Calibration and Validation of the Integrated Biosphere Simulator (IBIS) for a Brazilian Semi-arid Region

ANA PAULA M. A. CUNHA
Earth System Science Center, National Institute for Space Research, São José dos Campos, Brazil

REGINA C. S. ALVALÁ
Brazilian Center for Monitoring and Warning of Natural Disasters, São José dos Campos, Brazil

GILVAN SAMPAIO
Earth System Science Center, National Institute for Space Research, São José dos Campos, Brazil

MARÍLIA HARUMI SHIMIZU
University of São Paulo, São Paulo, Brazil

MARCOS HEIL COSTA
Federal University of Viçosa, Viçosa, Brazil

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ABSTRACT

The reliability of predictions from climate and weather models is linked to an adequate representation of the land surface processes. To evaluate performance and to improve predictions, land surface models are calibrated against observed data. Despite an extensive literature describing methods of land surface model calibration, few studies have applied a calibration method for semi-arid natural vegetation, especially for the semi-arid northeast of Brazil, which presents caatinga as its natural vegetation. Caatinga is a highly dynamic ecosystem with the physics at the land surface–atmosphere interface still poorly understood. Therefore, in this study a multi-objective hierarchical method, which provides means to estimate optimal values of the model parameters through calibration, is evaluated. This method is applied to caatinga by using the Integrated Biosphere Simulator (IBIS). Results demonstrated that the calibrated set of vegetation parameters produced a considerably different energy balance from the default parameters. In general, the model was able to simulate the partition of the available energy into sensible and latent heat fluxes when the calibrated parameters were used. The IBIS model was not able to capture short-term, intense changes in latent heat flux from a dry condition to a wetter condition, however, even when the new set of calibrated parameters was used. Therefore, the parameter optimization may not be sufficient if processes are missing or misrepresented. This study is one of the first to understand the physics at the land surface–atmosphere interface in the caatinga ecosystem and to evaluate the ability of the IBIS model to represent the biophysical interactions in this important ecosystem.

1. Introduction

The interactions at the interface between the land surface and the atmosphere are modeled using the surface component of climate models, which is known as a soil–vegetation–atmosphere transfer scheme. The need to improve the representation of land surface biophysical processes, terrestrial carbon flux, and vegetation dynamic in atmospheric general circulation models and regional models, mainly for climatic change studies, has stimulated the development of sophisticated surface parameterizations. The evolution of these parameterizations tends to add complexity to the models, increasing the number of parameters that must be set to describe the morphological and biophysical characteristics of the
surface (Demarty et al. 2004). An indicator of a model's complexity is the number of parameters that are used to characterize the various ecosystem processes (Wang et al. 2009). The Integrated Biosphere Simulator (IBIS; Foley et al. 1996), for example, requires 76 parameters to be specified, 14 related to soil, 12 specific to each plant functional type (PFT), and 50 related to morphological and biophysical characteristics of vegetation. These parameters can be physically realistic and observable or empirical. Even though the necessary data may be accessible, they may not be directly usable because of the difference in temporal and spatial scales between measurements and model. Small uncertainties in the parameters' values may propagate to generate a wide range of variability in the subsequent simulations of energy, water, and carbon balances, which reinforces the importance of the parameters' calibration.

The purpose of calibrating land surface models is to reduce errors of model output by matching simulations with observations through adjustment of the model parameters. Several optimization techniques have been developed to generate an optimal set of parameters for models' surface. These techniques can consist of a single objective function (Sellers et al. 1989; Rocha et al. 1996; Delire and Foley 1999; Cunha et al. 2008) or of a multiobjective calibration (Gupta et al. 1998, 1999b; Yapo et al. 1998; Houser et al. 2001; Engeland et al. 2006; Varejão et al. 2011). Calibration methods that consider a single objective function are inadequate for models that simulate different surface processes and several output fluxes, as highlighted by Vrugt et al. (2003). The problem of calibrating a model with many outputs is restricted to finding a set of parameters that simultaneously minimize a vector of objective functions. In general, the calibration algorithms determine a single optimum parameter set, which is often insufficient because of parameter uncertainties.

On the other hand, the method of multiobjective calibration is based on statistical analysis of different objective functions, and the number of the objective functions depends on the case studied, the model, and the availability of observed variables. Gupta et al. (1999a) showed that a multiobjective calibration incorporating at least one appropriate heat flux and one surface state variable is required to ensure adequate calibration of all model predictions. The multiobjective calibration has already been applied in different surface modeling contexts and has been shown to produce more accurate simulations of energy fluxes for different types of land cover (Gupta et al. 1998, 1999b; Yapo et al. 1998; Houser et al. 2001; Engeland et al. 2006; Varejão et al. 2011).

The current work extends this investigation by considering data that were collected in a semiarid region of Brazil. Typical vegetation occurring in and around semiarid Brazil is xeromorphic vegetation known as caatinga, which presents fast morphological and physiological responses to water supply. This trait makes the parameterization of the caatinga in the surface model a complex task. This semiarid region of Brazil was chosen because it presents an irregular climate, water shortages, and vulnerability of land to desertification, mainly because of the climate, the state of the soil and the natural vegetation, and the ways in which these two resources are used. Thus, the objective of this paper is to assess the possibility for improving the radiation and energy balances simulated by the IBIS model, for a semiarid region, through the estimation of model parameters by using the hierarchical multiobjective calibration method.

Moreover, the effort to improve the IBIS model representation for Brazilian ecosystems has a particular importance because this model is the basis of the surface scheme that is being developed and implemented in the scope of the Brazilian Earth System Model (Nobre et al. 2013).

