Atmos. Chem. Phys. Discuss., 14, 23995–24041, 2014
www.atmos-chem-phys-discuss.net/14/23995/2014/
doi:10.5194/acpd-14-23995-2014

Atmospheric Chemistry and Physics Discussions

Evaluation of MEGAN-CLM parameter sensitivity to predictions of isoprene emissions from an Amazonian rainforest

J. A. Holm[1], K. Jardine[1], A. B. Guenther[2,3], J. Q. Chambers[1,4], and E. Tribuzy[5]

[1]Lawrence Berkeley National Laboratory, Berkeley, California, 94720, USA
[2]Pacific Northwest National Laboratory, Richland, Washington, 99354, USA
[3]Department of Civil and Environmental Engineering, Washington State University, Pullman Washington, 99163, USA
[4]Department of Geography, University of California, Berkeley, Berkeley, California, 94720, USA
[5]National Institute for Amazon Research (INPA), Ave. Andre Araujo 2936, Campus II, Building LBA, Manaus, AM 69.080-97, Brazil

Received: 26 August 2014 – Accepted: 5 September 2014 – Published: 17 September 2014

Correspondence to: J. A. Holm (jaholm@lbl.gov)

Published by Copernicus Publications on behalf of the European Geosciences Union.

Abstract

Tropical trees are known to be large emitters of biogenic volatile organic compounds (BVOC), accounting for up to 75 % of the global isoprene budget. Once in the atmosphere, these compounds influence multiple processes associated with air quality and climate. However, uncertainty in biogenic emissions is two-fold, (1) the environmental controls over isoprene emissions from tropical forests remain highly uncertain; and (2) our ability to accurately represent these environmental controls within models is lacking. This study evaluated the biophysical parameters that drive the global Model of Emissions of Gases and Aerosols from Nature (MEGAN) embedded in a biogeochemistry land surface model, the Community Land Model (CLM), with a focus on isoprene emissions from an Amazonian forest. Upon evaluating the sensitivity of 19 parameters in CLM that currently influence isoprene emissions by using a Monte Carlo analysis, up to 61 % of the uncertainty in mean isoprene emissions was caused by the uncertainty in the parameters related to leaf temperature. The eight parameters associated with photosynthetic active radiation (PAR) contributed in total to only 15 % of the uncertainty in mean isoprene emissions. Leaf temperature was strongly correlated with isoprene emission activity ($R^2 = 0.89$). However, when compared to field measurements in the Central Amazon, CLM failed to capture the upper 10–14 °C of leaf temperatures throughout the year (i.e., failed to represent ~ 32 to 46 °C), and the spread observed in field measurements was not representative in CLM. This is an important parameter to accurately simulate due to the non-linear response of emissions to temperature. MEGAN-CLM 4.0 overestimated isoprene emissions by 60 % for a Central Amazon forest (5.7 mg m^{-2} h^{-1} vs. 3.6 mg m^{-2} h^{-1}), but due to reductions in leaf area index (LAI) by 28 % in MEGAN-CLM 4.5 isoprene emissions were within 7 % of observed data (3.8 mg m^{-2} h^{-1}). When a slight adjustment to leaf temperature was made to match observations, isoprene emissions increased 24 %, up to 4.8 mg m^{-2} h^{-1}. Air temperatures are very likely to increase in tropical regions as a result of human induced climate change. Reducing the uncertainty of leaf temperature in BVOC algorithms, as well as

ACPD
14, 23995–24041, 2014

improving the accuracy of replicating leaf temperature output in land surface models is warranted in order to improve estimations of tropical BVOC emissions.

1 Introduction

Vegetation is known to be a large emitter of non-methane, biogenic volatile organic compounds (BVOCs) (i.e., 1150 Tg C yr^{-1}), well exceeding chemical compounds that are emitted as a result of human activity by an estimated factor of ~ 10 worldwide (i.e., ~ 142 Tg C yr^{-1}) (Lamb et al., 1993; World Meteorological Organization, 1994; Goldstein and Galbally, 2007). BVOCs play a critical role in the atmospheric chemistry of the troposphere as their photochemical reactions influence the distribution and/or lifetime of gases; specifically ozone (O_3), methane (CH_4), hydroxide (OH), and carbon monoxide (CO), all which can alter the radiative balance of the atmosphere (Atkinson and Arey, 2003; Pacifico et al., 2009). In terms of influence on precipitation, BVOC oxidation can provide condensed matter for formation of secondary organic aerosols (Went et al., 1960), which is the fine particle predominantly serving as cloud condensation nuclei (CCN) over the Amazonian rainforest (Poschl et al., 2010). Hundreds of biogenic VOCs have been identified, yet isoprene is one of the dominant compounds representing the annual global flux to the atmosphere, and will be the focus of this study.

Tropical trees are estimated to account for 48 % of total global BVOC emissions, 60 % of terpenoid emissions (Guenther et al., 2012), and nearly 75 % of the global atmosphere isoprene budget (Guenther et al., 2006). A better understanding of the environmental and biological controls over isoprene emissions from forests are an interest of study because of the complex interactions and feedback processes linking increasing global temperatures, forest production and growth, and atmospheric production of secondary organic aerosols and ozone (Penuelas and Staudt, 2010; Nguyen et al., 2011; Kulmala et al., 2013).

