Sensitivity and uncertainty analysis of the carbon and water fluxes at tree scale in Eucalyptus plantations using a metamodeling approach

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Sensitivity and uncertainty analysis of the carbon and water fluxes at tree scale in *Eucalyptus* plantations using a metamodeling approach

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Abstract

Understanding the consequences of changes in climatic and biological drivers on tree carbon and water fluxes is essential in forestry. Using a metamodeling approach, sensitivity and uncertainty analyses were carried out for a tree scale model (MAESPA) to isolate the effects of climate, morphological and physiological traits, and inter-tree competition on the absorption of photosynthetically-active radiation (APAR), gross primary production (GPP), transpiration (TR), light use efficiency (LUE), and water use efficiency (WUE) in clonal *Eucalyptus* plantations. The metamodel predicting daily TR was validated using one year of sap flow measurements and showed close agreement with the measurements (mean percentage error = 11%, $n = 2155$). Simulations showed that APAR, GPP and TR were very sensitive to the tree morphology and to a competition index representing its local environment. LUE and WUE were, in addition, very sensitive to the natural variability of the physiological leaf and root parameters. A maximum percentage error of 10% in these parameters leads to a 18%, 17%, 16%, 9% and 18% uncertainty for APAR, GPP, TR, LUE and WUE, respectively. The uncertainties in TR were highest for the smallest trees. This study highlighted the need to take account of the spatial and temporal variability of tree traits and environmental conditions for simulations at tree scale.

**keywords**: meta-modeling; surrogate model; process-based model; MAESTRA; eucalypt;
Introduction

The variability of single-tree growth within a forest is the result of a complex interaction between many different factors, from genetics, through competition between trees, to climatic conditions. The local variability in tree functioning has implications at stand scale, and “perhaps the most fundamental question in forestry is why one tree grows faster than another” (Binkley et al. 2013). The resources (light, water and nutrients) available to individual trees will differ from tree to tree and vary with time as a result of competition with other plants and specific local conditions.

Process-based models (PBMs) are likely to become important tools in forestry as they are able to predict the response of trees to a range of conditions where empirical data are not available (Landsberg and Sands 2010). Nonetheless, PBMs are sometimes regarded as too complex to be used in forest management, requiring too many parameters (Bartelink and Mohren 2004). Natural and planted forest ecosystems present very variable local environmental conditions and tree characteristics: species, size, total leaf area, spatial distribution of leaves and many other traits. Some models simplify this local variability by assuming that the parameters and/or the functions within the stand canopy are uniform (Fontes et al. 2010; Hanson et al. 2004; Bukhart et al. 2012) to obtain simpler PBMs which can be used for forest management (e.g. 3-PG model, Landsberg and Waring 1997; CABALA, Battaglia et al. 2004; G'Day, Comins and McMurtrie 1993; Marsden et al. 2013) and whom complexity depends on the purpose and the scale of the study (Battaglia et al. 1998; Pretzsch et al. 2008). These simplified models are commonly used and have been shown to succeed in simulating light interception, gross primary production (GPP), ecosystem respiration, and evapotranspiration in many different types of forest (Hanson et al. 2004). However, they fail to simulate the local variability of tree functioning which is a key issue for predicting the growth of individual trees in non-uniform forests or to study the impact of forest management practices such as thinning (but see Makela et al. (2000) and Battaglia et al. (2015) for examples of modeling approaches where simple rules are used to disaggregate the stand-level outputs between individual trees). There are some very detailed 3D, structural-functional models that simulate the transpiration,
carbon budget and growth of each tree (and even each leaf) in a stand (Dauzat et al. 2001; Fernández et al. 2011; Griffon and de Coligny 2014), but they are computationally intensive, making long-term simulations difficult.

The computational efficiency of 3D PBMs can be improved by representing individual tree crowns as simple shapes such as ellipsoids or cones (e.g. MAESTRA model; Medlyn 2004; MAESPA model; Duursma and Medlyn 2012). Such models, however, require a larger set of parameters than stand scale PBMs, thus limiting their use in forestry. When input parameters are unknown, assumptions are often made to estimate their values. One standard approach is setting some tree scale parameters to values that are the same for all trees or values that do not vary with time. Such simplifications are likely to bias stand-scale simulations and to lead to considerable uncertainties at tree scale, thus representing a major issue for modeling forests at tree scale. A necessary step in any modeling study is, therefore, to estimate that part of the uncertainty (i.e. the possible error) of the model simulations, arising either from a lack of knowledge of parameter values or from deliberate simplifications (Smith 2013). Sensitivity and uncertainty analyses are accurate methods for identifying critical parameters that must be well described through time and/or space. Only those parameters that vary significantly in space and/or time and to which the model outputs are sensitive need to be taken into account in the model when simulating spatial and/or temporal variability (le Maire et al. 2005).

Previous sensitivity analyses of the tree scale MAESTRA model generally investigated local sensitivity and did not take the natural variability of the parameters into account (Bowden and Bauerle 2008), or were limited to a small number of physiological parameters (e.g. Bauerle and Bowden 2011). Some recent studies have shown the limitations of such local approaches, where the sensitivities of carbon and water fluxes to physiological parameters were strongly influenced by atmospheric CO₂ concentration or meteorological conditions such as light or temperature (Bauerle et al. 2014). The soil water balance was introduced in the new version of the model (MAESPA)
which affected many of the processes modeled and the previous sensitivity analysis for MAESTRA must, therefore, be confirmed and extended by taking into account the variability of both tree traits and meteorological conditions. Furthermore, so far as we are aware, no uncertainty analysis of the tree scale MAESPA model has yet been carried out. Such a study is, by definition, limited to the ecosystem where the model is applied. This study focused on tropical Eucalyptus plantations because the MAESTRA and MAESPA models have been used extensively in these planted forests (see the bibliography at http://maespa.github.io/bibliography.html), probably owing to the economic importance of eucalypts in tropical regions. Eucalyptus plantations cover more than 20 million hectares around the world and are expanding rapidly in tropical areas (Booth 2013).

The computational cost of complex PBMs is a serious constraint when carrying out global sensitivity analyses. A recent alternative approach is to build a metamodel (or surrogate model), which is a new computationally efficient model that gives almost the same results as the PBM but makes it easier to carry out sensitivity and uncertainty analyses (Faivre et al. 2013). The metamodel approach has recently started to be used in forest modeling to develop faster modules for light interception (Marie and Simioni 2014), biomass prediction (de-Miguel et al. 2014) or land use changes (Gilliams et al. 2005; Sieber et al. 2013.). In addition to facilitating sensitivity analysis, a metamodel of a tree scale PBM could give simple modules of carbon and water fluxes that are easier to couple with a tree scale allocation scheme for simulating individual tree growth.

Wood production is highly dependent on GPP, which is the amount of carbon assimilated by the trees. The dependence of GPP on incident radiation is usually represented by two factors: the amount of PAR absorbed by the tree (APAR) and the light use efficiency (LUE), which indicates how much absorbed light energy is required to produce carbohydrates and, consequently, GPP. GPP also depends on the amount of water used (transpired) by the trees (TR), through water use efficiency (WUE), defined here as the slope of the GPP / TR relationship. This study set out i) to explore the potential of simple metamodels as an easy means of predicting daily values for APAR,
GPP, TR, LUE and WUE at tree scale, ii) to use a metamodel approach to evaluate the sensitivity of the tree-scale MAESPA model outputs to the variability of inter-tree competition within a stand, and to meteorological, physiological and morphological drivers, and iii) to estimate the uncertainty of the simulations of GPP, TR, LUE and WUE at tree scale resulting from the uncertainty in the input parameters.