2. Materials and methods

a. Study area description

The semiarid region is characterized by the presence of the natural vegetation known as caatinga. Caatinga vegetation is composed of shrubs and small trees, usually thorny and deciduous, that lose their leaves in the early dry season. Nowadays, more than 10% of the semiarid area has already undergone a very high degree of environmental degradation, being susceptible to desertification (Oyama and Nobre 2004). Caatinga is a highly dynamic ecosystem that responds quickly to climatic conditions. The dominant factor that controls the structure and distribution of vegetation is the precipitation, with an annual mean of 500–800 mm and high spatial and temporal variability (Hastenrath and Heller 1977; Oliveira et al. 2006). The rainy season extends from February to May, when the intertropical convergence zone reaches its southernmost position. The adaption to the lack of water for several months of the year appears in the form, color, metabolism, and life cycles of plants. Caatinga, in comparison with other xeric areas in South America, presents climatic distinctiveness that resulted in numerous important morphological and physiological adaptations to aridity by many species of plants (Mares et al. 1985). Moreover, caatinga builds a continuous vegetation layer, and canopy density, height, and percentage of nondeciduous species generally increase with the amount of mean annual rainfall.

b. Experimental site and data acquisitions

The micrometeorological and hydrological data necessary for the IBIS calibration were obtained from the
caatinga experimental site, situated at the Agricultural Research Center of the Semiarid Tropics [Centro de Pesquisa Agropecuaria do Tropico Semi-Arido (CPATSA); 9°03'30.6"S, 40°19'45.1"W; 350 m], Petrolina, Pernambuco State, Brazil (Fig. 1). It represents an area of 600 ha of native caatinga, which presents thorny vegetation with small leaves, pertaining to the Leguminosae family (mostly Mimosa tenuiflora). Canopy height is 4.5 m, on average, and only 6% of species plants present heights between 6 and 8 m. Species taller than 8 m are not found. The soil of the experimental area is classified as argisol, which is characterized by low water retention and poor fertility.

In the study region, the rainfall shows high temporal variability. In terms of cumulative precipitation for the period from July 2004 to June 2005 (Fig. 2), it can be observed that rainfall is concentrated from January to April. Around 81% of the rainfall occurred in the first four months of the year, which clearly indicates the existence of an intense and longer dry season. The mean annual precipitation was about 300 mm, and the average temperature was 26°C. The lowest and highest temperatures recorded were 15.6°C and 37.8°C, respectively. The mean annual relative humidity was 59%.

A 9-m-height micrometeorological tower was installed on homogeneous and flat terrain of the natural caatinga. The data needed to force the IBIS model were obtained from the tower and consist of incoming solar radiation, downward longwave radiation, air temperature, relative humidity of air, horizontal wind speed, and precipitation. All components of short- and longwave solar radiation were measured with Kipp & Zonen, Inc., pyranometers and pyrgeometers facing up and down at a height of 9 m from the ground. Microclimatic measurements of air temperature and relative humidity were taken above the vegetation with Vaisala, Inc., model HMP 45C-L probe at the same height as the radiation sensors. Wind speed was measured with R. M. Young Company Wind Sentry anemometers. Rainfall data were collected using a Hydrological Services, Pty Ltd., TB4 rain gauge. The high-frequency data in the caatinga were collected at each minute, and 10-min averages were stored in a Campbell Scientific, Inc., CR23X datalogger.

The measured data used to calibrate the IBIS parameters were hourly time series of incoming and reflected photosynthetically active radiation (PARin and PARo, respectively), net radiation Rnet, friction velocity, sensible heat flux $H$, and latent heat flux LE. PAR was measured with a Kipp & Zonen PAR-Lite sensor. Rnet was acquired with one Kipp & Zonen NR-Lite net radiometer at 10 m above the ground. The eddy-covariance-method
system (EC) over the caatinga was installed at 11 m above the ground and consisted of a sonic Campbell Scientific CSAT3 anemometer and a Li-Cor, Inc., LI7500 gas analyzer connected to a Campbell Scientific CR10X datalogger. The distance from the tower to the border portion is 1000 m (fetch), more than 100 times the height of the flow measurement system, which certainly ensures that the measured fluxes are derived only from caatinga, even during stable conditions. The measured fluxes were corrected to minimize any systematic error arising from the EC system setup and flux-averaging method. The EC fluxes were calculated as 30-min block-averaged covariances between the scalars (or horizontal wind speed) and vertical wind velocity according to commonly accepted procedures (Aubinet et al. 2000). The coordinate rotation and the data frequency-response correction were done according to the Moore (1986) method. Temperature covariance was corrected for humidity as described by Schotanus et al. (1983). The soil heat flux $G$ was measured with one Hukseflux Thermal Sensors, BV, HFP01 flux plate at 5-cm soil depth; $G$ was not corrected for the heat storage above the plates.

c. Quality control for the energy balance data

The conservation of energy is usually expressed as energy balance closure, which can be formulated as follows:

$$\text{R}_{\text{net}} = H + LE + G + S + Q,$$

where $S$ is the heat storage within vegetation canopy and $Q$ is the sum of additional energy sources and sinks; $S$ and $Q$ are frequently neglected because of their small magnitudes.

Energy balance closure has been accepted as an important test of EC data (Anderson et al. 1984; Verma et al. 1986; Mahrt 1998; Wilson et al. 2002). In theory, the conservation of energy requires instantaneous closure. In practice, energy balance closure can be biased by up to 30% (Wilson et al. 2002). The reasons for the nonclosure are manifold and are not always known. In general, the causes for nonclosure as concluded from several studies can be summarized as follows: 1) equipment limitations, such as systematic bias and mismatch in source areas for the terms in the energy balance equation; 2) neglected energy sinks; 3) loss of low-and/or high-frequency contributions to the turbulent flux; and 4) neglected advection of scalars (Wilson et al. 2002; Schüttemeyer 2005; Xiao et al. 2012). In the context of semiarid environments, another explanation may be an underestimation of $G$ as a result of substantial heat gradients in the upper layers of the soil (Veenendaal et al. 2004). In general, the soil heat flux is often treated improperly, leading to neglect or underestimation of heat storage between the soil heat flux plate and the surface.