ACPD
14, 23995–24041, 2014

Increased aerosol loading reduces the amount of solar radiation reaching the Earth's surface by absorbing or reflecting radiation and increasing diffuse irradiance (Forster et al., 2007). Through the formation of clouds, CCN can increase the planetary albedo, leading to an increase in diffuse light, and a reduction in direct light. Studies have shown that diffuse light can propagate deeper into dense tropical forests and increase photosynthesis and canopy light use efficiency (Choudbury, 2001; Alton et al., 2007; Doughty et al., 2010). This in turn could create either a positive feedback for isoprene emissions through increased plant growth and carbon allocation to isoprene production, or a negative feedback as a result of decreased temperatures associated with increased diffuse light. Positive feedbacks on climate change are expected from the photochemical production of O_3, increasing lifetimes of CH_4, and release of latent heat of water condensation from enhanced CCN concentrations. Thus, isoprene mediated interactions between the terrestrial biosphere and the atmosphere is complex and is both sensitive to and driven by changes in climate (Pacifico et al., 2009).

1.1 Contributions leading to uncertainties in biogenic emission rates

Some of the main driving biophysical elements that lead to large variations in isoprene emissions are leaf temperate (T_{leaf}), light conditions, shading and related photosynthetically active radiation (PAR), internal leaf CO_2 concentration, LAI, and species composition and plant functional type (PFT) (Guenther et al., 2006). While at differing levels of intensity, these elements are also predicted to vary with a changing climate and therefore are critical factors to evaluate. Leaf temperatures and light intensity, the major environmental drivers of isoprene emissions are predicted to be substantially modified in tropical regions through climate change processes. In tropical forests additional variations in emissions can vary as a function of the seasonal transitions from the wet to dry season (Kuhn et al., 2004a; Baker et al., 2005), species composition and species-specific variations (Harley et al., 2004; Kuhn et al., 2004a), as well as a function of leaf age (Kuhn et al., 2004b; Alves et al., 2014). Isoprene emissions are known to be strongly light dependent and can show a lack of decreasing leaf-level emission at light

ACPD
14, 23995–24041, 2014

saturation in tropical systems (Lerdau and Keller, 1997). Sensitivities to temperature also have a major role in controlling isoprene emission rates, and could be the most influential variable (Monson et al., 1992; Wang et al., 2011).

Isoprene emissions are found to have an exponential response to increasing temperature (Loreto et al., 1996; Keller and Lerdau, 1999). Jardine et al. (2014) found that isoprene emissions in tropical mango trees (*Mangifera indica* L.) continued to increase at elevated leaf temperatures, $> 37.5\,^{\circ}C$, despite the fact that optimum temperature for net photosynthesis (30.0–32.5 °C) had already been surpassed. Rinne et al. (2002) found that measured isoprene flux in a Central Amazon forest correlated well with a light and temperature emission activity factor as calculated from a canopy model (Guenther, 1997), but had a stronger correlation with measured sensible heat flux. Many, but not all, emission rate models have been parameterized using the temperature and light algorithms of Guenther et al. (1995) (hereafter referred to as G95). Debate continues on whether the assemblage of emission models are in general agreement with each other or whether they differ from each other in emission rate estimates (Pouliot and Pierce, 2009; Arneth et al., 2011; Zare et al., 2012; comparing Baker, 2007 to Warneke et al., 2010) depending on the scale, land-use type, or climate used. A sensitivity analysis on the controlling environmental factors of isoprene emissions in models may help narrow the uncertainty and variability.

1.2 Modeling biogenic emissions

The need to accurately model biogenic emission rates is urgent and needed in order to assess the interactions with future changes in climate. We use the Model of Emissions of Gases and Aerosols from Nature version 2.1 (MEGAN 2.1; Guenther et al., 2012). MEGAN 2.1 is a biogenic flux global model that has been embedded in the land surface model, Community Land Model (CLM) which is part of the Community Earth System Model (CESM). Biogenic emission models are useful for global modeling, however when trying to match observational records, the G95 global model estimates of biogenic emissions have been reduced by 50 % for tropical regions (Prather et al.,

ACPD
14, 23995–24041, 2014

2001; von Kuhlmann et al., 2004). For example, the Intergovernmental Panel on Climate Change Third Assessment Report (IPCC TAR) suggested using global isoprene emission rates that are 56 % less than G95 estimates (Prather et al., 2001). In the past, many global three-dimensional chemistry-transport models assumed 20 % less BVOC emissions than G95 estimates. There have been efforts to modify G95 algorithms to fit the temperature and light response of tropical species (Keller and Lerdau, 1999) although it is not clear if the differences they observed were due to the inherent differences in tropical plants or due to the environmental growth conditions (e.g., high light and temperature). That study found that if the standard algorithms, developed using temperate species, were used for high-light and high-temperature tropical forests, isoprene was significantly underestimated.