1. Materials and Methods

1.1. Study site and measurements

The site was a 90 ha *Eucalyptus* plantation located in southeastern Brazil (São Paulo State), at 22°58’04”S and 48°43’40”W, 750 MASL, and managed as part of the Euclux project (http://www.ipef.br/eucflux/en/). A highly productive *E. grandis* clone was planted in November 2009 at an average spacing of 3 meters between rows and 2 meters within each row (1666 trees ha⁻¹) using standard forestry practices for Brazilian commercial *Eucalyptus* plantations (Gonçalves et al. 2013). *Eucalyptus* plantations in Brazil, and particularly in this region, are among the most productive forests in the world (Nouvellon et al. 2012), and are generally harvested at 6 years of age. Four permanent plots of 84 trees were inventoried at ages 5, 6, 9, 12, 15, 18, 21, 25, 31 and 37 months to measure tree height (H) and diameter at breast height (DBH). Destructive sampling of 10 trees (taken from outside the permanent plots) at each date were carried out to determine the allometric relationship for tree leaf area (LA), crown radius (D_C) and crown height (H_C), following the methodology described in detail in le Maire et al. (2013). Leaf inclination angles (LIA) were measured at 1, 2 and 3 years after planting using a clinometer. At each age LIA was measured on 10 trees of different sizes (72 leaves per tree). Vertical leaf area density distribution was calculated using the leaf area in the bottom, medium and upper third of the crown, using destructive sampling. The horizontal leaf area distribution was measured as part of another experiment with the same *Eucalyptus* species (Christina et al. 2015). Photosynthesis parameters used in the MAESPA model were measured for 6 trees (A-Ci curves for estimating J_MAX, V_CMAX, R_d, as defined in Table. 2) or 3 trees (A-PAR curves for estimating α, θ, as defined in Table. 2) of different heights, using a
portable gas exchange system (LI-COR 6400, LI-COR Inc., Lincoln, NE, USA). For each tree these photosynthesis parameters were measured at different heights within the crown (bottom, medium and upper part of the crown) and for two horizontal positions within the crown (inner and outer part of the crown). Water content reflectometers (CS616, Campbell Scientific, Shepshed, UK) were used to measure the soil water content every meter down to 10m depth over the first 5 years after planting. Half-hourly meteorological data (Table 1) were collected at the top of an eddy-flux tower in the same stand as the 4 permanent plots, from January 2010 to December 2014.

1.2. **MAESPA presentation**

The MAESPA model (Duursma and Medlyn 2012) coupled the soil water balance components of the SPA model (Williams et al. 1996) to the MAESTRA model (Medlyn 2004), with some major changes and additions. MAESTRA was a 3D single-tree and stand process-based model that calculated light interception and distribution within crowns, and used a leaf physiology sub-model to estimate photosynthesis and transpiration. The 3D model for calculating APAR was based on Norman and Welles (1983) and is described in other studies (Medlyn 1998). The spatial position, crown dimension and total leaf area of each tree of the stand were fixed as inputs in the model. APAR was calculated for specified “target” trees in the stand, taking into account the neighboring trees competing for light. The crown was discretized in a 3D grid with a given number of horizontal layers and a given number of points per layer. For each point in the grid, the leaf area was defined using normalized beta-distributions. A single leaf inclination distribution was specified for all trees within the stand. At each grid point, after calculating the PAR absorption, photosynthesis and transpiration were calculated using a combined stomatal conductance / photosynthesis / transpiration model based on Farquhar et al. (1980) for CO₂ assimilation and Tuzet et al. (2003) for stomatal conductance. The APAR, GPP and TR were calculated for each target tree at a half-hourly time step. The water balance sub-model was derived largely from the SPA model (Williams et al. 1996). The soil profile comprised various horizontally uniform soil layers, with specific characteristics and root densities (no competition between trees). The water balance sub-model was
based on the water potential of the soil, roots, leaves and air, and on the hydraulic conductivities between these different compartments. The transpiration was calculated by combining two methods, the first based on the Penman-Monteith equation applied to small volumes of leaves, and the second one based on the equations computing the water flow from the soil to the leaves. The leaf water potential was estimated iteratively by matching these two calculations of the transpiration rate, and used to compute the stomatal conductance (Tuzet et al. 2003). The water content in each soil layer was calculated from the infiltration, drainage, root water uptake and soil evaporation at the same time-step as the above-ground processes (half-hourly). Except for the soil water content, there are no memory effects in the model.

1.3. Building first level metamodels of MAESPA for tree scale APAR, GPP, TR, LUE and WUE

For the global sensitivity and uncertainty analyses, metamodels for APAR, GPP, TR, LUE and WUE were set up as a first simplification of the computationally intensive MAESPA model. These metamodels were based on empirical formulae and simplified parameter sets. A flowchart of the method used to build these first level metamodels is given in Fig. 1A.

1.3.1. Setting up 1500 virtual random stands

A large number of realistic virtual stands are required for calibrating the MAESPA metamodels. These must cover the widest possible range of virtual stands with trees of different morphologies and physiologies. Different meteorological conditions representative of the climate also need to be selected. 1,500 Eucalyptus stands of 576 trees (24 rows*24 trees/row) were generated pseudo-randomly. It has been shown that a purely random sampling is not the most computationally efficient method cost for calibrating metamodels or for uncertainty and sensitivity analyses (Marino et al. 2008). Using stratified sampling is likely to provide more efficient coverage of the parameter space. Consequently, Latin Hypercube Sampling (LHS, Mckay et al. 2000) was used to provide an efficient distribution of parameter values with only 1,500 scenarios. For each scenario, the average
DBH within the stands and the morphological and physiological parameters at stand scale were estimated. The ranges used in the latin hypercube for the values of these parameters are shown in Tables 1 and 2. Once the average DBH had been estimated, a realistic virtual stand was built with the DBH of each tree in the virtual stand being determined using a random normal distribution and a competition index (CI, Hegyi 1974; Mailly et al. 2003). The method is described in section "Tree positions and DBH" of the supplementary material. The tree morphology (height, leaf area, etc) was then calculated from the DBH using allometric relationships. Each virtual plantation was associated with half-hourly meteorological parameters for a given day, randomly selected from 5 years of data, in order to use the real variability of the meteorological parameters and the correlation that often occurs between them within a day.

1.3.2. MAESPA simulations

MAESPA simulations were performed in each virtual stand for one day. Simulations were performed on one target tree chosen at random from the central part of the stand (16 rows*16 trees/row), discarding the external 4 rows of trees in each stand to avoid border effects. APAR, GPP, TR, LUE and WUE for that tree were calculated at half-hourly time-steps and cumulated over the day to give the daily total APAR, GPP, TR, LUE and WUE for 1,500 different trees in 1,500 different virtual stands.

1.3.3. Polynomial first level metamodels

The 1,500 simulations performed with the MAESPA metamodel were used to build metamodels for APAR, GPP, TR, LUE and WUE at a daily time step based on second order polynomial regressions (Barton and Meckesheimer 2006; Faivre et al. 2013). Two types of parameter were used to calibrate the metamodels: i) MAESPA input parameters, such as the leaf area or the photosynthetic capacity of the tree, and ii) simplified or aggregated MAESPA input parameters, such as the half-hourly meteorological input parameters, which were aggregated into average daily conditions. The parameters describing all the neighboring trees were reduced to Hegyi’s competition index (1974;
Mailly et al. 2003, see supplementary material). In total there were 37 parameters (Tables 1 & 2).

For example, for GPP the polynomial equation was:

\[
GPP(X) = \alpha_0 + \sum_{j=1}^{K} (\alpha_j X_j + \beta_j X_j^2) + \sum_{j=1}^{K} \sum_{k=j+1}^{K} \gamma_{jk} X_j X_k + \varepsilon, \varepsilon \sim N(0, \sigma^2)
\]

(1)

where \(X_j\) (or \(X_k\)) are one of the 37 parameters and \(\alpha_0, \alpha_j, \beta_j, \gamma_{jk}\) are the regression coefficients.