To evaluate the EC estimates of LE and $H$, the energy balance closure was examined through the linear regression coefficient of turbulent energy ($\text{LE} + H$) against the available energy ($\text{R}_{\text{net}} - G$). Energy balance closure is obtained when $\text{R}_{\text{net}} - G$ (estimated from meteorological data) is equal to the outgoing energy ($\text{LE} + H$, as measured by EC). This is even more important because random errors for measured $\text{R}_{\text{net}}$ and $G$ cannot be specified properly. A second method
to evaluate closure was to calculate the cumulative sum of the available energy \((R_{\text{net}} - G)\) and the dependent fluxes \((LE + H)\) over the analyzed periods and then to calculate the energy balance ratio \((EBR; \text{Mahrt 1998; Gu et al. 1999; Wilson et al. 2002; Barr et al. 2006})\):

\[
EBR = \frac{\sum(H + LE)}{\sum(R_{\text{net}} - G)}.
\]  

(2)

The advantage of this method is that it neglects possible random errors in flux estimation. The third method, used as a reference factor for assessing the level of surface energy balance, was the energy balance residual:

\[
Res = R_{\text{net}} - G - H - LE.
\]  

(3)

According to Eq. (3), \(Res\) contains all unmeasured terms and various types of errors. The value of \(Res\) reflects the measurement status of the energy balance and can be the reference for evaluating the unmeasured energy items indirectly (Guo et al. 2008; Yue et al. 2011; Xiao et al. 2012).

The land surface models are usually based on conservation of energy, and the measured covariance data do not always indicate energy closure (as discussed above). This study used two types of data filtering before the model calibration to resolve this impasse. The first filter eliminates the periods with gaps in the input data series. The second filter is based on energy budget closure, which eliminates from the model-evaluation processes those days for which the energy budget closure is poor:

\[
(1 - \epsilon) \leq \frac{H + LE}{R_{\text{net}} - G} \leq (1 + \epsilon).
\]  

(4)

In this study, \(\epsilon = 0.2\) was used; that is, only the periods of data whose daily energy budget as measured by \(EC\) was within 80% of the budget energy measured by radiative instruments were used.

d. Model description

Version 2.6 of IBIS (Foley et al. 1996, 2005; Kucharik et al. 2000) was used in this study. IBIS is part of a new generation of global biosphere models, termed dynamic global vegetation models, that consider transient changes in vegetation composition and structure in response to environmental change. Much of the structure of the land surface module has been borrowed from a land surface transfer scheme (LSX; Thompson and Pollard 1995a,b), and it represents a wide range of processes, including land surface physics, canopy physiology, plant phenology, vegetation dynamics and competition, and carbon and nutrient cycling. The model is hierarchically organized and generates global simulations of the surface water balance, the terrestrial carbon balance, and vegetation structure (e.g., biomass, leaf area index, and vegetation composition). Each grid cell has the potential to represent two vegetation layers (corresponding to upper and lower canopies), and six soil layers extending to a depth of 4 m. The six soil layers that are the default in IBIS have top-to-bottom thicknesses of 0.10, 0.15, 0.25, 0.50, 1.0, and 2.0 m. For each soil layer, the model simulates temperature, volumetric water content, and ice content at each time step.

In IBIS the vegetation cover is represented as a combination of PFTs that are adapted from Prentice et al. (1992). PFTs are defined to resolve a few important features such as basic physiognomy, leaf habit, photosynthetic pathway, and leaf form (Foley et al. 1996). A more detailed description of the global version of IBIS can be found in Kucharik et al. (2000).

e. Multiobjective hierarchical calibration—Optis

To obtain the intended performance, the model should be calibrated in a way such that all of the processes are realistically simulated. In this study, the method used to calibrate the model was developed by Varejão et al. (2011). The method is based on a theory of ecosystems hierarchy to optimize processes simulated by the IBIS model automatically. Only a short description will be given here; for a full description, refer to Varejão et al. (2011).

The multiobjective optimization software Optis is founded on the nondominated sorted genetic algorithm-II (NSGA-II), which is a multiobjective calibration algorithm (Deb et al. 2002). NSGA-II is based on the Pareto frontier concept to find optimal solutions for multiobjective-optimization problems. Pareto solutions are those for which improvement in one objective can only occur with the worsening of at least one other objective. Thus, instead of a unique solution to the problem, the solution to a multiobjective problem is a set of Pareto points, also called a Pareto frontier. After defining the Pareto-frontier solution set, Optis returns the output as the preferred solution that symmetrically optimizes all of the objectives. To avoid any interference from the objective-function units or value scales, normalization of the algorithm output is performed before the choice of the optimal value. Thereafter, the point with the smallest Euclidean distance from the origin is
selected as the preferred solution for the optimization problem (Varejão et al. 2011). Optis works coupled with the IBIS model; during the calibration process, however, the IBIS model independently operates from Optis. The optimization algorithm interacts with the IBIS model only through reading output data and changing input data parameters. IBIS simulates processes that span through a range of time scales, from energy and mass fluxes (seconds) to carbon budget in soils and vegetation dynamics, including competition among plant functional types (decades). Therefore, the calibration algorithm employed a temporal hierarchical approach to separately calibrate each process, or set of processes, according to its hierarchical level. The number of objective functions is calibrated according to the availability of observed data. The hierarchical levels of calibration and the optimized output were defined as level 1: PARo fluxes and reflected solar radiation (reflsw), level 2: radiation fluxes (Rn), and level 3: turbulence (H and LE).

