estimation of the uncertainty from the first (expert-judgment based, likely too pessimistic) to the second (observation-based, perhaps too optimistic) approach.

### 2.5 Spatial sensitivity analysis (SA)

The first step in the sensitivity analysis also consists in generating parameters samples. The same parameters are considered for the SA as for the UA (Sect. 2.4), i.e. the 11 parameters (8 parameters from ORCHIDEE and 3 parameters from STICS) selected by the screening analysis.

As opposed to the UA where all parameters are considered together for their effect on the distribution of the harvested biomass output variable, the goal of the sensitivity analysis is to rank the influence of parameters based on their impact on the biomass and its spatial distribution obtained in the continental-scale 0.5° runs. The partial correlation coefficient (PCC) measures the correlation between an output variable and

GMDD

7, 1197–1244, 2014

Modeling sugar cane vield

A. Valade et al.

Title Page

Abstract Introduction

Conclusions References

Tables Figures

l∢ ⊳l

. →

Back Close

Full Screen / Esc

Printer-friendly Version



Interactive Discussion



a parameter after the correlation with other parameters has been eliminated (Marino et al., 2008). However, for monotonic but non-linear relationships, these measures perform poorly and a rank transformation needs to be applied to the data first to linearize the relationship. The correlation calculated between the rank-transformed data is then called partial rank correlation coefficients (PRCC). PRCC has been found to be an efficient indicator for the influence of parameters, because it is a measure of the sensitivity of the output to parameters (Saltelli and Marivoet, 1990) The larger the PRCC, the more important the parameter is with respect to the output variable. Here, the relationship between modeled biomass on a grid, and parameters is diagnosed through the calculation of the Partial Ranked Correlation Coefficients (PRCC) on each grid point between the output and parameter assuming a monotonic behavior of the model.

The SA is implemented from the results of the 0.7° simulations over Brazil and Australia (see Fig. 1 and Sect. 3.5). In this regional sensitivity analysis, ORCHIDEE-STICS is run for each region on a grid of 20 by 15 grid points and 13 by 20 grid points respectively, driven by gridded climate forcing fields from the reanalysis products ERA-Interim (Dee et al., 2011), with varying parameter values from a sampling where only bounds and no distributions were assigned to the parameters. The management information (date of planting, date of harvest, fertilization, irrigation) and the soil properties (as described in Valade et al., 2013) are assumed to be uniform across each region and were defined as typical of each area. The a priori bounds used for the parameters in the SA correspond to the first version of the parameters ranges considered in the uncertainty analysis (i.e. derived from expert knowledge). As cited by Wang et al. (2005), for sensitivity analyses, Bouman (1994) advises to use parameters ranges as broad as possible within the limits of the model validity domain. Once the parameters' a priori bounds have been set, ensemble runs are performed with all the parameter sets. From the distributions of input parameters and output variables obtained at each pixel, a spatial distribution of PRCC is obtained, which is interpreted in Sect. 3.5 in terms of regional differences of each parameter on modeled sugar cane yield.

**GMDD** 

7, 1197–1244, 2014

Modeling sugar cane vield

A. Valade et al.

Title Page **Abstract** Introduction

Conclusions References

**Figures** 

Back

Printer-friendly Version

### **GMDD** 7, 1197–1244, 2014

### Modeling sugar cane vield

A. Valade et al.

### Title Page Introduction **Abstract** Conclusions References **Figures** Back Full Screen / Esc

**Printer-friendly Version** 

# Interactive Discussion

The interest of carrying out such a regional sensitivity analysis is that it provides maps of the geographic patterns of the importance of each parameter, leading to a better comprehension of the mechanisms behind the parameter-related model sensitivity. These results can be very useful for planning purposes, for instance to quantify 5 what are the different factors that control sugar cane yield and ethanol production over a large region under future climatic conditions as compared to present-day conditions.

#### Results and discussion

### Screening

From the Morris screening method, we obtain for each parameter two indices  $\mu^*$  and σ, that measure the influence of each parameter and its degree of involvement in nonlinearities and interactions with other parameters, respectively. From  $\mu^*$  and  $\sigma$  values, we establish a ranking of the parameters by only considering parameters involved in limited interactions and/or non-linearities ( $\sigma < 2\mu^*$ ) and then we rank the remaining parameters based on their  $\mu^*$  index, a larger  $\mu^*$  being interpreted as a more influential parameter. The Morris parameters ranks for ORCHIDEE and STICS are respectively shown in Fig. 5a and b where each radar plot corresponds to one model. The axes refer to the parameters and the line colors to the sites. For STICS, for the sake of readability, not all of the initially selected 50 parameters are represented on the radar plot but only those parameters that pertain to the 10 top-ranked parameters at least at one site. The maximum number of 10 parameters was fixed based on examination of Morris indices  $\mu^*$  and  $\sigma$  at individual sites that only revealed 3 to 5 sensitive parameters each time. The positions and roles in the model of the parameters identified as most important are shown in Fig. 3. Figure 4 gives more details, with the main equations through which these parameters affect the output variables of STICS and of ORCHIDEE.

The 3 most influential parameters of STICS (Fig. 3a) reflect the way STICS and OR-CHIDEE are chained (Fig. 3). Indeed, from the chained model structure, the indirect



impact of STICS parameters on harvested biomass occurs through their effect on processes related to LAI, root growth and nitrogen stress, the only STICS variables passed to ORCHIDEE for calculating biomass. This chaining of the models through three variables is reflected in the identification of the 3 most important STICS parameters, which control the daily maximum rate of foliage production  $\delta_{\rm IAI}^{\rm max}$ , the growth rate of the root front,  $\kappa_{\text{root}}$  and the threshold of nitrogen nutrition index INN<sub>min</sub>.  $\delta_{\text{IAI}}^{\text{max}}$  and INN<sub>min</sub> parameters are both involved in LAI calculation. Indeed, the LAI equation has four members describing four processes of the sugar cane foliage development. First, the LAIdevelopment ( $\Delta_{LAL}^{dev}$  in Fig. 4) describes the potential LAI increase through the scaling of the daily maximum rate of foliage production by a function of the development stage  $(k_{\rm LAI})$ , and is logically directly controlled by the value of parameter  $\delta_{\rm LAI}^{\rm max}$ . The second member in the LAI defining equation in Fig. 4 represents the temperature effect on LAI growth through the accumulation of degrees above a temperature threshold ( $T_{min}$  in Fig. 3). The last two members of the equation represent processes that can limit LAI development and competition for light between plants due to planting density ( $\Delta_{I \Delta I}^{dens}$  in Fig. 4) and a limitation from trophic stress emerging from competition between plant components for nitrogen, based on the calculation of a nitrogen nutrition index limited by parameter INN<sub>min</sub>. The root growth rate  $\kappa_{root}$  has a less direct impact on LAI since it intervenes in the calculation of the root front depth, which then impacts the availability of nitrogen and water and therefore the stress status of the crop (impact on  $C_N^{\text{plant}}$  and  $W_{\rm s}$  in Fig. 4).