To limit the large number of possible two-way interactions between the 37 parameters, stepwise regression based on the Akaike information criterion (AIC) was used to remove non-significant interactions. Interactions were omitted if this did not significantly increase the AIC. For the particular case of APAR, the meta-model was built with only the parameter which had an influence on APAR in the model (competition index, morphological and meteorological parameters, as well as leaf transmittance and reflectance). The accuracy of the different first-level metamodels was evaluated through the R-squared (\(R^2\)) and the Root Mean Square Error (RMSE).

1.4. Global sensitivity analysis

The first level metamodels were accurate (see results) and could be used as substitutes for the MAESPA model for sensitivity analyses, considerably increasing the calculation speed. A global sensitivity analysis of the APAR, GPP, TR, LUE and WUE metamodels was performed using the Sobol approach (Sobol, 1993), which gives an estimate of the sensitivity based on the variance of the output. This time, 10,000 trees were randomly sampled from 10,000 different virtual stands built using the method described above (see section 1.3.1 and supplementary material). Taking the example of GPP, the main sensitivity index (\(S_i\)) of the \(i\)th parameter (\(X_i\)) for GPP was calculated as follows:

\[
S_i = \frac{\text{Var}(E(GPP|X_i))}{\text{Var}(GPP)}
\]

(2)
where the numerator is the variance of the expected GPP knowing the value of the parameter \(X_i\) and the denominator is the variance of GPP. This is the contribution of \(X_i\) to the GPP variance and represents the effect of varying \(X_i\) alone. A total sensitivity index \((ST_i)\) for each parameter was also calculated. \(ST_i\) was the sum of the main sensitivity index for parameter \(I\) and the sensitivity of the parameter \(i\) in interaction with all the other parameters. It was expressed as:

\[
ST_i = 1 - \frac{\text{Var}(E(GPP|X_{-i}))}{\text{Var}(GPP)}
\]

(3)

where the numerator is the effect of varying all parameters except \(X_i\). Consequently, the sensitivity of the interaction of parameter \(i\) with all the other parameters \((\text{Int}_i)\) was calculated as the difference between \(ST_i\) and \(S_i\). Sobol sensitivity indices for individual parameters were calculated with R.4.0 (Package sensitivity, function sobol2007 or sobol).

1.5. Local uncertainty analysis

1.5.1. Local uncertainty analysis for one particular tree

A local uncertainty analysis of the first level metamodels for APAR, GPP, TR, LUE and WUE was performed, for illustrative purposes, on one tree chosen from the tree database used in the global sensitivity analysis. The aim of the local uncertainty analysis was an estimation of the output error due to measurements uncertainty, and was therefore performed on little variations. It was possible that the values of the morphological, physiological and root parameters of this particular tree might be over- or under-estimated, leading to uncertainties on the model outputs. Note that the CI parameter of the model could also be over- or under-estimated, as a result of errors in the neighboring tree sizes and positions. Account was not taken of possible errors in meteorological variables in this analysis because they are difficult to quantify, and probably much smaller than the uncertainties on other parameters.

The uncertainty was expressed as the mean absolute percentage error for maximum error values from 0 to 10% with a 0.5 percentage point step to test the linearity of the relationship between model uncertainty and error in parameter values. For example, for a maximum error in the
parameters of ±5%, the value of each parameter varied in a uniform probability distribution from -5% to +5% around its initial value (the error could be zero). 5,000 simulations of the models were run with 5,000 scenarios using Latin hypercube sampling of the parameters between these 5% limits. The APAR, GPP, TR, LUE or WUE outputs were then compared with the simulations of the tree with all parameters set to their initial values (zero error). For a single tree \( i \) and a 5% maximum error, the mean absolute percentage error (MAPE\(_{\text{tree},5\%}\)) was calculated as follows (example for GPP):

\[
\text{MAPE}_{\text{GPP,\text{tree},5\%}} = \frac{1}{5000} \sum_{j=1}^{5000} \frac{|\text{GPP}_{\text{error,5\%,j}} - \text{GPP}_{\text{ini}}|}{\text{GPP}_{\text{ini}}}
\]  

(4)

where \( \text{GPP}_{\text{ini}} \) is the GPP simulation with the original set of parameter (no error) and \( \text{GPP}_{\text{error,5\%,j}} \) is the GPP for the \( j \)th scenario with maximum variations from -5% to +5%.

1.5.2. Generalization of the uncertainty analysis to trees of all ages

Because the uncertainty in APAR, GPP, TR, LUE and WUE may depend on the set of initial values of parameters selected, the uncertainty analysis for a single tree was repeated for 8 trees with different DBHs and then for all the 10,000 trees in the global sensitivity dataset, which covers trees from 6 months old to 3 years old. The median, 10\(^{th}\) and 90\(^{th}\) percentiles of the uncertainty is shown as a function of the maximum error in the parameters and as a function of DBH in Fig. 4.

1.6. Second level metamodel for TR and comparison with measurements

After the global sensitivity analysis, a second level metamodel for TR was built (Fig. 1B), by pruning the same parameter set than the first level meta-model. The aim was to include the least possible number of parameters in order to facilitate the presentation and the use of the metamodel, without adversely affecting the general performance. This metamodel was obtained by removing parameters that had a Sobol index less than 0.02 in the first level metamodel. Predictions from the second level metamodel for TR were compared with daily-averaged sap flow measured for individual trees over one year in another Eucalyptus grandis plantation. This second site was
located at 15 km from the Eucflux study site. The structure of this second plantation was comparable with the Eucflux site in terms of tree density and tree age (Christina et al. 2015). Sap flow was measured for 10 trees representing the whole range of DBH from January to December 2012. Every tree was equipped with a sensor protected from external temperature variations and water intrusion by a reflective foil. The sensor output voltage was recorded every 30 seconds and the average was stored every 30 minutes (CR1000 dataloggers and AM16/32 multiplexers, Campbell Scientific Inc., Logan, UT, USA). The sap flow density was calculated using a calibration equation taking into account the thermal dissipation of the sensors for *E. grandis* trees (Delgado-Rojas et al. 2010). The mean percentage error between the model predictions and the measurements were calculated for daily, weekly, monthly and annual time scales. For example, the daily mean percentage error for tree transpiration (MPE\(_{\text{TR,Day}}\)) was calculated as:

\[
MPE_{\text{TR,Day}} = \frac{1}{N} \sum_{i=1}^{N} \frac{TR_{\text{DaySim},i} - TR_{\text{DayMeas},i}}{TR_{\text{DayMeas},i}} \tag{5}
\]

where \(N\) is the number of trees, \(TR_{\text{DaySim},i}\) is the daily simulated transpiration of tree \(i\) and \(TR_{\text{DayMeas},i}\) is the daily measured transpiration of tree \(i\).

In addition, the measurements were compared to the MAESPA model predictions which had been precisely parameterized for this study site in a previous study (Christina et al. 2015).

### 2. Results

#### 2.1. Global sensitivity analysis of APAR, GPP, TR, LUE and WUE

The first level metamodels for APAR, GPP, TR, LUE and WUE reproduced MAESPA predictions accurately (Fig. 2). The best fits for metamodels were found for APAR (\(R^2 = 0.92\), RMSE = 12.6 MJ d\(^{-1}\) tree\(^{-1}\)) and GPP (\(R^2 = 0.91\), RMSE = 18.1 gC d\(^{-1}\) tree\(^{-1}\)), while the fit accuracy was lower for TR (\(R^2 = 0.84\), RMSE = 9.4 L\(_{\text{H}_2\text{O}}\) d\(^{-1}\) tree\(^{-1}\)), LUE (\(R^2 = 0.87\), RMSE = 0.20 gC MJ\(^{-1}\)) and WUE (\(R^2 = 0.77\), RMSE = 1.13 gC L\(_{\text{H}_2\text{O}}^{-1}\)).