In the hierarchical levels 1 and 2, it is possible to use two adjustment metrics: the mean absolute error (MAE) and the maximum bias (Bmax). MAE and Bmax are respectively given by

\[ \text{MAE} = n^{-1} \sum_{i=1}^{n} |P(i) - O(i)| \]  
\[ \text{Bmax} = \max_{i=1}^{n} \left[ \sum_{j=1}^{n} (P_j - O_j) \right] \]  

where \( n \) is length of series, \( P \) indicates predicted data, and \( O \) indicates observed data. In level 3, only MAE was applied. As the name suggests, the mean absolute error is an average of the absolute errors. MAE is not ambiguous—it conveys the mean errors in absolute values. Since it is clearer to interpret, MAE is more appropriate to the evaluation method. Bmax is a cumulative value able to identify small changes in data distribution. It indicates the greatest accumulated error between the predicted and observed ones. Therefore, the cumulative sum is used for calibration to minimize the maximum distance between an observed data curve and predicted data curves. Table 1 presents the objective functions and the parameters identified for calibration by hierarchical level.

The choice of the parameters to be calibrated was based on the results of the sensitivity analysis made by Varejão et al. (2011). The sensitivity analysis was performed to select, efficiently, the most important parameters for each model output. The sensitivity analysis uses the Morris (1991) method with the calculation of the sensitivity index adapted for land surface models. This method determines an importance ranking for

<table>
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<tr>
<th>Hierarchical level</th>
<th>Objective function</th>
<th>Parameter</th>
<th>Possible range</th>
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<td>1</td>
<td>MAE&lt;sub&gt;PARo,reflsw&lt;/sub&gt;, Bmax&lt;sub&gt;PARo,reflsw&lt;/sub&gt;</td>
<td>rhoveg&lt;sub&gt;_vis&lt;/sub&gt;</td>
<td>Reflectance of an avg leaf/stem (VIS)</td>
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<td>tauveg&lt;sub&gt;_vis&lt;/sub&gt;</td>
<td>Transmittance of an avg leaf/stem (VIS)</td>
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<td>chilfz</td>
<td>Lower canopy leaf orientation factor</td>
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<td>root coef</td>
<td>Carbon allocation fraction to fine roots coef (s&lt;sup&gt;–1&lt;/sup&gt;)</td>
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<td>growth coef</td>
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<td>rhoveg&lt;sub&gt;_NIR&lt;/sub&gt;</td>
<td>Reflectance of an avg leaf/stem (NIR)</td>
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<td>Specific leaf area (m&lt;sup&gt;2&lt;/sup&gt;kg&lt;sup&gt;–1&lt;/sup&gt;)</td>
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<td>avmuir coef</td>
<td>Coef to calculate canopy emissivity</td>
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<td>dispu coef</td>
<td>Zero-plane displacement height for upper canopy (m)</td>
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<td>MAE&lt;sub&gt;Rn&lt;/sub&gt;, Bmax&lt;sub&gt;Rn&lt;/sub&gt;</td>
<td>vmin_pft</td>
<td>Nominal vmax of top leaf at 15°C (molCO&lt;sub&gt;2&lt;/sub&gt; m&lt;sup&gt;–2&lt;/sup&gt;s&lt;sup&gt;–1&lt;/sup&gt;)</td>
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<td>coefmls</td>
<td>m coef for stomatal conductance relationship</td>
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<td>tempvm coef</td>
<td>Stress max vmax coef</td>
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<td>tauleaf</td>
<td>Foliar biomass turnover time constant (yr)</td>
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<td>stressf coef</td>
<td>Coef for soil water stress</td>
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<td>aleaf</td>
<td>Carbon allocation fraction to leaves</td>
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<td>alogl coef</td>
<td>Coef for roughness length of lower canopy</td>
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<td>beta1</td>
<td>Parameter for Jackson rooting profile, lower canopy</td>
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parameters in terms of their mean effect on output as well as their nonlinear and interaction effects on output. After the sensitivity analysis, the nonsignificant parameters of the model for a specific output are disregarded during the calibration procedure, and then the parameters related to each IBIS output variable were grouped. The results obtained by Varejão et al. (2011) showed that 23 parameters are sensitive to 9 IBIS output variables. Of them, 9 were shown to affect more $H$ (rhoveg_NIR, coefmub, beta, chifuz, tauveg_NIR, tauleaf, dispu_coef, rgrowth_coef, and avmuir_coef). For LE, the parameters with the highest index sensitivity were beta, chifuz, rgrowth_coef, tauleaf, vmax_pft, and coefmub. From these 23 analyzed parameters, a total of 18 model parameters were applied in this study. So, the number of parameters evaluated was smaller because some of them are related to variables that do not have field measurements from the associated experimental site. The 18 parameters were selected because of their importance in driving main components of the energy balance as well as the high level of uncertainty in their specification in situ.

The calibration was performed using the IBIS model in “offline” mode (on a single grid point), forced with hourly data from July 2004 until June 2005. This period covers the transition time from the dry season to the wet season in the studied region. In all simulations, the model was run with static vegetation (i.e., vegetation fixed at the present-day state). The model was initialized with the measured value of soil water content of 0.30 m$^3$ m$^{-3}$ and observed data of the particle size of six soil layers from the studied area (percentages of sand and clay).

### 3. Results and discussion

#### a. Energy balance closure from observational data

To investigate the energy balance closure and its residual energy component, half-hourly datasets were processed. Figure 3 shows the monthly-mean diurnal cycles of Rnet, $H$, LE, $G$, and Res, representing the main characteristics of surface energy partitioning in semiarid regions. During both seasons, $H$ is distinctly larger than LE, with the energy transport dominated by $H$ in the near-surface layer. Despite Rnet being higher during the wet season than during the dry season, because the wet season includes summer months $H$ is slightly reduced and LE has doubled its value because of higher soil moisture availability. As illustrated in Figs. 3a and 3b, Res was close to zero until the sunrise. Afterward, it slowly increases, reaching its maximum value at 1200 local time, decreasing in the afternoon, and becoming negative from 1600 to 2100 local time. The level of the energy balance closure is greater during the night than during the day for both seasons, showing that the available energy exceeds turbulent energy at that time. This result indicates that the surface energy balance closure varies during different periods of time, which is consistent, for example, with the experimental findings of Oncley et al. (2007) and Gao et al. (2010). This pattern was also observed by Yue et al. (2011) in semiarid grassland.