The 8 most influential parameters that control harvested biomass in ORCHIDEE, are identical for all sites except for the Colimaçons site (where only 7 parameters are identified as influential by the Morris method). The Morris top ranked parameters of ORCHIDEE control photosynthesis and water budget equations as well as respiration processes (Fig. 4). Three of those (the minimum and optimal temperatures for photosynthesis,  $T_{\min}$ ,  $T_{\text{opt}}$ , the maximum rate of carboxylation  $V_{\text{Cmax}}^{\text{opt}}$ ) affect directly the rate of carboxylation V<sub>c</sub> that is calculated from the maximum rate of carboxylation weighted by a mean leaf efficiency and scaled by a limiting factor depending on the optimum and

**GMDD** 

7, 1197–1244, 2014

Modeling sugar cane vield

A. Valade et al.

Title Page Introduction **Abstract** 

References

**Figures** 

Full Screen / Esc

Back

Paper

GMDD

7, 1197–1244, 2014

# Modeling sugar cane yield

A. Valade et al.

Full Screen / Esc

Back

Printer-friendly Version

Interactive Discussion



minimum temperatures for photosynthesis. The stomatal conductance  $g_s$  that links assimilation and transpiration is defined by the Ball–Berry equation (Ball et al., 1987) as a function of assimilation and depends on the air relative humidity and  $CO_2$  concentration, scaled by a slope factor, called the Ball–Berry slope ( $\beta$ ). The root profile constant ( $\kappa_{\text{hum}}$ ) describes the exponential distribution of root density in the soil and is involved in the definition of available water and root temperature. Finally, the extinction coefficient ( $\kappa_{\text{ext}}$ ) intervenes in an equation derived by Monsi and Saeki (1953), similar to Beer's law, which describes the attenuation of light with depth in the canopy.

Two ORCHIDEE parameters controlling autotrophic respiration also stand out, with the maintenance respiration coefficient ( $\alpha_{\rm Mresp}$ ) and the fraction of biomass allocated to growth respiration ( $f_{\rm Gresp}$ ). The leaf parameter that is involved in the biomass allocation also ranked high (5th most important) but only for one site and is therefore not retained for the rest of the study.

For the chained model STICS-ORCHIDEE, the 11 most influential parameters show a good agreement between sites for the most important parameters as seen on Fig. 5 where ranking lines overlap for most of the parameters. Building on the results of the Morris screening analysis, we select the 8 top ranked parameters for ORCHIDEE and 3 for STICS that were revealed as influential for biomass for further uncertainty and sensitivity analysis.

### 3.2 Uncertainty analysis: parameters controlling biomass uncertainty at a typical site

In this section, we attribute the harvested biomass uncertainty to the uncertainty of the ORCHIDEE vs. STICS parameters. The simulated biomass uncertainty is a function of time during the growing season, and it differs between sites. In Fig. 6, we show the contributions of ORCHIDEE and STICS parameters respectively to the total uncertainty for one typical site, Grafton, Australia, during the 1994–1995 growing season, which has climate conditions within the range of other sites. Figure 6a–c displays the

Interactive Discussion



normalized frequency distributions of simulated biomass obtained from ensemble runs for three times in the growing season: (1) very early in the cycle in Fig. 6a, at 100 days after planting (DAP), (2) during the peak growing season in Fig. 6b, at 200 DAP and (3) short before harvest in Fig. 6c, at 350 DAP. We distinguish between the normalized frequency distributions of simulated biomass when considering the uncertainty propagated from STICS parameters alone (green), ORCHIDEE parameters alone (yellow), and from ORCHIDEE and STICS parameters together (brown), along with their best-fit normal distributions overlaid. These distributions were obtained by Monte Carlo LHS ensemble runs (Sect. 2.4) with a sampling of parameters of STICS alone, ORCHIDEE alone and of both models together. We consider uncertainties starting from the time when biomass reaches 50 g C m<sup>-2</sup> in order to discard the emergence phase during which biomass is very low and uncertainties are therefore not significant.

At 100 DAP (Fig. 6a), the uncertainty distribution of biomass related to ORCHIDEE parameters U(O) spans a slightly larger range than the distribution related to STICS, U(S), and it has more extreme values. The U(O) distribution is symmetrical around the mean value, with a standard deviation of 86.9 g C m<sup>-2</sup>. The U(S) distribution is nonsymmetric, skewed towards larger values of biomass, and it has a slightly smaller standard deviation (76.5 g C m<sup>-2</sup>) than that of U(O). Combining U(O) and U(S) in Monte Carlo runs by varying the parameters of both models at the same time gives the total uncertainty distribution, U(O+S), shown in brown in Fig. 6. This distribution has more extreme values and a higher standard deviation (112.0 g C m<sup>-2</sup>), i.e. U(O + S) > U(O) + U(S).

At 200 DAP (Fig. 6b), and later at 350 DAP (Fig. 6c), the picture has changed. First, all uncertainties distributions are wider than at 100 DAP. Secondly, the means of U(O) and U(S) are no longer in agreement, with the asymmetric U(S) distribution being even more shifted towards high values of the harvested biomass. The reason for this shift is that among the variables transmitted from STICS to ORCHIDEE in the chain of models. the only one that can act to increase the biomass calculated by ORCHIDEE in the later phase of the growing season, near 350 DAP, is LAI. This is because a higher LAI will

**GMDD** 

7, 1197–1244, 2014

Modeling sugar cane vield

A. Valade et al.

Title Page **Abstract** Introduction

References Conclusions

**Figures** 

Back

Printer-friendly Version

**GMDD** 

7, 1197–1244, 2014

Modeling sugar cane vield

A. Valade et al.

Title Page

Introduction **Abstract** 

References

**Figures** 

Back

Full Screen / Esc

**Printer-friendly Version** 

Interactive Discussion



result into increased photosynthesis and therefore biomass in ORCHIDEE. However, passed a certain threshold, the LAI impact saturates when the foliage is sufficient for all incoming light to be captured, and therefore, uncertainty on the STICS parameters that impact LAI will not increase the uncertainty of biomass any longer. Unlike LAI, the nitrogen stress and root profile variables controlled by the parameters of STICS continue to act as limiting factors on biomass throughout the peak and late growing season. The saturation of the biomass uncertainty associated with STICS parameters is stronger at 200 DAP than at 300 DAP, when biomass increase has slowed down and the role of LAI for driving biomass is less important.

On Fig. 6d, the total uncertainty U(O + S) is given for the reference simulation (with parameters at their maximum likelihood values, red line) and the uncertainty on harvested biomass can be defined as a percentage of the harvested biomass in the reference simulation. For the Grafton site, at harvest, the overall uncertainty is 26.%. The relative contributions of ORCHIDEE and STICS to the total uncertainty,  $\alpha_0$  and  $\alpha_{\rm S}$  respectively, are defined by  $\alpha_{\rm O} = \frac{{\rm U(O)}}{{\rm U(O+S)}}, \ \alpha_{\rm S} = \frac{{\rm U(S)}}{{\rm U(O+S)}}$ . The evolution of these contributions to the total uncertainty is shown in Fig. 6e. We can see in this example that U(O) > U(S) during the entire growing season, but with a decrease of U(S), and an increase of U(O) such that the increase in biomass uncertainty seen on Fig. 6d becomes increasingly dominated by uncertain ORCHIDEE parameters. The progressive increase in the weight of ORCHIDEE parameters uncertainties is due to the reduction in the role played by LAI for biomass increase along the growing season. Indeed, if early in the season the foliage is crucial to allow photosynthesis and carbon allocation, later in the cycle, other processes become important as well and passed a certain LAI for which all incoming light is captured, it might not even play a role anymore and then the STICS parameters only impact biomass accumulation through nitrogen stress index and root depth.