APAR, GPP and TR were very sensitive to meteorological parameters (Fig. 3). In particular, APAR and GPP were sensitive to global radiation (RAD) and the beam fraction of radiation (\(F_{\text{BEAM}}\)).
was also sensitive to soil water content at the beginning of the day (SWC), air temperature (T_{AIR}) and relative humidity (RH). Moreover, tree APAR, GPP and TR were sensitive to morphological parameters such as tree leaf area (LA) and height (H), as well as the close environment of the tree (competition index CI). GPP was also sensitive to the parameters controlling the photosynthetic capacity of the leaves (J_{MAX}, V_{CMAX} and quantum yield \( \alpha \)). TR was highly sensitive to physiological parameters controlling the tree (K_{P}) and leaf (g_{0}, g_{1} and \( \Psi_{w} \)) conductivities, and to a lesser extent by the root mass density (RMD).

Tree light use efficiency (LUE) was highly sensitive to meteorological parameters, with a much higher sensitivity to F_{BEAM} and SWC than GPP. LUE was also highly sensitive to physiological parameters, in particular the minimum stomatal conductance (g_{0}), J_{MAX}, V_{CMAX}, \( \alpha \) and \( \theta \). LUE was less sensitive to morphological (LA, LIA, LAD_{V} and LAD_{H}) and root parameters (RMD and \( \theta_{R} \)). LUE was not strongly affected by CI, indicating that GPP was sensitive to CI through light absorption only.

Tree water use efficiency (WUE) was highly sensitive to many meteorological and physiological parameters. Some meteorological parameters also affected TR (SWC, RAD, T_{AIR}, F_{BEAM}), but unlike TR, WUE was also highly sensitive to relative air humidity (RH) and wind speed (Wind). WUE was highly sensitive to g_{0} and K_{P} as well as to interactions with J_{MAX}, V_{CMAX}, R_{d}, and Refl. WUE was also sensitive to root parameters such as RMD and \( \theta_{R} \) but insensitive to CI and morphological parameters.

2.2. Local uncertainty analysis of GPP, TR, LUE and WUE

The local uncertainty of the MAESPAMetamodel predictions resulting from errors in the input parameters varied between trees. A few examples of uncertainties for a few trees are given in Table 3. The uncertainty, expressed in mean absolute percentage error (MAPE_{tree}), depended on the initial values of the tree parameters. These examples show that the output uncertainty was strongly dependent on the tree being simulated. The variability in the uncertainties in the predicted values of
GPP, TR, LUE and WUE for 10,000 different trees depended on the output and the error in the parameters (Fig. 4A). With a maximum error in the parameters of 10%, the median MAPE\textsubscript{tree} was 18%, 17%, 16%, 8% and 18% for APAR, GPP, TR, LUE and WUE respectively with uncertainty values up to 40% for APAR, GPP, TR and WUE for certain trees (Fig. 4A). The uncertainty was linearly dependent on the error up to 10% maximum error.

The median uncertainty slightly increased with tree DBH for APAR, GPP and LUE simulations. It was independent of tree size for WUE (Fig. 4B). For TR, the median uncertainty slightly decreased with tree DBH, and the variability of the uncertainty was much higher for trees with a DBH less than 8cm.

### 2.3. Validation of the second level metamodel for TR

After removing parameters with low sensitivity indices, the second level metamodel used only 11 parameters. The sensitivity indices for these parameters are shown in Fig. 5A. Annual simulations of TR using this daily metamodel at tree scale over one year showed good agreement with the measured sap flow (Fig. 5B). The tree transpiration time series was well represented with a slight decrease during the dry season in the middle of the year. The accuracy of transpiration simulations depended on the simulation time scale (Fig. 5C). At daily time-scale, the average mean percentage error at tree scale (MPE) was 11%, with a strong variability depending on the tree simulated and the day. The MPE decreased as the time scale increased. The MPE for tree scale TR simulations fell to 9% for weekly and monthly simulations and 4% for annual simulations. The MAESPA model showed the same accuracy at daily time-scale (MPE 11%) but was slightly better for weekly and monthly simulations (MPE 6%) and annual simulations (MPE 2%).

### 3. Discussion

#### 3.1. Dealing with temporal and spatial parameter variability for tree scale modeling
3.1.1. Tree scale parameter variability

Unlike the traditional view of uniform *Eucalyptus* planted forests, this study highlights the need to take the local variability of the trees into account to give an accurate prediction of carbon and water fluxes at tree scale in monoclonal plantations. This local variability results from both inter-tree competition for resources (light, water and nutrients) as well as morphological tree traits. Competition between trees has been commonly used as an empirical indicator (e.g., for the effect of thinning, Forrester et al. 2013a) or a predictor (e.g. Vanclay 2006) of tree growth in *Eucalyptus* planted forests. This study showed that a competition index can be used in metamodels to replace and/or describe some processes of competition for light commonly used in PBMs. Carbon and water fluxes in this study were highly sensitive to Hegyi’s competition index (1974). This competition index reflects the effect of the size of the surrounding trees (based on their DBH), relative to the size of the target tree, as well as the effect of the distance from the target tree. Smaller trees of a stand are generally associated with a high competition index as observed in our *Eucalyptus* plantations (described in eq. S3). Many competition indices have been used in the literature. While distance-dependent indices are not always the best indicators of growth (e.g. Biging and Dobbertin 1995), they are generally useful proxies (Contreras et al. 2011). This dependence on the competition index emphasizes the importance of taking surrounding trees into account to predict carbon and water fluxes at tree scale, even in relatively uniform clonal *Eucalyptus* plantations.

Another component of the local variability that appeared important for predicting carbon and water fluxes was the variability of the crown architecture. For example, leaf inclination angles (LIA) and leaf area density had a significant effect on light use efficiency. Plants adapted to low light environments tend to have more horizontal leaves than those adapted to sunlight (Mc Millen and Mc Clendon 1979; King 1997). This behavior has been also observed in *Eucalyptus* plantations at the experimental site where suppressed trees had more horizontal leaves than dominant trees (data not shown). Similar behavior was observed within the tree crown where leaves at the bottom of the
crown were more horizontal than upper leaves (le Maire et al. 2011). The same attention should be
paid to parameters describing leaf distribution within the crown which might vary between clones
or sites (Alcorn et al. 2013).

While a simple indicator like the competition index may be sufficient for predicting tree growth in
empirical models or metamodels, it is important that certain morphological tree traits (in particular
tree height and leaf area), and the distance between trees, are accurately parameterized when
simulating the carbon and water fluxes in complex tree-scale PBMs such as MAESPA. Other
morphological tree traits do not require as much accuracy (e.g. crown height for predicting GPP in
this study). Dimensions of trees within planted forests are generally estimated through allometric
relationships (O’Brien et al. 1995) which are often associated with high uncertainties (Chave et al.
2014). Multiple allometric relationships calibrated for different ages and for different plots are
needed for tree-scale PBMs. Some previous studies of light use with the MAESTRA/MAESPA
model assumed a nominal position for trees within the stands (Christina et al. 2015; le Maire et al.
2013), while others estimated the tree position using in situ measurements, aerial photography or
very high resolution satellite images (Charbonnier et al. 2013; Forrester et al. 2013b; Gspaltl et al.
2013). The assumption of a regular spacing could bias the competition environment of the trees and
in consequence the prediction of carbon and water fluxes at tree scale.

3.1.2. Parameters set constant across the stand

This study highlights the importance of some parameters that are commonly held constant between
trees in PBMs for accurate predictions of carbon and water fluxes at tree scale.

