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Multi-site land surface model optimization: An exploration of objective functions

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ABSTRACT

Land surface/ecosystem models are important tools for understanding the dynamic interactions between land surface and the atmosphere. However, to be effective these models must be carefully calibrated to accurately represent ecosystem processes. Generally, such models are calibrated for one site and then run with the same set of calibrated parameters, either for other sites or for a whole region with the same plant functional type. Here we investigate an alternative approach to the challenge of calibration. We perform multi-site calibration of net ecosystem exchange for two pasture sites in Amazonia. Twenty different objective functions (five adjustment measures subject to four calibration options) are evaluated to investigate the consistency and sensitivity of the results in a multi-site model calibration. Our results indicate that, with some restrictions regarding the choice of objective function, multi-site calibration is possible and produces consistent results across sites. Ultimately, the choice of objective function should be based on the intended use of the model. We recommend that the site-weighted method using mean absolute error as objective function should be used for shorter time scales and the site-weighted maximum bias error as objective function is better for longer time scales.

1. Introduction

Land surface models are an essential tool in climate modeling, and coupled climate-vegetation models have been widely used in investigations about the effects of changes in land use, land surface processes, carbon cycle and its implications for the Earth's climate (Costa and Pires, 2010; Foley et al., 2000; McGuire et al., 2001; Williams et al., 2009). Coupled climate-biosphere models can be used in various scenarios of land use change. However, to provide realistic results and forecasts, models must be carefully calibrated to accurately represent ecosystem processes (Liu et al., 2003).

In terrestrial ecosystem models several processes are represented by parameters (affecting the performance of the model) which need to be specifically obtained for each ecosystem (Groenendijk et al., 2011). Given the frequent lack or inability to obtain direct measurements, some of these parameters must be calibrated through optimization methods in order to minimize the differences between observed data and the model outputs. Several optimization methods have been used for parameter estimation in ecosystems models, such as genetic algorithms (D'heygere et al., 2006), gradient methods (Rayner et al., 2005; Wang et al., 2001), Kalman filters (Ju et al., 2009; Mo et al., 2008; Zhu et al., 2009) and global search methods (Braswell et al., 2005; Gupta et al., 1999; Knorr and Kattge, 2005). However, it is the choice of objective function rather than the choice of optimization method that has the greatest impact on model results (Trudinger et al., 2007).

Various objective functions have been proposed to identify and account for errors between simulated and observed data sets. The most commonly used measures are the correlation coefficient (r), mean absolute error (MAE), root mean square error (RMSE), mean bias error (MBE), slope of the least-squares regression between simulated and observed data (Willmott, 1982; Willmott and Matsuura, 2005), coefficient of efficiency (Legates and McCabe, 1999), and average error. This final measure and other key objective functions are reviewed by Janssen and Heuberger (1995).

Another important issue in model optimization is that models are generally calibrated for a single site that is characterized by a particular vegetation class or plant functional type (PFT). After calibration, the model is applied to other sites or to an entire region with the same PFT. The calibrated parameter set, however, may not be representative for other sites or for the wider region

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(Groenendijk et al., 2011). Alternative solutions that perform multi-site calibration (simultaneous calibration at two or more sites) are therefore desirable.

Multi-site calibration (≥2 sites) has recently become more common due to greater data availability, improved model sophistication and better computing capabilities (White and Chaubey, 2005). Indeed, several different approaches to multi-site model calibration have been considered (Bekele and Nicklow, 2007; Cao et al., 2006; White and Chaubey, 2005; Zhang et al., 2008, 2010), although most examples come from the hydrology literature. In one of the earliest studies, White and Chaubey (2005) applied multi-site calibration to a watershed model, using an objective function that simultaneously calculated statistical tests to minimize errors to several variables and sites. They concluded that multi-site calibration more accurately predicted measured values and could be used to accurately predict watershed response for various outputs.

Bekele and Nicklow (2007) considered two calibration methods for a watershed model; the first method used specific objective functions to fit different segments of the time series. In the second method, the calibration was performed by simultaneously using data from multiple gauging stations. The results indicated that the second calibration method outperformed the first. Zhang et al. (2008) attempted to optimize 16 parameters of a watershed model through the application of a single objective optimization method and a multi-objective optimization algorithm for a single site and for three sites concurrently. They concluded that parameters estimated by optimizing the objective function at three sites consistently produced a better goodness-of-fit than those obtained by optimization at a single site.