Table 3 summarizes the results of the overall parametric uncertainty analysis at the 7 sites, including Grafton. The total uncertainty U(O+S) ranges between 25.5% of biomass at Piracicaba, Brazil during 2004–2005 and 44.26% of harvested biomass at Tirano, La Réunion in 1998–1999 yielding an average uncertainty on biomass at harvest due to uncertain parameter values of the chained model ORCHIDEE-STICS of 34.0% of harvested biomass across the 7 sites, in the order of previous results on different variables in similar studies using process-based models such as (Dufrêne et al., 2005) who found an uncertainty of 30% on modeled NEE for a forest sites in France with the CASTANEA model.

As for the ORCHIDEE vs. STICS relative contributions to the uncertainty of simulated biomass at all sites, the results at each site are not identical but display a similar general pattern shown by Fig. 7. For all sites, the ORCHIDEE parameters contribution to total uncertainty increases during the cycle, or remains approximately constant for Ingham in 1992–1993, and increases during the growing cycle to dominate entirely the total uncertainty at the end of the cycle compared to STICS parameters. The STICS contribution to overall uncertainty decreases during the growing season to reach a minimum by the end of the growing season. For sites Piracicaba during 2004–2005, Tirano in 1998-1999 and Colimaçons during 1994-95, during the beginning of the cycle the U(S) is even larger than U(O). The results for Ayr in 1991-1992 display a less clear pattern. Indeed, at the end of the cycle, the contributions of ORCHIDEE and STICS to the total uncertainty are almost equal, due to an increase in STICS contribution during the second half of the cycle. This result confirms a hypothesis made in Valade et al. (2013) where the difficult calibration of LAI at this site was attributed to the simulation by STICS of an important stress. Indeed if a large stress is simulated by the phenological module, this can impede ORCHIDEE processes of biomass growth and therefore increases the weight of STICS parameters with respect to ORCHIDEE ones.

GMDD

7, 1197–1244, 2014

Modeling sugar cane vield

A. Valade et al.

Title Page

Abstract Introduction

Discussion Paper

Discussion Paper

Discussion

Pape

Conclusions References

Tables Figures

I∢

→ -

Back Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



Optimizing the 11 ORCHIDEE-STICS parameters selected from the screening analysis at 7 sites leads to a reduction of the width of the a priori uncertainty distribution of the parameters (Table 2). Carrying out the same uncertainty analysis with a narrower uncertainty range of parameters (thanks to their site calibration) leads to an important reduction of uncertainties of biomass both for the STICS and ORCHIDEE components of uncertainty. This can be seen by comparing Fig. 6 (initial range of parameters) with Fig. 8 (narrower range after parameters calibration at the sites). For site Grafton during 1994–1995 for example, U(O+S) gets reduced from 26% to 17% of the reference harvested biomass, U(O) from 24% to 15% and U(S) from 14% to 10%. Figure 9 and Table 3 (bottom section) show the uncertainty contributions and overall uncertainty estimates for the 7 sites after observation-based reduction of the a priori uncertainty on parameters. The overall parametric uncertainty of biomass defined as the 1-sigma standard deviation of the (O+S) distribution has thus been reduced to 21% in average, to 11.48% when attributed to STICS alone, and to 17.15% when attributed to ORCHIDEE alone, (Table 3).

The ORCHIDEE and STICS contributions to the total uncertainty keep the same general pattern as with the initial parameters uncertainty distribution, with a domination of ORCHIDEE parameters in the uncertainty towards the end of the growing season (Fig. 9). Compared with the first uncertainty budget with expert-based parameters uncertainties (Fig. 8), there is generally a slight decrease in the STICS contribution at the end of the season.

We have thus established full uncertainty budgets for the two components of the ORCHIDEE-STICS chain of models, which has revealed variations in the uncertainty in the biomass simulation from site to site. The next step is to discriminate between the different parameters the ones that contribute most to the overall uncertainty through a sensitivity analysis at regional scale.

GMDD

Paper

Discussion Paper

Discussion Paper

Discussion

Paper

7, 1197-1244, 2014

Modeling sugar cane vield

A. Valade et al.

Title Page

Abstract Introduction

Conclusions References

Tables Figures

l∢ ≯l

- →

Back Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



The overall parametric uncertainties have been quantified at 7 sites and attributed to either STICS or ORCHIDEE. The sensitivity analysis (SA) in this section will go a step further and leads to discriminate the different parameters that contribute to the spatial distribution of uncertainty over the two regions considered. This sensitivity analysis is performed at regional scale because from the previous section, we have seen that the uncertainty in the biomass simulation varies from site to site.

Ensemble runs at regional scale were realized over Brazil and Australia each with different value combinations for the 11 parameters previously selected through the Morris screening analysis (Table 1). The Partial Rank Correlation Coefficients (PRCC) were then calculated for each pixel in each of the two regions (see Sect. 2.5), and the SA results are discussed for two dates during the growing season, 200 and 350 days after planting (DAP). The SA results express the strength of the relationship between an uncertain parameter and the simulated biomass at harvest at each pixel. The statistical significance of the PRCC calculated for each grid cell is tested with the associated p values, and non-significant PRCC are removed (p value < 0.05). The first date 100 DAP examined for site scale UA studies (Sect. 2.3) is not shown here, because no statistical significance was found in the correlations between the parameters and the harvested biomass at 100 DAP. Then, the pixels statistically significant PRCC calculated for each parameter can be analyzed both in a geographical projection (latitude, longitude) (Figs. 11 and 12, columns 1–2 and 4–5) and in a (Temperature, Precipitation) climatic space projection (Figs. 11 and 12, columns 3 and 6). The regional sensitivity analysis thus carried out for sugar cane growing areas in Brazil and Australia shows the magnitude, spatial distribution and climatic dependency of the sensitivity of harvested biomass to the 11 parameters previously selected through the Morris screening analysis (Table 2).

GMDD

Paper

Discussion Paper

Discussion Paper

Discussion Paper

7, 1197–1244, 2014

Modeling sugar cane vield

A. Valade et al.

Title Page

Abstract Introduction

Conclusions References

Tables

Figures

I₫

►I

- ◀

•

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



Printer-friendly Version

Interactive Discussion



Across both regions in Brazil and Australia, we find that the sensitivity of biomass to the model parameters is not uniformly distributed. This means that the simulated yield depends on different parameters within different parts of the same region. This result shows that applying a model at one site to determine the most important parameters, and generalizing its conclusion across a region generates biased conclusions. Considering only the first most important parameter in each pixel (Fig. 10), we can see that early in the cycle (200 DAP, Fig. 10a) four parameters dominate the spatial distribution of the U(O + S) uncertainty of biomass at 200 DAP, both over Brazil and Australia. These parameters are three ORCHIDEE parameters involved in the photosynthesis process, the minimum and optimum temperature for photosynthesis  $T_{\min}$ ,  $T_{\rm opt}$ , and the maximum rate of carboxylation  $V_{\rm Cmax}^{\rm opt}$ , and one parameter from STICS  $\delta_{\text{IAI}}^{\text{max}}$ , defining the maximum rate of increase of LAI and only appearing in the Australian region. In Brazil, the parameter  $V_{\text{Cmax}}^{\text{opt}}$  is the first most important parameter for 93% of the area, whereas the optimum and minimum photosynthesis temperatures parameters only dominate in respectively 3 and 4% of the area. In Australia, the parameters' domination is more balanced with 37.5 % for each of  $V_{
m Cmax}^{
m opt}$  and  $\delta_{
m LAI}^{
m max}$  and 25 % for  $T_{\rm min}$ .