Despite similar pattern of Res for both seasons, Res is larger than $G$ and LE during the dry season and is larger than $G$ during the wet season. The monthly average Res was 17.7 and 23.15 W m$^{-2}$ in the dry and wet seasons, respectively. From Fig. 3a it is possible to observe that $G$ and Res are not in phase with Rnet, $H$, and LE. For $G$ it
is due to the time difference of energy transfer from the surface to the flux plate (G is delayed when compared with Rnet). Soil heat flux sensors can introduce important heat flow distortion induced by the difference in conductivity between the plates and the surrounding soil. The phase delay of G further results in the phase lead of Res and thereby contributes to the decline in the closure level of energy balance closure, mainly from the period from 0600 to 1000 local time, and also from the period from 1500 to 2000 local time.

Figure 4 shows the linear regression analysis results of \((H + LE)\) against \((R_{net} - G)\) and energy closure level. Seen is an incomplete energy balance closure with \((H + LE)\) being up to around 17% lower than \((R_{net} - G)\), with this imbalance tending to be greatest during the high insolation time. In an ideal case of energy balance, the slope of the regression straight line is 1, and its intercept is zero. Energy balance closure analysis resulted in a slope of 0.83 and intercept of 4.37 W m\(^{-2}\), with a coefficient of determination \(R^2\) equal to 0.96 for caatinga. These values are consistent with those found by Yue et al. (2011) for a semiarid grassland (slope, intercept, and correlation equal to 0.84, 18.88, and 0.98, respectively), those found by Williams et al. (2004) for an Agdal olive orchard site in a semiarid Mediterranean climate (slope = 0.74; \(R^2 = 0.94\)), and those found by Scott et al. (2006) for a semiarid riparian environment (slope equal to 0.76 over a grassland and slightly better for the shrubland, equal to 0.81).

The EBR, which should not be affected by random errors, showed an average value of 0.83 for the whole period. The annual ratio of total turbulent heat flux to total available energy was similar to the ones found by Wilson et al. (2002) for 50 “FLUXNET” sites in the United States of America (0.82).

As expected, the energy balance is clearly not closed. The lack of energy balance closure found in this study is commonly reported for other semiarid sites (Veenendaal et al. 2004; Schüttemeyer et al. 2005; Hastings et al. 2005; Xiao et al. 2012). The improper surface energy balance closure in semiarid regions is attributed, among other factors, to the underestimation of \(G\) as a result of intense heat gradients in the upper layers of the soil because of high insolation. It must result in substantial energy storage \(S\) in the soil layer above the sensor (Veenendaal et al. 2004). Assuming a specific heat capacity of the soil for the studied area (dry sandy soil) equal to 1.28 MJ m\(^{-2}\)C\(^{-1}\) and given the mean observed maximum temperature change of 4.6°C during high insolation, the heat storage in the 2–5-cm layer was on the order of 100 W m\(^{-2}\). Oliveira et al. (2006) showed that, after addition of the heat storage to the energy balance, the sum of \(H + LE + G + S\) represented 94% of the Rnet. This result indicates that the EC estimates of LE and \(H\) are, in general, consistent. Moreover, while the imbalance introduces some degree of uncertainty in the results that are presented here, the magnitude is such that it does not significantly alter the conclusions.

b. Calibration

Table 2 presents IBIS hierarchical calibration results for the caatinga site. The initial and calibrated parameter values are shown. The most modified parameters, after calibration, are chiflz, rroot_coef, and rgrowth_coef for the hierarchical level 1; avmuir_coef for the hierarchical level 2; and alogl_coef for the hierarchical level 3. The chiflz is an optical parameter of the canopy, which influences the amount of light absorbed. According to Varejão et al. (2011), chiflz is one of the parameters that most influence the estimation of PARo. Both rroot_coef and rgrowth_coef are important in the calculation of \(H\) and LE. The avmuir_coef is the average diffuse optical depth, which is directly related to the radiative transfer within vegetative canopies and consequently is related to Rnet.

The best MAE value was obtained by minimizing objective function \(\text{MAE}_{\text{LE}}\) (about 19 W m\(^{-2}\)), followed by \(\text{MAE}_H\) (about 30 W m\(^{-2}\)) and \(\text{MAE}_{\text{Rnet}}\) (about 40 W m\(^{-2}\)). Varejão et al. (2011) used the same hierarchical calibration for Tapajós National Forest site, finding \(\text{MAE}_{\text{LE}}, \text{MAE}_H\), and \(\text{MAE}_{\text{Rnet}}\) equal to 36.53, 40.57, and 21.54 W m\(^{-2}\), respectively.

Figure 5 presents observed and simulated PARo. PAR is a key variable to be used to verify the interaction
of radiation with the ecosystem. In general, during the dry season, when the canopy is reduced, PARo usually presents a gradual increase, whereas the values of this radiation component in the beginning of the rainy season are reduced because of the recovery of the photosynthetic activity, which causes a higher PARin absorption.

Figure 5 indicates that most of the inconsistency of simulated PARo occurred during the day, when the value is greatest. PARo is overestimated during both the dry and wet seasons and especially during the rainy season. This error is reduced when the calibrated parameters are used in the simulation. After the calibration procedure, the chiflz parameter, which has an impact on the PARo simulation, was reduced. As a result, the leaf orientation has changed, making the leaves more upright, reducing the incidence of solar radiation and, thus, reducing PARo.