Parameters controlling stomatal conductance and plant conductance had, as expected, a significant
effect on TR, WUE, and LUE. While high sensitivity to \( g_1 \) (the slope between the GPP and TR) as
shown by (Bauerle and Bowden 2011) was expected, the minimum stomatal conductance \( g_0 \) had a
greater effect on TR, LUE and WUE. The minimum stomatal conductance \( g_0 \) has commonly been
assumed to be close to zero with little effect on water fluxes (Caird et al. 2007; Zeppel et al. 2010).
However, recent studies have shown that $g_0$ could be higher than previously expected in many ecosystems (Ogle et al. 2012) and that its value could change seasonally (Barnard & Bauerle 2013). In a recent study using MAESTRA, it was shown that $g_0$ had a large effect on TR (Bowden and Bauerle 2008). Stomatal conductance is driven by $g_0$ or $g_1$ depending on the assimilation (A) conditions in the Ball-Berry type model of Tuzet et al. (2003) model ($gs = g_0 + g_1*A/Cs * f(\Psi_{leaf})$; where Cs is the CO$_2$ concentration at the stomata surface and $f(\Psi_{leaf})$ is a function of the leaf water potential). Bauerle et al. (2014) showed that the importance of $g_0$ depended on the meteorological conditions. For instance, TR was more sensitive to $g_0$ in low light (e.g. in canopies with a high LAI) than high light conditions. A lower sensitivity to $g_1$ and a higher sensitivity to $g_0$ have also been observed for red maple which has a higher LAI (Bauerle and Bowden 2011). In these low photosynthesis situations, $gs$ is mostly driven by $g_0$. The high sensitivity to $g_0$ in the Eucalyptus plantation in this study supports the conclusions of Barnard and Bauerle (2013) who stressed the necessity of measuring $g_0$ accurately. An estimate of $g_0$ using linear extrapolation from stomatal conductance model regression underestimated the minimum stomatal conductance by more than 50% compared to direct measurements.

This study showed that the photosynthetic parameters (within the range of values measured at the site) had little effect on TR. Photosynthetic parameters may affect $gs$, since assimilation is one of the parameters used to calculate $gs$ in the Ball-Berry model of stomatal conductance. Nevertheless, for conditions of low assimilation (A) (e.g. when the irradiance is low) or low $f(\Psi_{leaf})$ (when leaf water potential is low), $g_0$ dominates the $gs$ calculation. GPP, LUE, and to a lesser extent WUE, were, however, highly sensitive to $J_{MAX}$, $V_{CMAX}$ and quantum yield ($\alpha$). Bauerle et al. (2014) underlined that, in the Farquhar model, the sensitivity to photosynthetic parameters was dynamic in response to light and temperature changes owing to the transitory nature of light versus CO$_2$ limitations. In low light conditions, photochemical reactions (influenced by $J_{MAX}$ and $\alpha$) will limit photosynthesis. For strong light conditions, or under water stress (which decreases substomatal CO$_2$ concentrations as the stomata close), it is more likely that photosynthesis will be limited by the
carboxylation capacity. The influence of $\alpha$ seems rather more complex but evidence suggests that $\alpha$ could have a higher influence on photosynthesis than $J_{MAX}$ or $V_{CMAX}$ under low light conditions and high temperatures (Bauerle et al., 2014).

The fine root parameters also affected the predictions at tree scale even though they were constant across the stand. In the model, fine root biomass affect the water status of trees, affecting the leaf water potential and, consequently $f(\Psi_{\text{leaf}})$, stomatal conductance and WUE. Root parameters are very difficult to measure, and the use of typical values constant in time and space is generally assumed a priori. However, this study showed that fine roots have to be accurately measured to give reliable predictions of WUE. Moreover, although not having a great effect in the short term, long-term variations (as a result of tree growth) of root traits such as root distribution could result in large changes in carbon and water fluxes in *Eucalyptus* plantations.

3.1.3. Variability of meteorological parameters with time

The variability of meteorological parameters with time was a major factor driving APAR, GPP, TR, LUE and WUE predictions at tree scale. Meteorological parameters showed a high variability over the year owing to seasonal changes as well as day-to-day variability. Some of these parameters had the effects that were expected on carbon and water fluxes. This was the case, for example, for the effect of global radiation (RAD) on GPP and the effect of soil water content (SWC) on TR. The relative humidity (RH) had little effect on GPP and TR but a major effect on WUE. This is explained by the stomatal conductance which scales linearly with photosynthesis (depending on the atmospheric CO$_2$ concentration at the leaf surface) and the slope between them is strongly dependent on the relative humidity.

The beam fraction ($F_{BEAM}$) strongly affected carbon and water fluxes by decreasing LUE and WUE. This is recognized behavior in natural and planted forests. In boreal, temperate and tropical forests, Alton et al. (2007) showed that LUE increased from 6% to 33% when incoming global radiation
was dominated by diffuse light, and a similar trend was reported by Zhou et al. (2011) for temperate, subtropical and tropical forests in China. This is partly explained by the fact that the diffuse light tends to cause less saturation of photosynthesis in individual leaves in the canopy (Gu 2002; Charbonnier et al. 2013). \( F_{\text{BEAM}} \) affected GPP in this study but this effect was limited as, even though a lower \( F_{\text{BEAM}} \) tend to increase LUE, it is generally associated with a decrease in global radiation (RAD). The beam fraction of incoming light is often estimated using the approximation of Spitters et al. (1986) based on total incident global radiation (Forrester et al. 2013b; le Maire et al. 2013; Forrester and Albrecht 2014; Christina et al. 2015). The high sensitivity of the model to this parameter alone suggests that studies dealing with LUE should measure \( F_{\text{BEAM}} \) to high precision (e.g. Charbonnier et al. 2013) rather than approximating it.

3.2. The use of metamodels in forestry

This study developed a metamodeling approach for carrying out sensitivity analyses of complex, computationally intensive PBMs for trees. While such an approach has already been used with success in engineering disciplines and for energy analyses (Marrel et al. 2009; Tian 2013), it is not common in PBMs field of research, especially for sensitivity analysis purposes. In engineering studies the commonly used metamodels for sensitivity analysis use regression splines, smoothing operators or Gaussian processes (Tian 2013). This study showed that polynomial metamodels could be used as surrogates for complex tree scale PBMs for evaluating the sensitivity of carbon and water fluxes as well as the uncertainties.

One major objective of metamodeling is to obtain simple and parsimonious modules compared to the original PBMs. The second-level metamodel presented in this study gave accurate predictions of carbon and water fluxes at tree scale using far fewer parameters than the original MAESPA model, while keeping the interactions between them. For example, a complete parameterization of MAESPA would require ~200 parameters to fully parameterize 24 trees but the simple second level metamodel for TR required only 11 parameters because shading trees are summarized by the competition index. In the current study second level metamodels for APAR, GPP, LUE and WUE
were also created but were not presented in this article due to the unavailability of a proper validation dataset. Similarly to our second level metamodel, simple metamodels are generally built after removing parameters with low sensitivity and by using aggregated parameters (e.g. Lafond et al. 2015). The difference between our approach and the one of Lafond et al. (2015) is that they performed the sensitivity analysis on the original model and built a metamodel using the selected inputs, while we have built our first metamodel using almost all inputs of the original model and simplified it afterwards.

Metamodels are also often used as powerful tools to obtain surrogate models much faster than the original models. As an example, Marie and Simioni (2014) built a metamodel of the light interception module of a forest PBM (noTG) 62 times faster than the original model. But the use of metamodels is no limited to speeding-up a model, it could also be used for model coupling. For example, a metamodel for tree light interception could be coupled with tree scale PBMs which simulate growth of individual, rather than computing light interception at canopy scale (e.g. GOTILWA+ model, Keenan et al. 2008). Similarly, simple metamodels for tree light use efficiency could be coupled with tree scale PBMs of tree growth by using the light use efficiency as an input (e.g. PICUS model, Seidl et al. 2005). This approach combining models and metamodels has already been applied at stand scale. For example, Härkönen et al. (2010) and Härkönen et al. (2011) used a summary model of light use efficiency to estimate whole canopy GPP as a function of climatic conditions in various pine and spruce forests in Finland. Nevertheless, metamodels are usually only applicable to the species and parameter space for which they were calibrated. More general metamodels could be developed by increasing the parameter space, but their accuracy is more difficult to assess since they must be tested in many different types of forests and under many different climatic conditions.