Later in the growing season (350 DAP, Fig. 10b), consistently with the results of the site-scale uncertainty analysis, the influence of the STICS parameters decreases until no STICS parameters appear any longer as a dominant parameter in any of the regions. At this later stage in the season, two parameters stand out as explaining most of the uncertainty in most pixels of both regions,  $V_{\rm Cmax}^{\rm opt}$  and  $T_{\rm min}$ . In Brazil,  $V_{\rm Cmax}^{\rm opt}$  is still the most sensitive parameter for most of the region, but  $T_{\mathrm{opt}}$  disappeared and the area dominated by  $T_{\min}$  expanded and now covers the cooler area of the southeast coastal zone. In Australia, the area dominated by  $V_{\rm Cmax}^{\rm opt}$  expanded into most of the region and now covers 83% of the area. In the coolest pixels, the soil-related parameters appear with the two root profile parameters from STICS and from ORCHIDEE,  $\kappa_{\rm root}$  and  $\kappa_{\rm hum}$ .

### **GMDD**

7, 1197–1244, 2014

### Modeling sugar cane vield

A. Valade et al.

Title Page Introduction **Abstract** References **Figures** 

Full Screen / Esc

Figures 11 and 12 focus on the values of the PRCC for each parameter as well as their spatial distribution. Their projection in a Temperature-Precipitation space for a given time (Fig. 11 for 200 DAP, Fig. 12 for 350 DAP) give more insights on the dependency of the sensitivity to the climatic conditions along the growing cycle. As an example, the sensitivity of the simulated biomass to  $T_{\rm opt}$  is highly sensitive to the average temperature of the location. At low-temperature sites, where temperature is a limiting factor for crop growth (below 17 °C), the PRCC is higher than 0.8, whereas at high-temperature sites (above 22 °C) the PRCC is below 0.3. Sites with temperatures above 25 °C do not even show significant correlations (grey symbols on the scatter plot).

For the parameter  $\kappa_{\text{hum}}$ , which describes the root profile of the cane (inverse of root depth), the dependency is most obvious on precipitation amount. For annual precipitations above 2500 mm, no significant correlation is found.

Comparing the regional sensitivities at two times in the growing season shows again the decrease in the importance of STICS parameters whereas all of most important ORCHIDEE parameters have larger RPCC than earlier in the season.

### 4 Concluding remarks

In the perspective of applying spatially explicit mechanistic vegetation models such as ORCHIDEE-STICS to biofuel yield simulations we have sought the quantification and understanding of parametric uncertainty propagation in the model, both at site level and at continental scale over two large regions, Australia and Brazil. For this, a rigorous analysis of the uncertainty budget of simulated sugar cane biomass has been established, using a step by step tracking of uncertainty in the model.

The main parameters from the two chain components of the model responsible for most of the uncertainty propagation have been identified through a Morris screening analysis. For the ORCHIDEE model, the most influential parameters are those involved in photosynthesis equations,  $T_{\min}$ ,  $T_{\text{opt}}$ ,  $V_{\text{Cmax}}^{\text{opt}}$ , the radiation interception parameter  $k_{\text{ext}}$ ,

GMDD

7, 1197–1244, 2014

Modeling sugar cane vield

A. Valade et al.

Title Page

Abstract Introduction

Conclusions References

Tables Figures

l∢ ⊳l

•

Back Close

Full Screen / Esc

Printer-friendly Version



Discussion

Interactive Discussion



the root profile constant  $\kappa_{\text{hum}}$ , the parameters for respiration, slope of the Ball-Berry relation  $\beta$ , maintenance and growth respiration parameters  $f_{\text{Gresp}}$  and  $\alpha_{\text{Mresp}}$  for the ORCHIDEE carbon, water and energy model. For the STICS model, the most influential parameters are those responsible for simulation of phenology, nitrogen and water stress, the parameters describing the maximum rate of carboxylation, the maximum growth rate of the root front and the threshold for nitrogen stress have been found to have the greatest role.

We used two approaches for estimating the total uncertainty propagated from the parameters into the model by assigning uncertainties on parameters with two methods, one "pessimistic", in which a priori parameter uncertainty bounds are set based on expert judgment, and one optimistic where smaller uncertainty are derived by an optimization of the model parameters at several sites and this providing a smaller arguably more realistic a priori uncertainty range.

We found that all these parameters together contribute to an overall uncertainty of 21 % on sugar cane biomass simulations with an agro-LSM model and that this amount is variable among sites with different climatic, edaphic and management situations. We also analyzed this uncertainty separately for each component of the model and found that whatever estimate chosen for the parameters uncertainty, by the end of the growing season, the uncertainty propagated from the phenology module STICS decreases and the overall uncertainty is almost totally explained by the ORCHIDEE uncertainty.

The overall origin of uncertainty has then been diagnosed in even more detail through a regional sensitivity analysis allowing the identification of the parameter for which harvested biomass is most sensitive for each pixel within regions of Australia and Brazil. We revealed a strong heterogeneity of the results based on climatic conditions and also variability in time that confirms the results of the uncertainty analysis, by showing a decrease in the importance of the STICS parameters along the growing season.

We believe that our results for the sugar cane crop simulated with the model ORCHIDEE-STICS are relevant to other agro-LSM with different crops. All these results prove the importance of establishing clear uncertainty budgets for highly parameterized

**GMDD** 

7, 1197–1244, 2014

Modeling sugar cane vield

A. Valade et al.

Title Page Introduction **Abstract** 

References

**Figures** 

Back

Full Screen / Esc

**GMDD** 7, 1197–1244, 2014

### Modeling sugar cane vield

A. Valade et al.

Title Page **Abstract** Introduction References **Figures** Back

Full Screen / Esc

**Printer-friendly Version** Interactive Discussion



models such as agro-LSM, especially when applying these models to answer questions related to political decisions such as biofuels burning topics.

As an example, combining our optimistic uncertainty estimation with the results from (Lapola et al., 2009) for irrigated sugar cane (obtained with the model LPJml, very sim-5 ilar to ORCHIDEE-STICS), we can evaluate the range assorted with their estimation of land requirements to fulfill the demand in ethanol in Brazil. They found a mean yield of 74.36 tha<sup>-1</sup>, and conclude that to fulfill government targets, the sugar cane areas would need to expand by 2.8 million hectares. With the hypothesis that our uncertainty calculation is applicable to the LPJml results, we can translate the potential mean production uncertainty as a range of (59–90 tha<sup>-1</sup>). The land requirements when including parameters uncertainty would then becomes (2.3-4 million ha), almost a 2 to 1 ratio. To go further in the application of this result, and assuming that sugar cane expansion results in deforestation through direct or indirect land use change, we can translate the land expansion of sugar cane for biofuels into carbon emissions from deforestation. Several estimates of carbon emissions associated with conversion of tropical forest to croplands have been published and their results span a large range revealing the large uncertainties in this area (BSI, 2008; Cederberg et al., 2011; Searchinger et al., 2008) Discussing the uncertainty on this estimate is beyond the scope of this paper so we will only consider the value from (Searchinger et al., 2008), of 604 t CO<sub>2</sub> eq ha<sup>-1</sup>. Using this conversion factor, the expansion of sugar cane calculated by (Lapola et al., 2009) would result in CO<sub>2</sub> eq emissions of 1.68 Gt CO<sub>2</sub> eq whereas including the parametric uncertainty of the model we obtain a range of 1.2 to 2.4 Gt CO<sub>2</sub> eg provoked by Brazilian government's ethanol targets with our calculation of uncertainty.