In contrast to hydrological studies, multi-site calibration of land surface ecosystem models is still in an early stage of development and many questions remain unanswered. It is still unclear, for example, if model parameters should have the same calibrated value at different sites with the same PFT. Some parameters may be strongly species-dependent and their true value may vary according to the composition at each site, even for the same PFT. This effect could potentially be isolated by using different sites covered by the same single species – a common situation for agricultural land uses. However, parameters that are dependent on soil characteristics and the management history of sites cannot be adequately controlled. Moreover, even if isolation of ecosystem composition is possible other questions arise such as how model parameters will vary according to the objective function used during multi-site calibration.

The aim of this article is to assess the performance of a terrestrial ecosystem model that has been calibrated for two sites using a range of objective functions and analyze the difference between individual and multi-site calibration. Specifically, we use the SITE model (Santos and Costa, 2004) to perform the single and multi-site calibration of net ecosystem exchange (NEE) for two pasture sites in Amazonia. Model performance is optimized using 20 different objective functions: Five adjustment measures subject to four calibration options – two single-site calibrations (one per site) and two multi-site calibrations (varying on the weight given to each site: the same weight or a weight proportional to the duration of the time series in each site).

2. Material and methods

2.1. Experimental sites

The calibration was performed for two experimental pasture sites located in the Amazon region. The sites are part of the Large-Scale Biosphere-Atmosphere Experiment in Amazonia (LBA) towers network and are used in the Data Model Intercomparison Project (see LBA-DMIP editorial by Costa in "2013").

The first pasture site is located at the Fazenda Nossa Senhora ranch (hereafter referred to as site FNS) (10°45′S, 62°21′W, 230 m), in Ouro Preto d'Oeste, Rondônia, Brazil. This site is in the center of a deforested area with an approximate radius of 50 km – deforestation was caused by a fire in 1977 to clear land for crop cultivation. Since the early 1980s the area has been uniformly covered by the *grass Brachiaria brizantha*. Nobre et al. (1996) describe the climate in the site as follows: annual mean air temperature ranging from 23 to 24 °C, monthly mean precipitation of 200 mm from November to April, and 20 mm from July to August – being as low as 5 mm in July.

The second site is on a farm 77 km along the Santarém-Cuiabá highway (hereafter referred to as site K77) (03°01′S, 54°53′W), near Santarém, Pará State, Brazil. The forest was cleared in 1990, after which the field was planted with the same grass species as the first site, *Brachiaria brizantha*. In November 2001 the site was burned and plowed for rice cultivation.

2.2. Model description

SITE is a simplified dynamic vegetation model of tropical ecosystems developed by Santos and Costa (2004). This model is based on previously developed models, mainly LSX (Pollard and Thompson, 1995), LSM (Bonan, 1996), IBIS (Foley et al., 1996) and SiB2 (Sellers et al., 1996) and provides a simple simulation of the fluxes of CO_2, water and energy, as well as the dynamics of carbon in the ecosystem. It operates through modeling the relationships between several fundamental ecosystem processes: canopy infrared radiation balance, solar radiation balance, aerodynamic processes, canopy physiology and transpiration, balance of water intercepted by the canopy, transport of mass and energy in the atmosphere, soil heat flux, soil water flux and carbon balance. Although SITE is an intentionally simple model, it has the necessary complexity to represent the main processes responsible for ecosystem functioning.

SITE is a dynamical single point model that uses an integration time step (dt) of one hour. The model is structured with one layer of canopy and two layers of soil. The main output variables of the model are latent heat flux, sensible heat flux, water vapor flux and net ecosystem exchange (NEE). In this study, we only optimize for NEE.

A full specification of the SITE model is provided by Santos and Costa (2004). Here, we present a brief description of the part of the model that is relevant to understand the calibration of parameters and the optimized output. For convenience, the calibrated parameters (summarized in Table 1) are identified by a superscript asterisk (*).

NEE is expressed as the difference between soil heterotrophic respiration (R_H) and the net primary production (NPP) (Eq. (1)). Negative values of NEE indicate assimilation of carbon by the

Table 1
Parameters calibrated and range of values tested.

Calibrated parameters	Range of values tested
γ	0.010–0.050 (changing 0.005, dimensionless)
m	1.0–10.0 (changing 1.0, dimensionless)
V_{max}	10.0–120.0 (changing 5.0, μmol-CO_2 m^{-2} s^{-1})
St_m	−1.0–−7.0 (changing 1.0, dimensionless)
K_u	1.0–5.0 (changing 0.5, dimensionless)
K_f	1.0–5.0 (changing 0.5, dimensionless)