Conclusion

Using metamodels for sensitivity analyses showed that carbon and water fluxes at tree scale in *Eucalyptus* plantations are controlled by key sets of parameters that were different for APAR, GPP,
TR, LUE and WUE. Uncertainty on the measurements of morphological, physiological and fine root parameters could cause a significant uncertainty on APAR, GPP, TR, LUE and WUE. This study showed that the natural variability of both tree traits and meteorological conditions must be taken into account in global sensitivity analyses. Moreover, metamodeling was shown to be a powerful method for future process-based modeling studies for forests, reducing the degree of complexity of the original model without significant loss of precision.

Acknowledgements

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References


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### Tables

Table 1. List of parameters used for constructing the MAESPA metamodels with their symbols and definitions, as well as the range of values and references. Part 1: competition, meteorological and morphological parameters.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description and units</th>
<th>Range of values</th>
<th>Source or details</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>CI</strong></td>
<td>Competition index (m², Heigy 1974)</td>
<td>3 to 8</td>
<td>Calculated based on tree density</td>
</tr>
<tr>
<td><strong>SWC</strong></td>
<td>Average soil water content at the beginning of the day (m³ m⁻³)</td>
<td>0.1 to 0.2</td>
<td>Taken from a 5-year dataset</td>
</tr>
<tr>
<td><strong>RAD</strong></td>
<td>Daily global radiation (W m⁻²)</td>
<td>18 to 370</td>
<td>&quot;</td>
</tr>
<tr>
<td><strong>T_AIR</strong></td>
<td>Daily average air temperature (°C)</td>
<td>10 to 27</td>
<td>&quot;</td>
</tr>
<tr>
<td><strong>RH</strong></td>
<td>Daily average relative humidity (%)</td>
<td>34 to 99</td>
<td>&quot;</td>
</tr>
<tr>
<td><strong>Press</strong></td>
<td>Daily average atmospheric pressure (kPa)</td>
<td>91.8 to 93.8</td>
<td>&quot;</td>
</tr>
<tr>
<td><strong>Wind</strong></td>
<td>Daily average wind speed (m s⁻¹)</td>
<td>0.3 to 6</td>
<td>&quot;</td>
</tr>
<tr>
<td><strong>F_BEAM</strong></td>
<td>Beam fraction of PAR</td>
<td>0 to 0.5</td>
<td>&quot;</td>
</tr>
<tr>
<td><strong>PPT</strong></td>
<td>Daily precipitation (mm d⁻¹)</td>
<td>0 to 124</td>
<td>&quot;</td>
</tr>
<tr>
<td><strong>DBH</strong></td>
<td>Diameter at breast height (cm)</td>
<td>4 to 18</td>
<td>This study</td>
</tr>
<tr>
<td><strong>H</strong></td>
<td>Tree height (m)</td>
<td>4 to 20</td>
<td>&quot;</td>
</tr>
<tr>
<td><strong>LA</strong></td>
<td>Tree leaf area (m²)</td>
<td>1 to 90</td>
<td>&quot;</td>
</tr>
<tr>
<td><strong>D_C</strong></td>
<td>Crown diameter (m)</td>
<td>2 to 5</td>
<td>&quot;</td>
</tr>
<tr>
<td><strong>H_C</strong></td>
<td>Crown height (m)</td>
<td>4 to 14</td>
<td>&quot;</td>
</tr>
<tr>
<td><strong>LIA</strong></td>
<td>Average leaf inclination angle (°)</td>
<td>20 to 80</td>
<td>li Maire et al. 2013; Christina et al. 2015; this study</td>
</tr>
<tr>
<td><strong>LAD_V</strong></td>
<td>Relative height within the crown of the maximum of vertical leaf area density</td>
<td>0.2 to 0.8</td>
<td>&quot;</td>
</tr>
<tr>
<td><strong>LAD_H</strong></td>
<td>Relative distance from trunk of the maximum of horizontal leaf area density bearing</td>
<td>0.2 to 0.7</td>
<td>&quot;</td>
</tr>
<tr>
<td></td>
<td>Bearing of the x-axis from south (°)</td>
<td>-180 to 180</td>
<td>This study</td>
</tr>
</tbody>
</table>
Table 2. List of parameters used for constructing the MAESPA metamodels with their symbols and definitions, as well as the range of values and references. Part 2: physiological and fine root parameters.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description and units</th>
<th>Range of values</th>
<th>Source or details</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Physiological parameters</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$g_0$</td>
<td>Minimum stomatal conductance (mol m$^{-2}$ s$^{-1}$)</td>
<td>0.01 to 0.08</td>
<td>Medlyn et al. 2007; Barnard and Bauerle 2013; Christina et al. 2015</td>
</tr>
<tr>
<td>$g_i$</td>
<td>Slope between stomatal conductance and photosynthesis (d.u.)</td>
<td>5 to 20</td>
<td>”</td>
</tr>
<tr>
<td>$S_f$</td>
<td>Slope of the response to leaf water potential (MPa$^{-1}$)</td>
<td>0.4 to 6</td>
<td>Tuzet et al. 2003</td>
</tr>
<tr>
<td>$\psi_W$</td>
<td>Reference water potential (MPa)</td>
<td>-1 to -3</td>
<td>”</td>
</tr>
<tr>
<td>$J_{\text{MAX}}$</td>
<td>Maximum rate of photosynthetic electron transport at 25°C (µmol m$^{-2}$ s$^{-1}$)</td>
<td>60 to 230</td>
<td>Grassi et al. 2002; Whitehead and Beadle 2004; Medlyn et al. 2007; Wullschleger 1993; Christina et al. 2015; this study</td>
</tr>
<tr>
<td>$V_{\text{CMAX}}$</td>
<td>Maximum rate of Rubisco carboxylase activity at 25°C (µmol m$^{-2}$ s$^{-1}$)</td>
<td>40 to 126</td>
<td>”</td>
</tr>
<tr>
<td>$R_d$</td>
<td>Dark respiration at 25°C (µmol m$^{-2}$ s$^{-1}$)</td>
<td>0.3 to 3</td>
<td>Grassi et al. 2002; Medlyn et al. 2007; Alcorn et al. 2008; Christina et al. 2015; this study</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>Quantum yield of electron transport (mol mol$^{-1}$)</td>
<td>0.2 to 0.4</td>
<td>Grassi et al. 2002; Medlyn et al. 2007; Christina et al. 2015; this study</td>
</tr>
<tr>
<td>$\theta$</td>
<td>Curvature parameter of the light response of photosynthesis (d.u.)</td>
<td>0.2 to 1</td>
<td>Grassi et al. 2002; Christina et al. 2015; this study</td>
</tr>
<tr>
<td>Trans</td>
<td>Leaf transmittance</td>
<td>0.01 to 0.1</td>
<td>Richards and Schmidt 2010; le Maire et al. 2013</td>
</tr>
<tr>
<td>Refl</td>
<td>Leaf reflectance</td>
<td>0.025 to 0.27</td>
<td>”</td>
</tr>
<tr>
<td>Wleaf</td>
<td>Leaf width (m)</td>
<td>0.02 to 0.06</td>
<td>Christina et al. 2015</td>
</tr>
<tr>
<td>$K_p$</td>
<td>Leaf-specific total plant conductivity (mmol m$^{-2}$ s$^{-1}$ MPa$^{-1}$)</td>
<td>0.2 to 3</td>
<td>”</td>
</tr>
<tr>
<td><strong>Fine root parameters</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$R_{\text{RAD}}$</td>
<td>Root radius (mm)</td>
<td>0.1 to 1</td>
<td>Christina et al. 2011; Christina et al. 2015</td>
</tr>
<tr>
<td>SRL</td>
<td>Specific root length (m g$^{-1}$)</td>
<td>5 to 80</td>
<td>”</td>
</tr>
<tr>
<td>RMD</td>
<td>Root mass density (g m$^{-2}$)</td>
<td>40 to 1100</td>
<td>”</td>
</tr>
<tr>
<td>$R_{\text{Depth}}$</td>
<td>Maximum root depth (m)</td>
<td>2.5 to 18</td>
<td>Christina et al. 2011</td>
</tr>
<tr>
<td>$R_{\text{Dis}}$</td>
<td>Root distribution using the beta parameter of Jackson et al. 1996</td>
<td>0.94 to 0.99</td>
<td>This study; Christina et al. 2011</td>
</tr>
<tr>
<td>$\theta_R$</td>
<td>Average residual SWC (m$^{-3}$ m$^{-3}$)</td>
<td>0.08 to 0.18</td>
<td>Marsden et al. 2013; Christina et al. 2015, this study</td>
</tr>
</tbody>
</table>
Table 3. Uncertainty in daily tree absorbed photosynthetically active radiation (APAR, MJ d\(^{-1}\) tree\(^{-1}\)), gross photosynthesis (GPP, gC d\(^{-1}\) tree\(^{-1}\)), transpiration (TR, LH2O d\(^{-1}\) tree\(^{-1}\)), light use efficiency (LUE, gC MJ\(^{-1}\)) and water use efficiency (WUE, gC L\(_{H2O}\)\(^{-1}\)) for 8 trees sampled with different diameters at breast height (DBH, as a proxy of tree age), for a ±5% or a ±10% maximum error on morphological, physiological and root parameters. The single-tree output value is given for zero error and the uncertainty is expressed as mean absolute percentage error (MAPE\(_{\text{tree,x\%}}\)).