This quick application of our uncertainty calculation proves how important it is to consider the uncertainty when addressing issues aimed at decision-makers.

Supplementary material related to this article is available online at http://www.geosci-model-dev-discuss.net/7/1197/2014/ amdd-7-1197-2014-supplement.pdf.

### Modeling sugar cane vield

A. Valade et al.

- Title Page Abstract Introduction Conclusions References **Figures** 
  - Full Screen / Esc

Back

- Printer-friendly Version
- Interactive Discussion



the simulations and figures.

#### References

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GMDD

7, 1197–1244, 2014

Modeling sugar cane vield

A. Valade et al.

Title Page

- Abstract Introduction
- Conclusions References
  - nclusions
  - Tables Figures
  - I◀
- **→**
- Back Close
  Full Screen / Esc
- Printer-friendly Version
- Interactive Discussion
  - © O

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Printer-friendly Version

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Modeling sugar cane vield

A. Valade et al.

Title Page Introduction Abstract

References Conclusions

**Figures** 

Back

Full Screen / Esc

Discussion

Pape



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Title Page Introduction Abstract

Conclusions References

**Figures** 

Back

Printer-friendly Version

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Title Page Abstract Introduction Conclusions References

**Figures** 

Back

Printer-friendly Version

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Modeling sugar cane vield

A. Valade et al.

**Abstract** Introduction

Conclusions References

> **Tables Figures**

> I⋖ ►I

Back

Full Screen / Esc

Printer-friendly Version



**Table 1.** Description of climate and management for the sites used in this study in Australia (Ayr, Ingham, Grafton), Brazil (Piracicaba) and La Réunion (Colimaons, Tirano).

		Planting and harvest dates		Mean annual precipitation	Average temperature	irrigation	Fertilization
Australia	Ayr	19 Apr 1991	13 Aug 1992	964	23.4	irrigated	no
	Ayr	22 Apr 1992	13 Aug 1993	560	23.6	irrigated	yes
	Grafton	28 Sep 1994	19 Sep 1995	768	19.6	irrigated	yes
	Ingham	23 Jul 1992	21 Oct 1993	1294	24.2	irrigated	yes
Brazil	Piracicaba	29 Oct 2004	26 Sep 2005	1230	21.6	irrigated	
La Réunion	Colimacons	3 Aug 1994	1 Dec 1995	989.5	19	rainfed	yes
	Tirano	26 Nov 1998	26 Nov 1999	813	22.34	irrigated	yes

**GMDD** 

7, 1197–1244, 2014

# Modeling sugar cane yield

A. Valade et al.

Title Page

Abstract Introduction

Conclusions References

Tables Figures

l∢ ►l

▶

Close

Full Screen / Esc

Back

Printer-friendly Version



Discussion Paper

Discussion Paper

Discussion Paper

Printer-f

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**Table 2.** List of parameters from STICS and ORCHIDEE included in each step of the analysis with their ranges of variation. All listed parameters are considered for the screening analysis. Only parameters in bold are considered in the uncertainty and sensitivity analyses.

		expert jubased ra	udgment anges distribution	Uncertainty analysis	Observations constrained ranges
	STICS				
Water budget	psisto	5	15		
	psiturg	1	5		
	Hinitf1	11	22		
	Hinitf2	11	22		
	Hinitf3	10	21		
	Ninitf1	0	30		
	Ninitf2	0	30		
Initial conditions	Ninitf3	0	30		
	afpf	0.15	0.5		
	afruitpot	0.0015	0.2		
	allocamx	0.63	0.86		
	bfpf	1	10		
	coefb	0.0015	0.0815		
	dureefruit	2850	3000		
	efcroijuv	1.7	2.3		
	efcroirepro	2	6		
	efcroiveg	3.2	6		
	nboite	12	25		
	pgrainmaxi	1200	2000		
	ratiosen	0	1		
	remobil	0.728	0.92		
	sdrpnou	552.5	747.5		
	splaimin	0	0.3		
	stlevsenms	400	800		
	stpltger	50	200		
	teopt	15	34.4		
	teopt	35	50		
Biomass conversion	vitirazo	0.0085	0.0115		
	stamflax	1000	2100		
	stlevamf	50	400		
	stlevdrp	1000	1740		
	tdmax .	28	40		

### **GMDD**

7, 1197-1244, 2014

# Modeling sugar cane yield

A. Valade et al.

Title Page

Abstract Introduction

Conclusions References

Tables Figures

l∢ ⊳i

- ◆

Back Close

Full Screen / Esc

Printer-friendly Version

Table 2. Continued.

		expert jubased ra	udgment anges distribution	Uncertainty analysis	Observation ranges	is constrained
Development stages	tdmin	10	14			
Radiation interception	extin	0.424	0.699			
	adens	-1	-0.2			
	bdens	2	10			
	dlaimax	0.0002	0.0015	uniform	0.00022	0.0011
	sbv	127.5	172.5			
	tcmax	35	42			
	tcmin	10	14			
Foliage	tutressmin	0	1			
· ·	Norg	0.05	0.2			
Mineralization	tref	15	27			
	croirac	0	0.2	uniform	0.07	0.092
	zlabour	17	23			
	zpente	24	110			
Roots	zprlim	111	140			
Soil	epc3	5	60			
	absodrp	0	1			
Water/Nitrogen stress	INNmin	0	0.5	uniform	0.3	0.3
	ORCHIDEE					
	f_ fruit	0.05	0.5			
	lai_ max	3	9			
	leaf_ age_ crit	30	200			
	max_ Ito_ Isr	0.25	0.5			
	min_lto_lsr	0.05	0.24			
	R0	0.05	0.5			
Allocation	S0	0.05	0.5			
	ext coef	0.5	0.9	uniform	0.5	0.72
	gsslope	7	11	beta(2,2)	7.7	9.5
	tphoto_ max	30	45	( , ,		
	tphoto_ min_ c	12	19	uniform	12	16.7
	tphoto_ opt	24	36	uniform	24	36
Photosynthesis	vcmax opt	40	100	beta(2,2)	64	81.3
-,	frac_ growthresp	0.2	0.5	beta(2,2)	0.23	0.3
Respiration	maint_resp_slope1	0.08	0.16	beta(2,2)	0.11	0.12
Water budget	humcste	0.8	7.2	uniform	3.2	4.1

7, 1197-1244, 2014

# Modeling sugar cane yield

A. Valade et al.

•

Back Close

Full Screen / Esc

Printer-friendly Version



**Table 3.** Uncertainty associated with *STICS*, *ORCHIDEE*, or *ORCHIDEE* + *STICS* parameters uncertainties expressed as percentage of the reference harvested biomass for each site and for each of the two uncertainty analysis.