The measured fluxes and simulations of the main components of the energy balance, using the calibrated and uncalibrated parameters, are compared using two-dimensional plots that show the time of day and day number (starting 1 July 2004), with the flux magnitude represented in color (Figs. 6–9). The two-dimensional plots were constructed by calculating 10-day diurnal averages of the hourly fluxes. Thus, they consist of 24 averages in the x dimension (hourly averages) and 36 averages in the y dimension (10-day averages over 1 yr). The measured and simulated fluxes using calibrated and uncalibrated parameters are also compared in a difference plot (uncalibrated minus measured and calibrated minus measured). In this way, it is possible to evaluate the calibration results in a diurnal and seasonal context for each variable. Figures 6f, 7f, 8f, and 9f show a conventional scatterplot of the simulated minus calibrated values and measured fluxes.

The seasonal variation of Rnet follows the seasonal variation of solar radiation (not shown). It gradually increases through spring and into summer (September–March, days 90–240) and tends be smaller during the winter. In the simulation using the default parameters set of the model, the model underestimates Rnet around 1200 local time for the whole period of integration (Fig. 6b). Rnet is strongly dependent on radiative properties of vegetation, especially concerning the leaf reflectance. After calibration, near-infrared reflectance (rhoveg_NIR) decreased by approximately 25% from its default value. Although this parameter was not severely modified, if compared with the other ones, it is the most important one for the calculation of Rnet. Figure 6c shows the simulated Rnet after calibration. The overall results of simulations show a good fit between observed and simulated Rnet, and a nearly perfect linear regression line is verified (Fig. 6f). Furthermore, the simulated Rnet was well adjusted to the observed fluxes, with a satisfactory long-term adjustment (Fig. 10a).

Table 2. IBIS hierarchical calibration results for the caatinga site.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Initial</th>
<th>Calibrated range</th>
<th>Calibrated</th>
</tr>
</thead>
<tbody>
<tr>
<td>rhoveg_vis</td>
<td>0.062</td>
<td>0.05–0.057</td>
<td>0.05</td>
</tr>
<tr>
<td>tauveg_vis</td>
<td>0.07</td>
<td>0.03–0.034</td>
<td>0.03</td>
</tr>
<tr>
<td>chiflz</td>
<td>–0.5</td>
<td>From –1.0 to –0.567</td>
<td>–0.9996</td>
</tr>
<tr>
<td>beta1</td>
<td>0.95</td>
<td>0.987–0.99</td>
<td>0.9899</td>
</tr>
<tr>
<td>rroot_coef</td>
<td>1.25</td>
<td>0.6635–2.474</td>
<td>2.474</td>
</tr>
<tr>
<td>rgrowth_coef</td>
<td>0.3</td>
<td>0.1636–0.5907</td>
<td>0.5498</td>
</tr>
<tr>
<td>rhoveg_NIR</td>
<td>0.6</td>
<td>0.4029–0.4698</td>
<td>0.4515</td>
</tr>
<tr>
<td>tauveg_NIR</td>
<td>0.25</td>
<td>0.1412–0.1862</td>
<td>0.1637</td>
</tr>
<tr>
<td>specla</td>
<td>12.5</td>
<td>1.10–19.94</td>
<td>19.066</td>
</tr>
<tr>
<td>avmuir_coef</td>
<td>1</td>
<td>4.27–10.0</td>
<td>9.999</td>
</tr>
<tr>
<td>dispu_coef</td>
<td>0.7</td>
<td>0.3075–0.947</td>
<td>0.8195</td>
</tr>
<tr>
<td>vmax_pft</td>
<td>2.75 × 10⁻⁵</td>
<td>From 1.85 × 10⁻⁵ to 4.0 × 10⁻⁵</td>
<td>3.973 × 10⁻⁵</td>
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<tr>
<td>coefmls</td>
<td>9.0</td>
<td>5.002–9.99</td>
<td>5.058</td>
</tr>
<tr>
<td>tempvm_coef</td>
<td>3000</td>
<td>1750–2939</td>
<td>2398</td>
</tr>
<tr>
<td>tauleaf</td>
<td>1.5</td>
<td>0.6025–1.336</td>
<td>0.9795</td>
</tr>
<tr>
<td>stressf_coef</td>
<td>–5.0</td>
<td>From –3.5404 to –3.50</td>
<td>–3.5</td>
</tr>
<tr>
<td>aleaf</td>
<td>0.45</td>
<td>0.1563–0.4481</td>
<td>0.2384</td>
</tr>
<tr>
<td>alogl_coef</td>
<td>0.1</td>
<td>0.0205–2.484</td>
<td>1.259</td>
</tr>
</tbody>
</table>
fraction consequently tends to increase. A similar pattern of the partition of available energy into $H$ and $LE$ was reported by Chen et al. (2009) and by Rotenberg and Yakir (2011) for other semiarid ecosystems. In general, the model was able to simulate the partition of the available energy into $H$ and $LE$ for the caatinga (Figs. 7 and 8), especially using the calibrated parameters in the simulations.

It is highlighted that the model underestimated $H$ for the period from 0600 to 1500 local time (at ~100 W m$^{-2}$) with the default parameters (Figs. 7b,d), which may have occurred as an underestimation result of the Rnet. This difference was reduced in the simulation considering the calibrated parameters (Fig. 7e). Simulated $H$ had good adjustment to the observed $H$, with a linear regression line close to the 1:1 ratio (Fig. 7f) and a high correlation coefficient, similar to the simulated Rnet. Figure 10b shows a slight bias between the observed data and the simulated data at the end of the simulation. The sensible heat flux is directly dependent upon the amount of net radiation available, such that during dry months it accounts for nearly all of the net radiation. Thus, the related parameters to the calculation of Rnet are dominant in the calculation of $H$. According to sensitivity analyses made by Varejão et al. (2011), among the nine parameters considered to be more relevant for simulation of $H$ values, rhoveg_NIR is the most important as well as Rnet. In the IBIS model, the sensible heat fluxes from vegetation to air are functions of leaf and stem temperature; these two are dependent on the solar fluxes absorbed by the canopies and soil as well as on net absorbed fluxes for infrared radiation. The rhoveg_NIR and other parameters related to leaf reflectance and transmittance were reduced after calibration (Table 2), which contributed to the increase of $H$.