<table>
<thead>
<tr>
<th>Tree DBH (cm)</th>
<th>APAR (MJ d(^{-1}) tree(^{-1}))</th>
<th>GPP (gC d(^{-1}) tree(^{-1}))</th>
<th>TR (L(_{H2O}) d(^{-1}) tree(^{-1}))</th>
<th>LUE (gC MJ(^{-1}))</th>
<th>WUE (gC L(_{H2O})(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>6</td>
<td>41 (±5%)</td>
<td>57.5 (±4%)</td>
<td>16.2 (±8%)</td>
<td>1.39 (±3%)</td>
<td>3.83 (±5%)</td>
</tr>
<tr>
<td>8</td>
<td>27 (±8%)</td>
<td>52.9 (±8%)</td>
<td>36.8 (±5%)</td>
<td>1.66 (±4%)</td>
<td>1.67 (±14%)</td>
</tr>
<tr>
<td>12</td>
<td>54 (±11%)</td>
<td>76.2 (±16%)</td>
<td>24.3 (±12%)</td>
<td>1.44 (±6%)</td>
<td>3.09 (±9%)</td>
</tr>
<tr>
<td>14</td>
<td>69 (±12%)</td>
<td>90.0 (±15%)</td>
<td>33.1 (±13%)</td>
<td>1.23 (±8%)</td>
<td>3.07 (±12%)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Tree DBH (cm)</th>
<th>APAR (MJ d(^{-1}) tree(^{-1}))</th>
<th>GPP (gC d(^{-1}) tree(^{-1}))</th>
<th>TR (L(_{H2O}) d(^{-1}) tree(^{-1}))</th>
<th>LUE (gC MJ(^{-1}))</th>
<th>WUE (gC L(_{H2O})(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>7</td>
<td>53 (±12%)</td>
<td>69.7 (±15%)</td>
<td>17.7 (±18%)</td>
<td>1.42 (±8%)</td>
<td>4.12 (±21%)</td>
</tr>
<tr>
<td>9</td>
<td>41 (±12%)</td>
<td>60.1 (±18%)</td>
<td>16.2 (±22%)</td>
<td>1.45 (±8%)</td>
<td>3.73 (±10%)</td>
</tr>
<tr>
<td>11</td>
<td>33 (±32%)</td>
<td>87.8 (±32%)</td>
<td>27.6 (±19%)</td>
<td>1.96 (±8%)</td>
<td>2.56 (±22%)</td>
</tr>
<tr>
<td>13</td>
<td>107 (±24%)</td>
<td>136.2 (±20%)</td>
<td>33.5 (±20%)</td>
<td>1.28 (±14%)</td>
<td>3.09 (±22%)</td>
</tr>
</tbody>
</table>
Figure legends

Fig. 1. Flowchart of the method used to build the MAESPA metamodels (A) and their use in the global sensitivity and uncertainty analysis (B). Separate first level metamodels were built for tree absorbed photosynthetically active radiation (APAR), gross primary production (GPP), transpiration (TR), light use efficiency (LUE) and water use efficiency (WUE). Some of the parameters used by the metamodels were simplified. For example, the daily average temperature was used in the metamodels while the hourly temperature was required in the MAESPA model. The second level metamodel was obtained by removing the least sensitive parameters.

Fig. 2. Comparison of the MAESPA and the first-level metamodel simulations for daily absorbed photosynthetically active radiation (APAR, A), gross primary production (GPP, B), transpiration (TR, C), light use efficiency (LUE, D), and water use efficiency (WUE, E). The kernel density estimation of simulations are shown in blue. The R-squared ($R^2$) and the Root Mean Square Error (RMSE) are presented for each metamodel ($n=1500$).

Fig. 3. Global sensitivity analysis of the first level MAESPA metamodels for daily absorbed photosynthetically active radiation (APAR), gross primary production (GPP), transpiration (TR), light use efficiency (LUE) and water use efficiency (WUE). The sensitivity to the individual parameters was estimated using the Sobol index. The sensitivity to the interaction with all other parameters was calculated as the difference between the total sensitivity index (ST) and the main sensitivity index (S) (equations 2 and 3). Individual parameters are grouped into meteorological (Meteo.), morphological (Morpho.), physiological (Physio.) and root parameters. $R^2$ for each metamodel is shown in the column heading. “+” and “-” indicate whether the relationship between the input parameter and the output value is positive or negative. 10,000 daily simulations were performed in the sensitivity analysis.
Fig. 4. Uncertainty analysis of the MAESPA metamodels for daily tree absorbed radiation (APAR), gross photosynthesis (GPP), transpiration (TR), light use efficiency (LUE) and water use efficiency (WUE). Uncertainty is expressed in mean absolute percentage error of the output for a single tree (MAPE_{tree}) as a function of the maximum error applied to model parameters (A) or as a function of the tree DBH (B). The medians of MAPE_{tree} calculated for 10,000 trees are shown as a black line and the 10th and 90th percentiles enclose the shaded area. 5,000 daily simulations were performed for each of the 5,000 trees in the uncertainty analysis.

Fig. 5. Validation of the MAESPA second level metamodel of tree transpiration (TR). Sensitivity of the metamodel to parameters using Sobol index (A), time series of daily simulated tree transpiration and sap flow measurements from 1.5 to 2.5 years after planting (B) and mean percentage error, with standard deviation, between simulated and measured tree TR depending on the time scale (C). The lines in B show the average of 10 trees and the grey areas are the standard deviations. The TR simulations of the original MAESPA models (Christina et al. 2015) were also compared with measurements (C).
Fig. 1
Fig. 2.
Fig. 3
Fig. 4.
Fig. 5.
Supplementary material

Building a single virtual random plantation

Tree positions and DBH

A virtual random plantation was designed as a *Eucalyptus* stand of 576 trees. All the allometric relationships used in this section to build the random plantation were established in the Euclflux *Eucalyptus* plantation between 0.5 and 3 years. The trees were first positioned, not in a perfectly regular 3*2 grid, but considering the small variations in distances which occurs in the field. For this, the lines were first placed every 3 m and then the trees were placed within the line with a distance between trees (d) sampled in a uniform distribution from 2 to 4 m (d~U(2, 4 m)). A random factor on (x,y) coordinates of each tree was finally assumed (ε = d/5) because trees were never perfectly aligned in these types of plantations.