		Total Uncertainty (% of observed value)	ORCHIDEE Uncertainty (% of observed value)	STICS Uncertainty (% of observed value)
Expert-based parameters' uncertainties	Ayr 91–92	35.11	20.43	20.73
	Ayr 92–93	27.21	25.26	9.31
	Ingham 92-93	38.60	31.42	21.04
	Grafton 94-95	26.05	23.92	14.07
	Piracicaba 04-05	25.49	23.36	14.00
	Colimacons 94-95	41.21	41.87	18.61
	Tirano 98–99	44.26	36.80	30.61
Optimization-based parameters' uncertainties	Ayr 91–92	31.20	14.01	25.64
	Ayr 92–93	15.84	15.60	4.58
	Ingham 92-93	21.66	22.35	9.19
	Grafton 94-95	16.84	15.25	9.81
	Piracicaba 04-05	14.67	14.80	5.84
	Colimacons 94-95	21.31	20.01	10.28
	Tirano 98-99	22.26	18.06	15.03

**GMDD** 

7, 1197–1244, 2014

# Modeling sugar cane yield

A. Valade et al.

Title Page

Abstract Introduction

Conclusions References

Tables Figures

l∢ ⊳i

•

Back Close

Full Screen / Esc

Printer-friendly Version



Back

Interactive Discussion



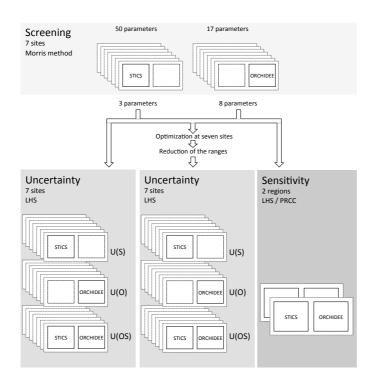


Fig. 1. Flowchart of the analysis carried out in this study. The first step is the separate screening for 7 sites of the STICS and ORCHIDEE parameters. The selection of parameters obtained from the screening are then used for two uncertainty analysis, one with the same parameters ranges of variation as for the screening, the other with parameters ranges of variation constrained by the optimization of the model at 7 sites. Each uncertainty analysis is decomposed in three parts, one including only ORCHIDEE parameters, one including only STICS parameters and one including parameters from both ORCHIDEE and STICS. Finally a sensitivity analysis is carried out for two small regions in Australia in Brazil for all parameters together.

**GMDD** 

7, 1197–1244, 2014

Modeling sugar cane vield

A. Valade et al.

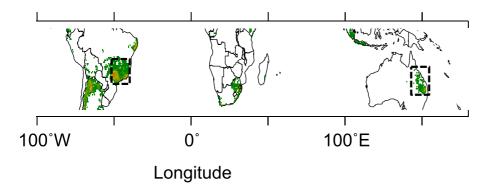
Title Page

Introduction **Abstract** 

References

**Figures** 

Printer-friendly Version



**Fig. 2.** Spatial distribution of the sites (dots) and regions (dashed rectangles) used in this study overlaid on a map of the distribution of sugar cane growing areas indicated in green.

**GMDD** 

7, 1197–1244, 2014

Modeling sugar cane yield

A. Valade et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

145100

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**■** 



Back



Full Screen / Esc

Printer-friendly Version



Discussion Paper

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



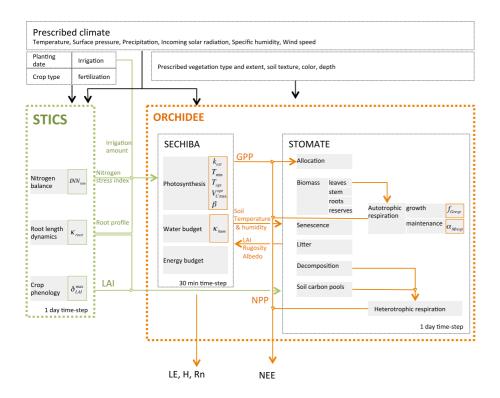


Fig. 3. Structure of the ORCHIDEE-STICS chain model. STICS calculates the crop phenology, water and nitrogen requirements and passes LAI, root profile, irrigation and Nitrogen nutrition index to ORCHIDEE. ORCHIDEE consists in the coupling of two module. SECHIBA simulates the photosynthesis process, water and energy budgets, STOMATE is a carbon module and calculates carbon fluxes and to the atmosphere (respiration) and carbon accumulation in the carbon pools (biomass compartments, litter, soil).

#### **GMDD**

7, 1197–1244, 2014

#### Modeling sugar cane vield

A. Valade et al.

Title Page

**Abstract** Introduction

References

**Figures** 

Back

Saeki, 1953)

(Krinner et al.,

al., 1996)

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$\Delta_{IAI}^{uv} \cdot \Delta_{IAI}^{v} \cdot \Delta_{IAI}^{uv} \cdot \Delta_{IAI}^{uv} \cdot \Delta_{IAI}^{uv}$ splai.dt		a	: Sowing density (pit.in )	
	(m. gemin to m. segren	$\alpha_{don}, \beta_{don}$	: Parameters describing competition from planting density(unitless, plt.m <sup>-2</sup> )	
$\alpha_{dem} \log \frac{d}{\beta_{dem}}$	$\Delta_{LAI}^{T} = \begin{cases} T_{crop} - T_{crop}^{\min} & \text{if } T_{crop} \leq T_{crop}^{\max} \\ T_{crop}^{\max} - T_{crop}^{\min} & \text{if } T_{crop} \geq T_{crop}^{\max} \end{cases}$	$T_{cnp}$ , $T_{cnp}^{min}$ , $T_{cnp}^{max}$	: Actual, minimum and maximum temperature for crop growth (°C)	
$\Delta_{LM}^{dens} = e^{-i \left(\beta_{dens}\right)} \cdot d$	$T_{cross}^{max} - T_{cross}^{min}$ if $T_{cross} \ge T_{cross}^{max}$	$k_{LM}$	: LAI development stage (unitless)	
		LAI	: Leaf area index (m <sup>2</sup> .m <sup>2</sup> )	(Brisson et al.,
	$\Delta_{LM}^{stress} = \min \left\{ INN = \max \left( \frac{C_N^{stess}}{C_N^{(r)}}, INN_{min} \right) \right\}$	$INN,W_s$	: Nitrogen nutrition index, water stress	2009)
$\Delta^{dev} = \frac{\delta_{LM}}{}$	$\Delta_{t,t}^{sress} = \min \left\{ \frac{HVV - Hax}{C_N^{crit}}, \frac{HVV}{min} \right\}$	$C_N^{orb}$ , $C_N^{pp}$	: Actual and critical nitrogen concentration in the plant (%)	
$\Delta_{LM} = \frac{1}{1 + e^{f(k_{LM})}}$	$\{W_i\}$	splai	: Stress index for competition between foliage and sugar accumulation (unitless)	
		of Dead	Charles and Control of the Control o	

: Air (soil for belowground compartments) temperature (°C)