A significant bias is observed in simulated values of LE (Figs. 8b,c), since the model underestimated observed annual total by approximately 11% and 26%
with the default and calibrated parameters, respectively. The statistical $R^2$ (equal to 0.55) value was also low. For the default parameters, IBIS overestimates the values of LE from 0700 to 1200 local time ($\sim 20 \text{ W m}^{-2}$), mainly during the drought months (1–130 days), and underestimates LE from 1000 to 1500 local time ($\sim 34 \text{ W m}^{-2}$) during the rainy season (days from 240 to 330; Figs. 8a,b).

The beta1, rgrowth_coef, and tauleaf parameters are those that affect the calculation of LE in the IBIS model, especially the first one (Varejão et al. 2011), which acts in the control of water-stress responses. It is used to calculate the water uptake by roots and is consequently used to calculate the plant transpiration.

After calibration, the parameters beta 1 and rgrowth_coef increased by 5% and 83%, respectively, while tauleaf decreased by 35%. The changes in these parameters after the calibration contributed to the reduction of LE from 0700 to 1200 local time (Figs. 8c–e). The difference between the values of simulated LE and observed LE is slightly reduced during the drought months; the difference increases during the rainy season, however. Note that even after calibration the model continues to present errors in simulating the variability and intensity of LE throughout the year, which can also be noted in the cumulative sum graph (Fig. 10c). These results suggest that the IBIS model has deficiencies in simulating the abrupt change from dry to wet conditions for the studied area. To test this hypothesis, key variables for the calculation of LE were evaluated in this study.

As highlighted above, the caatinga is a xeromorphic vegetation, which loses its leaves during the dry season and quickly blossoms during the rainy season. Abrupt changes occur in leaf area index (LAI) during the year. To assess the seasonal variability of the LAI that was simulated for the studied area, a time series of LAI (from July 2004 to June 2005) derived from Moderate Resolution Imaging Spectroradiometer (MODIS) images (MOD15A2), considering the pixels over the experimental caatinga flux site, was used. More detail information about MODIS LAI processing, as well as about the evaluation for a semiarid environment, can be found in Myneni et al. (2003) and Fensholt et al. (2004), respectively.

Figure 11 presents the values of simulated LAI for the mentioned period, showing very little seasonal variation for the uncalibrated and calibrated parameters. MODIS LAI responds much faster and more intensely to the seasonality of rain, reaching a peak in April ($1.85 \text{ m}^2 \text{ m}^{-2}$) and a minimum value at the end of the dry season ($0.74 \text{ m}^2 \text{ m}^{-2}$). Considering that the increase of vegetation cover and LAI values is directly linked to higher latent heat fluxes, it seems that the
model underestimates LAI during the wet season and overestimates it during the dry season. The parameters `rgrowth_coef` and `tauleaf` are related to LAI calculations; the modifications that occurred in these parameters were not sufficient to correct errors associated with the simulations, however.

The determination of LE is directly proportional to total transpiration and soil evaporation. For semiarid...
environments, evapotranspiration is an important component of the hydrological cycle, which often consumes a large part of precipitation (Güntner 2002). Figure 12 shows the temporal evolution of the total transpiration, soil evaporation, and volumetric water content simulated using calibrated and uncalibrated parameters. Note that transpiration is dominant in the first months simulated (dry months) and that soil evaporation becomes dominant during wet months (Figs. 12a,b). Because the transpiration was low during the wet months, the soil evaporation is greater, because more energy is available for this component. According to the measured LE, however, it was expected that LE simulated for the wet period would be higher. In a similar way, it was expected that the total transpiration would be higher. Considering that the seasonal variation of LAI has an important effect on the evapotranspiration, if LAI is not well simulated by the model, the errors can be propagated to the partitioning of evapotranspiration into evaporation and transpiration.

Furthermore, it is noteworthy that from dry to wetter soils the soil moisture availability may also be an important factor for stomata regulation and, thus, for evapotranspiration. The total volumetric water content simulated using the calibrated and uncalibrated parameters shows a small difference (Fig. 12c).

The simulated LAI, which was probably overestimated for the dry season, allowed larger water vapor release, leading to overestimation of LE. On the other hand, the lower soil wetness availability simulated for...
the wet season, relative to the driest months, should lead to lower LE values almost linearly. These results suggest that the model underestimates the total volumetric water content during the wet months. The difficulty in simulating LE in semiarid regions was also highlighted in the study performed by Hogue et al. (2005). In that study, the authors calibrated and rigorously evaluated the performance of the "Noah" land surface model (Ek et al. 2003) at two semiarid sites in southern Arizona. The Noah model performed well during the dry periods when $H$ is the dominant energy component, but during the wet monsoon periods the model did not capture the dramatic change in the energy balance and did not capture this variability in LE as well. Kahan et al. (2006) also showed the difficulties of the simplified Simple Biosphere (SSiB) model (Xue et al. 1991) to simulate the energy balance in the semiarid region of the Sahel.

Simulations using default and calibrated parameters versus observed soil heat flux $G$ are presented in Fig. 9.