A given average diameter at breast height (<DBH>) was sampled from a uniform law between 5 and 15 cm as observed between 6 months and 3 years of growth in these *Eucalyptus* plantations. This average <DBH> is afterwards considered as a good proxy of stand age. Tree-scale DBH were assumed to follow a normal distribution within the planted forests. An empirical relationship between the standard deviation of DBH (ε_{DBH}) within a given planted forest and its average diameter (<DBH>) was established over 3 years of growth in the Euclflux site:

\[ ε_{DBH} = a_{DBH} + b_{DBH} * <DBH> + N(0, c_{DBH}) \]  

(1)

where a_{DBH}, b_{DBH}, c_{DBH} are parameters (Table S1), and N is a normal distribution of mean 0 and standard deviation c_{DBH}. ε_{DBH} is therefore the sum of a deterministic value directly function of the stand randomly chosen <DBH>, and a random value independent of <DBH> and also randomly chosen for this stand.
Values of DBH of each tree were initially allocated randomly for all trees within the plantation following a normal distribution of medium $<\text{DBH}>$ and standard deviation $\varepsilon_{\text{DBH}}$. To build realistic planted forests taking into account the spatial structure which exist between neighbor trees, we computed the competition index of (Hegyi 1974):

$$C_{i} = \sum_{j=1}^{8} \frac{DBH_{j}}{DBH_{i} * L_{ij}}$$

(2)

where $C_{i}$ is the competition index for the tree $i$, $DBH_{i}$ is the diameter at breast height of the tree $i$, $DBH_{j}$ is the diameter at breast height of the nearest neighbor tree number $j$ (here 8 trees are taken into account), and $L_{ij}$ the distance between tree $i$ and $j$. An empirical relationship between $C_{i}$, $DBH_{i}$ and the $<\text{DBH}>$ has been established at all ages for Eucalyptus plantations using inventory data over 3 years:

$$\tilde{C}_{i} = a_{1_{CI}} * <\text{DBH}> + a_{2_{CI}} + \frac{b_{1_{CI}} * <\text{DBH}> + b_{2_{CI}}}{DBH_{i}^{c_{CI}}}$$

(3)

where $a_{1_{CI}}$, $a_{2_{CI}}$, $b_{1_{CI}}$, $b_{2_{CI}}$ and $c_{CI}$ are parameters calibrated on Eucflux site (Table S1). $\tilde{C}_{i}$ was an estimation of realistic competition index for a given tree which has a diameter of $DBH_{i}$, within a stand of average diameter $<\text{DBH}>$. We calculated the $C_{i}$ associated for all tree $i$ within the randomly designed stand, with eq. 2. If this $C_{i}$ was outside the 99% quantile of the fitted relationship producing realistic $\tilde{C}_{i}$ (eq. 3), we randomly sampled a new $DBH_{i}$ for the target tree, using the same normal distribution described before, until the condition was reached. The order of the target tree ($i$) selection was randomly chosen to avoid any tree ordering issue in this sequential algorithm. At the end of this first step, the positions of trees within the virtual plantation are defined, together with realistic DBH (in terms of distribution and spatial structure).
Morphological parameters dependent on DBH

Tree height ($H_i$), leaf area ($LA_i$), crown diameter ($D_{C,i}$) and crown height ($H_{C,i}$) of each tree were then estimated using allometric relationship established in the *Eucalyptus* plantation at all ages using data covering 3 years of growth. The equations were based on classically used deterministic equations function of tree height ($H$) and DBH (Saint-Andre et al. 2005) associated with a tree-scale random term selected from the error term (normally distributed variability):

$$H_i = a_H + b_H \cdot DBH_i + N(0, \varepsilon_H)$$ (4)

$$LA_i = a_{LA}(DBH_i^2 \cdot H_i)^{b_{LA}} + N(0, \varepsilon_{LA})$$ (5)

$$D_{C,i} = a_{DC}(DBH_i^2 \cdot H_i)^{b_{DC}} + N(0, \varepsilon_{DC})$$ (6)

$$H_{C,i} = a_{HC}(DBH_i^2 \cdot H_i)^{b_{HC}} + N(0, \varepsilon_{HC})$$ (7)

where $a$, $b$ and $\varepsilon$ (with subscripts) are parameters calibrated on Eucflux site (Table S1). The $\varepsilon$ term was used to include a probabilistic variability that exists between trees (spatial variability) as well as the possible parameter changes between seasons. Typically, $\varepsilon_{LA}$ is large compared to other $\varepsilon$ values compared to their average.

Finally, stand root mass density (RMD) was estimated using two allometric relationships, one between leaf dry mass ($M_{leaf}$) and the product between the squared diameter and the eight, and another between $M_{leaf}$ and RMD:

$$M_{leaf} = a_{leaf} (DBH^2 \cdot H)^{b_{leaf}} + N(0, \varepsilon_{leaf})$$ (8)

$$RMD = a_{RMD} \cdot \sum M_{leaf} \cdot Area + N(0, \varepsilon_{RMD})$$ (9)

where $a$, $b$ and $\varepsilon$ (with subscripts) are parameters calibrated on *Eucalyptus* plantations in the same region (Laclau et al. 2008), and $\text{Area}$ the plot area (Table S1). Note that $a_{RMD}$ was obtained from (Laclau et al. 2008) and $\varepsilon_{RMD}$ was fixed.
Other morphological and physiological parameters

The values for the other morphological and physiological input parameters of MAESPA model were uniformly sampled within the range that was measured in this study or observed in literature. We assumed that these parameters were independent and could be sampled individually, and were common for all trees in the virtual plantation. These independent parameters were stand scale parameters. Parameters names, threshold values and their sources are presented in Table 1 & 2. The leaf area distribution within the crown was computed horizontally (H_{LAD}) and vertically (V_{LAD}) as a beta-distribution:

\[ V_{LAD} = a_{LADV} \times X_{LADV}^{b_{LADV}} \times (1 - X_{LADV})^{c_{LADV}} \]  

\[ H_{LAD} = a_{LADH} \times X_{LADH}^{b_{LADH}+1} \times (1 - X_{LADH})^{c_{LADH}} \]

where \( X_{LADV} \) is the relative height within the crown, \( X_{LADH} \) the relative distance from the trunk to crown envelope, and \( a, b \) and \( c \) (with subscripts) are parameters of the beta-distribution, calibrated on the Euclflux site. In the Table 1, \( \text{LAD}_V \) and \( \text{LAD}_H \) were defined as the position in height and radius of the maximum of these functions and could be expressed as:

\[ \text{LAD}_V = \frac{b_{LADV}}{b_{LADV} + c_{LADV}} \]  

\[ \text{LAD}_H = \frac{b_{LADH} + 1}{b_{LADH} + 1 + c_{LADH}} \]

The value of \( \text{LAD}_V \) and \( \text{LAD}_H \) were sampled in a uniform distribution with threshold defined in Table 1. The parameter \( b_{LADV} \) and \( b_{LADH} \) were sampled in normal distribution established on measurements in our \textit{Eucalyptus} plantations (\( b_{LADV} \sim N(0.54,0.41) \) and \( b_{LADH} \sim N(-0.61,0.19) \)). Once the \( b_{LADV} \) and \( b_{LADH} \) parameters were sampled, the \( c_{LADV} \) and \( c_{LADH} \) parameters were calculated using the \( \text{LAD}_V \) and \( \text{LAD}_H \) equations 12 and 13. Finally, the \( a_{LADV} \) parameter was then calculated to reach an integral of \( V_{LAD} \) equal to 1. The \( a_{LADH} \) parameter was calculated to reach an integral of \( H_{LAD} \) equal to \( 1/(2\pi) \).
In total, there was 7 morphological characteristics which changed between trees (presented above), and 23 morphological and physiological parameters which were common for all trees in the virtual plantation.

_Table S1. Parameter values of the allometric relationship used in this study. When available, the number of data used for the regression (n) as well as the root mean square error (RMSE) are shown._

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_n.a._ denotes not available.
References