Maintenance respiration (gC.m<sup>-2</sup> dt<sup>-1</sup>)

light: Light fraction that goes through the vegetation

#### $z_{max}^{of} = \int_{a}^{T} \kappa_{max} f_{AJ} \cdot pfz f_{max} \cdot dt$ $\kappa_{max}$ : root growth rate (Brisson et al. $f_{\Delta T}$ : Minimum temperature for emergence of the crop (°C) pfz : Water status of the soil layer (unitless) 2009) ORCHIDEE ker : extinction coefficient (unitless) $light = e^{-k_{co} L t t}$

 $LAI = \int_{0}^{T} \Delta_{LAI}^{der} \cdot \Delta_{LAI}^{T} \cdot \Delta_{LAI}^{dens} \cdot \Delta_{LAI}^{stress} .splai.dt$ 

 $Mresp = \frac{1}{\Delta t} \left( \sum_{i \neq loof} c_i \cdot B_i + c_{loof} \cdot B_{loof} \cdot \frac{0.3 \cdot LAI + 1.4 \left(1 - e^{-k \cdot LAI}\right)}{LAI} \right)$ 

 $\varepsilon = f(T \cdot T \cdot T)$ 

STICS

 $\delta_{i,i}^{max}$ : daily maximum increment

INN .... threshold for nitrogen nutrition index (unitless)

T<sub>min</sub> / T<sub>min</sub> : Minimum / Optimal

respiration coefficient (K1)

of LAI (m2 plt 1 deg day 1)

photosynthesis temperatures (°C)	$\varepsilon_{temp} = f\left(I_{air}, I_{min}, I_{cyc}\right)$	ε <sub>seep</sub> : Limitation of photosynthesis capacity by temperature	2005)
$V_{Cmax}^{sys}$ : Rate of carboxylation in optimal conditions ( $\mu$ mol·m <sup>-2</sup> ·s <sup>-1</sup> )	$V_{Cmax} = V_{Cmax}^{ops} \cdot \varepsilon_{ever} \cdot \varepsilon_{ever} \cdot \varepsilon_{linf}$	$V_{c_{\text{EMS}}}$ : Effective rate of carboxylation $(\mu\text{mol.m}^2 s^4)  \varepsilon_{seen}$ : Water and nitrogen limitation (unitless $\varepsilon_{seq}$ : Temperature limitation (unitless) $\varepsilon_{teq}$ : Limitation from leaf age (unitless)	(Ishida et al., 1999)
$\beta$ : Ball-Berry slope (unitless)	$\mathbf{g}_{s}=\beta\frac{h_{c}}{C_{s}}A+\mathbf{g}_{s}^{other}$	$\begin{array}{lll} g_s: & Sommala conductance (\mu mol.m^s s^t) & A & : Assimilation (\mu mol.m^s s^t) \\ h_s: & Air relative humidity (kg.kg^t) & g_s^{the}: & Offset constant (unitless) \\ C_s: & Air CO_s concentration (ppm) & & & & & & & & \\ \end{array}$	(Ball et al., 1987)
$\kappa_{\rm hm}$ : Root profile description (m $^{\circ}$ )	$\begin{split} T_{ij} &= \frac{1}{K_{ii}} + \sum_{i=1}^{n_{ii}} T_{i} \cdot \left( e^{-s_{ii} - c_{i,i}} - e^{-s_{ii} - c_{i}} \right) \\ f_{ii} &= \alpha_{iii} \cdot e^{-\alpha_{ii} - b_{ij}} + \left( 1 - \alpha_{iii} \right) \cdot e^{-s_{ii} - b_{ii}} \end{split}$	$T_{s_0} \qquad : \text{Temperature for below-ground biomass } (K) \\ K_{s_0} \qquad : \text{Integration constant (unitiess)} \\ n_0, z_0 \qquad : \text{Number of soil layers, depth of the $k$}^n \text{ soil layer (n)} \\ T_4 \qquad : \text{Soil temperature for $k$}^n \text{ layer } (K) \\ f_5 \qquad : \text{Water fraction available for the plant (unitiess)} \\ n_{s_0} \qquad : \text{Normalizing coefficient related to wetness of the top soil layer (unitiess)} \\ h_{s_0}, h_{teasts} \qquad : \text{Depth of dry soil in the top and bottom layers (m)} \\ }$	(Krinner et al., 2005)
$f_{Gresp}$ : fraction of GPP lost as growth respiration (dimensionless)	$Gresp = \frac{1}{\Delta t} \Big( f_{Grego} \cdot B_{attice} \Big)$	$\begin{array}{ll} \textit{Gresp} : \; \textit{Growth respiration} \; (gC \cdot m^1 \cdot df^4) \\ B_{\mathit{slw}} : \; \; \textit{Allocatable biomass} \; (gC \cdot m^2) \end{array}$	(Ruimy et al., 1996)
$\alpha_{Mesop}$ : slope of the dependance on temperature of maintenance	$c_i = \max \left[ \begin{matrix} 0 \\ c_i^o (1 + \alpha_{\mathit{Meep}} T_i) \end{matrix} \right]$	c, : Fraction of biomass lost as maintenance respiration for part i (unitless) c, <sup>0</sup> : Prescribed maintenance respiration coefficients at 0 Degree Celsius (unitless)  T : Air (coil for belowering comparing the propertiess (C))	(Krinner et al., 2005; Ruimy et

Fig. 4. Main parameters for simulation of sugar cane yield with ORCHIDEE-STICS with the equations in which they are involved.

**GMDD** 

7, 1197-1244, 2014

# Modeling sugar cane vield

A. Valade et al.

Title Page

**Abstract** 

Introduction

References

Figures

Back

Full Screen / Esc

**Printer-friendly Version** 



Full Screen / Esc

Printer-friendly Version

Interactive Discussion



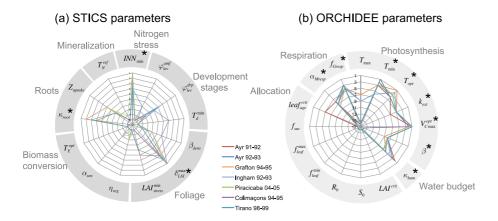


Fig. 5. Parameters rankings derived from the Morris screening analysis for STICS parameters (a) and ORCHIDEE parameters (b) for 7 sites (color lines). Each axis of the radar plot corresponds to the rank of a parameter, the lower the rank, the more important the parameter. The parameters identified as most important from this analysis are highlighted with stars.

**GMDD** 

7, 1197-1244, 2014

### Modeling sugar cane vield

A. Valade et al.

Title Page

**Abstract** 

Introduction

References

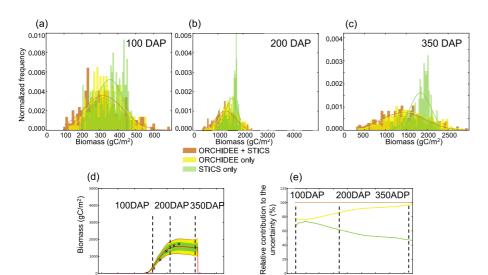
**Figures** 

**▶**I









**Fig. 6.** Uncertainty analysis for the site Grafton 94–95. **(a–c)** probability distributions of harvested biomass simulated after parameters uncertainty (from *STICS*:green, from *ORCHIDEE*: yellow, from *ORCHIDEE* + *STICS*: brown) has been propagated into the model. **(d)** reference simulation of harvested biomass (red) and uncertainty from *ORCHIDEE*, *STICS*, *ORCHIDEE* + *STICS*. **(e)** Contribution (%) of *ORCHIDEE* (yellow) and *STICS* (green) to the total uncertainty (brown) over the length of the growing season.