In general, the amplitude of $G$ is overestimated during daytime hours for most of the period ($\sim 15 \text{ W m}^{-2}$), and the model underestimates it from the late afternoon ($\sim 16 \text{ W m}^{-2}$). The differences in the values of $G$ simulated using the calibrated and default parameters are minimal, which is expected since the calibrated parameters are not directly linked to $G$. The statistical $R^2$ between observed and calibrated values was 0.8. Other studies considering data from different regions of the globe also showed overestimated values of $G$ (Delire and Foley 1999; El Maayar et al. 2001; Kahan et al. 2006),

![Image of diagram](image_url)

**Fig. 11.** Time series of simulated LAI, LAI MODIS, and cumulative precipitation (bars) for the caatinga site.

**Fig. 12.** Evolution of (a) total evapotranspiration, (b) total soil evaporation, and (c) volumetric moisture content, simulated by IBIS with default parameters (SoilWet uncalibrated) and with calibrated parameters (SoilWet calibrated) in the top 2.0 m. (d) Daily cumulative precipitation.
highlighting that the overestimation of $G$ is a common problem in many land surface models. According to El Maayar et al. (2001), one of the reasons for this problem is the poor numerical resolution of soil temperature near the surface, which causes an amplification of $G$ and a delay of turbulent fluxes. On the other hand, because the observational data are also subject to significant error, any discussions about model errors should take into account these errors. Since the long-term mean of the ground heat flux should be close to zero, the mean value of 15 W m$^{-2}$ is very likely to have a contribution for the measurements errors.

c. Validation of the calibrated parameter set for a different surface scheme

To check if the new set of calibrated parameters is also valid for a similar surface model, simulations were performed using the Community Land Model (CLM; Dai et al. 2001, 2003). Biogeophysical processes simulated by CLM include solar and longwave radiation interactions with vegetation canopy and soil, momentum and turbulent fluxes from canopy and soil, heat transfer in soil, hydrological processes of canopy and soil, and stomatal physiology and photosynthesis (Lawrence et al. 2011). The meteorological forcing dataset for the caatinga site was used to force the CLM model. Furthermore, 11 calibrated parameters for the IBIS model (rhoveg_vis, tauveg_vis, chiflz, rgrowth_coef, rhoveg_nir, tauveg_nir, specla, avmuir_coef, dispu_coef, aleaf and beta1) were used in the simulations with the CLM, since these parameters are common to both models.

Figure 13 shows the surface energy balance components simulated using calibrated and uncalibrated parameters. In general, the CLM was able to simulate the seasonal pattern of energy balance components. For the dry months, the CLM overestimated net radiation. For the calibrated parameters, $R_{net}$ decreases, mainly between August 2004 and April 2005. On annual average, $R_{net}$ simulated with the calibrated parameters (135 W m$^{-2}$) is closer to the observed value (128.5 W m$^{-2}$). Using the calibrated parameters, $R_{net}$ decreases, mainly between August 2004 and April 2005. In comparing these results with those obtained with the IBIS model, it is observed that $R_{net}$ simulated by CLM was closer to the observed values for the months from August to January. On the other hand, between February and July, the simulated values of $R_{net}$ by the IBIS model were closer to the observed values. For the sensible heat flux, the CLM underestimated values for the entire period of simulation. For the calibrated parameters, however, the simulated values of $H$ were closer to the observed. The simulated values of $H$ for the period January–May were better than those simulated by the IBIS model. The same inefficiency in simulating LE presented by the IBIS model was also found in the simulations using the CLM. The CLM overestimated the LE between July and December and underestimated it during the wet months. With use of the calibrated parameters, simulated LE had a small improvement. In general, the seasonal LE variability pattern simulated by the CLM model was better than that of the IBIS model. This result was expected since the CLM was initialized with monthly LAI data from MODIS, and, as discussed previously, the IBIS presented inefficiency in simulating the seasonal variability of LAI. In general, the parameters calibrated also presented improvements in the components of the energy balance simulated by CLM.

4. Conclusions

High-quality land surface energy balance simulations are essential because they determine the performance of regional weather and climate models. The land surface
models that simulate these processes generally utilize a large number of parameters, many of which are not regularly measured. Thus, there is a strong need to validate and calibrate these models with experimental data. The aim of this study was to provide an accurate set of parameters of the vegetated surface so as to make improvements in the simulation of the radiation and energy balance in a complex ecosystem that surrounds the caatinga vegetation of the semiarid region of Brazil. Few studies involving the validation and calibration of land surface models had been performed that consider semiarid regions. This study employed a multiobjective hierarchy calibration system for the IBIS model. The hierarchical calibration procedure was based on hierarchical temporal organization of natural systems, which is also reflected in the structure of the IBIS model. Thus, this procedure provided a more realistic model calibration.

The overall results show a good estimation of the net radiation and sensible heat flux. On a diurnal scale, the greatest difference between the simulated and observed $R_{\text{net}}$ and $H$ exists during the day. This difference was reduced in $R_{\text{net}}$ and $H$ simulated using the new set of calibrated parameters. The greatest bias is noticed in LE. The IBIS model was not able to efficiently simulate the annual variability of LE, even using the new set of calibrated parameters. This seems to be a problem that results from prior to the calibration procedure. Results found in this study and other studies performed for other semiarid regions of the globe emphasize that the current parameterization schemes applied to semiarid vegetation require improvements, especially concerning the energy partitioning at the surface during abrupt changes from dry to wet conditions in the study area. Thus, the parameter optimization may not be sufficient if processes are missing or misrepresented.

To allow a model to represent accurately the vegetation dynamics of a semiarid region, it is necessary to associate the calibration with improved parameterizations within these models. For the IBIS model, these improvements should be made primarily in the phenology module that is coupled to the IBIS. Other parameters that were not calibrated in this study may be considered, however, since the choice of parameters to be calibrated might also depend on the ecosystem.

One problem typically encountered in model calibration is that observations of only one or a couple of variables are normally available. Moreover, it is necessary to install more micrometeorological towers as a source of data to support these studies and to enable the calibration of other processes simulated by IBIS. There currently is a lack of micrometeorological data for semiarid regions in Brazil. Because of the scarcity of data, this study involved only data from a single experimental site.

This study was a first attempt to improve the representation of biophysical processes for a semiarid region of Brazil through use of multiobjective hierarchical calibration. These investigations allowed a better understanding of the energy fluxes and the physical vegetation properties that affect these exchange processes in the caatinga ecosystem. Such understanding is crucial to simulate semiarid climate processes.

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