**GMDD** 

7, 1197-1244, 2014

Modeling sugar cane yield

A. Valade et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

▶I

4



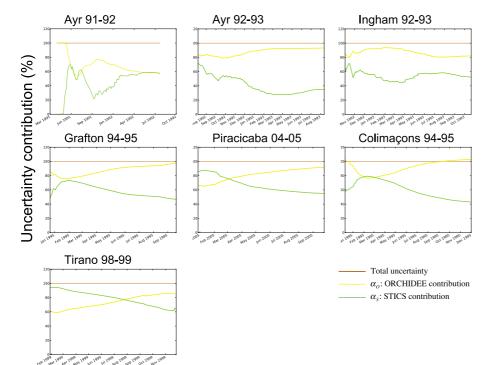
Back



Full Screen / Esc

**Printer-friendly Version** 





**Fig. 7.** Contribution (%) of *ORCHIDEE* (yellow) and *STICS* (green) to the total uncertainty (brown) over the length of the growing season for 7 sites.

**GMDD** 

7, 1197-1244, 2014

Modeling sugar cane yield

A. Valade et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

14

- ---

- 4

•

Back

Close

Full Screen / Esc

Printer-friendly Version





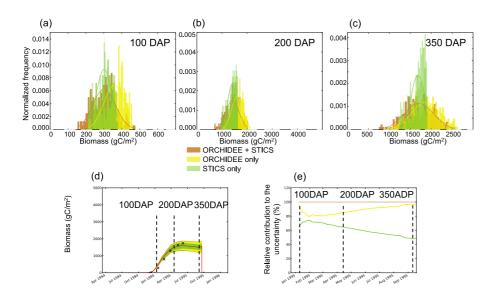


Fig. 8. Uncertainty analysis for the site Grafton 94–95 after parameters uncertainty ranges have been constrained through optimization at 7 sites. (a-c) Probability distributions of harvested biomass simulated after parameters un- certainty (from STICS: green, from ORCHIDEE: yellow, from ORCHIDEE + STICS: brown) has been propagated into the model. (d) Reference simulation of harvested biomass (red) and uncertainty from ORCHIDEE, STICS, OR-CHIDEE + STICS. (e) Contribution (%) of ORCHIDEE (yellow) and STICS (green) to the total uncertainty (brown) over the length of the growing season.

### **GMDD**

7, 1197–1244, 2014

#### Modeling sugar cane vield

A. Valade et al.

Title Page Introduction **Abstract** 

References

**Figures** 

Full Screen / Esc

Printer-friendly Version



Back

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



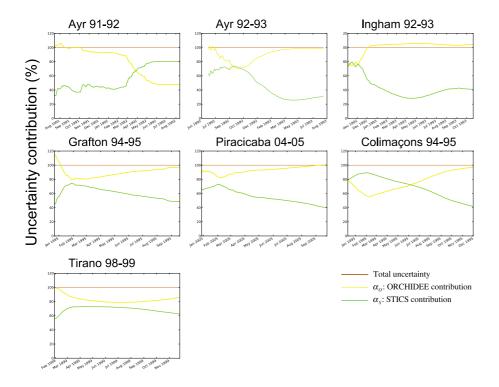


Fig. 9. Contribution (%) of ORCHIDEE (yellow) and STICS (green) to the total uncertainty (brown) over the length of the growing season for 7 sites after parameters uncertainty ranges have been constrained through optimization at 7 sites.

# **GMDD**

7, 1197-1244, 2014

## Modeling sugar cane yield

A. Valade et al.

Title Page

**Abstract** 

Introduction

Conclusions

References

**Tables** 

**Figures** 



Interactive Discussion



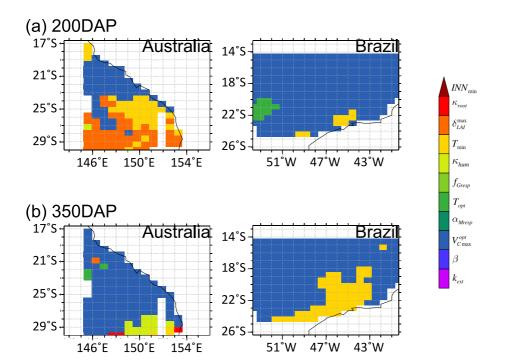


Fig. 10. Spatial distribution of the most influential parameters for the simulation of harvestable biomass for two milestones during the growing season, 200 days after planting (DAP) and 350 DAP.

# **GMDD**

7, 1197-1244, 2014

# Modeling sugar cane yield

A. Valade et al.

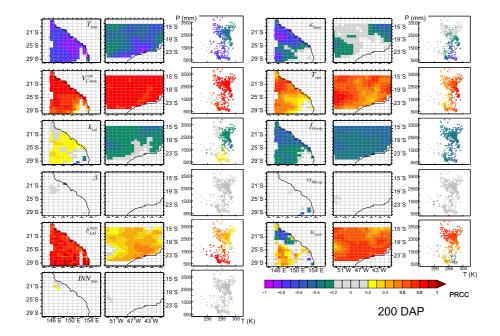
Title Page **Abstract** Introduction

References

**Tables Figures** 

Back

Printer-friendly Version



**Fig. 11.** Sensitivity of *ORCHIDEE-STICS* to its main parameters at 200 days after planting, as measured with Partial Ranked Correlation Coefficients (PRCC). The color indicates the strength of the relation between the parameter and the harvestable biomass, which is represented spatially (columns 1, 2, 4, 5) and in a (Temperature, Precipitation) referential (columns 3, 6). PRCC data points shown in grey are not statistically significant.

**GMDD** 

7, 1197-1244, 2014

Modeling sugar cane yield

A. Valade et al.

Title Page

Abstract Introduction

Conclusions References

Tables Figures

l∢ ≯l

Back Close

Full Screen / Esc

**Printer-friendly Version** 



7, 1197-1244, 2014

# Modeling sugar cane yield

**GMDD** 

A. Valade et al.



Printer-friendly Version



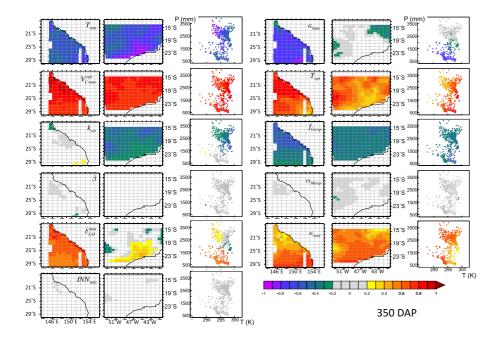


Fig. 12. Sensitivity of ORCHIDEE-STICS to its main parameters at 350 days after planting, as measured with Partial Ranked Correlation Coefficients (PRCC). The color indicates the strength of the relation between the parameter and the harvestable biomass, which is represented spatially (columns 1, 2, 4, 5) and in a (Temperature, Precipitation) referential (columns 3, 6). PRCC data points shown in grey are not statistically significant.