In addition to uncertainties in observational and modeled isoprene emission rates, there are also large uncertainties associated with terrestrial components estimates (i.e., net primary productivity (NPP), LAI, T_{leaf}) and climate projections in global Earth System Models (ESMs). This is particularly true for tropical forests (Friedlingstein et al., 2006; Cox et al., 2013), as seen by substantially high LAI and gross primary productivity (GPP) estimates for the Amazon (Lawrence et al., 2011). For example the disagreement in projections of precipitation and temperature from 18 models used in the Coupled Model Intercomparison Project phase five (CMIP5) can result in large differences in the total carbon uptake of tropical forests (Ahlström et al., 2012). Improving the terrestrial representation and land–atmosphere interactions of ESMs are important for improving prognoses of future climate change under multiple scenarios.

The objectives of this study will aid in evaluating the strengths, weaknesses, and sensitivities of current leaf-level BVOC emission models in an ESM, and how they can be improved. A baseline evaluation of MEGAN-CLM for tropical forests is necessary for improving leaf-level BVOC emission algorithms for the coupled plant-ecosystem-atmosphere-cloud system. The main research questions of this study are: (1) which biophysical parameters in CLM have the strongest control on landscape scale isoprene emissions, (2) which biophysical parameters contributes the most variability in isoprene

ACPD
14, 23995–24041, 2014

emissions and leads to the largest uncertainty in emissions, and (3) how well do driving variables in MEGAN-CLM compare to in situ measurements? Results from the model evaluation and sensitivity analysis will be used to develop a detailed plan for recommended parameter and structural changes to MEGAN-CLM to improve simulation of tropical forest isoprene emissions.

2 Methods

2.1 Model description

2.1.1 Model of Emissions of Gases and Aerosols from Nature (MEGAN)

MEGAN 2.1 was used to test variations and sensitivities in isoprene emissions from tropical forests. MEGAN 2.1, also available as a stand-alone model, is a biogenic flux global model that has: (1) been updated to estimate emissions from urban, rural, and agricultural ecosystems, (2) been expanded to estimate emissions of 147 chemical species, and (3) been embedded in the land surface model, Community Land Model (CLM 4.0 and CLM 4.5). The genesis of MEGAN 2.1 is developed from MEGAN 2.0 (Guenther et al., 2006), based off of emission algorithms originally developed in Guenther et al. (1995). The global emission of isoprene predicted by G95 was 503 Tg C yr^{-1}. Estimates from the first version of MEGAN similarly ranged from 440–660 Tg C yr^{-1}, depending on the landcover and climate driving variables used, and annual estimates from MEGAN 2.1 had a similar range and an average of 471 Tg C (equivalent to 534 Tg).

The MEGAN approach calculates a whole canopy emission rate based on whole canopy flux measurements. This allows the model to account for all ecosystem emission sources such as vegetation, including woody tissues, roots, and flowers, as well as accounting for varying biophysical controls on emission processes and sources. The whole canopy approach has benefits and drawbacks due to a lack of understanding re-

ACPD
14, 23995–24041, 2014

garding the contribution of each ecosystem as an emission source and the influence of environmental controlling forces on emission rates (Harley et al., 2004; Pacifico et al., 2009). Two major factors are taken into consideration and required for modeling BVOC emissions from terrestrial sources (Guenther et al., 1995, 2012). They are (1) defining an emission factor (ε) based on observations for each emission type, and (2) simulating the environmental processes controlling the variation in emissions, also know as the emission activity factor, (γ, unitless). The emission activity factor accounts for changes in atmospheric, biophysical, and phenological conditions, all of which control emission responses. The emissions activity factor (γ, Eq. 1) considers emissions in response to a canopy environment coefficient (C_{CE}), leaf area index (LAI) defined as γ_L (Eq. 2), photosynthetic active radiation, PAR (γ_P, Eq. 3), leaf temperature (γ_T, Eq. 4), leaf age (γ_A), soil moisture (γ_{SM}), and CO_2 inhibition (γ_C).

$$\gamma = \gamma_L \times \gamma_P \times \gamma_T \times \gamma_A \times \gamma_{SM} \times \gamma_C \quad (1)$$

$$\gamma_L = C_{CE} \times \mathrm{LAI} \quad (2)$$

The C_{CE} was assigned a constant value of 0.3 in MEGAN-CLM used here, and assigned 0.57 for the MEGAN canopy environment model (Guenther et al., 2012). This coefficient forces the emission activity factor to a value of 1.0 and so accounts for the differences in the canopy environment models used for CLM and for Guenther et al., 2012. In this current modeling framework, for a tropical Amazonian forest γ_A and γ_{SM} are held constant at 1.0. This rationale is based on the assumption that leaf age is assumed to be constant for tropical evergreen canopies, and soil moisture is assumed to have no affect because soil moisture is considered to be greater than wilting point in

ACPD
14, 23995–24041, 2014

the tropics.

$$\gamma_P = C_P \left[\frac{\alpha \times \mathrm{PAR}}{\left(1 + \alpha^2 \times \mathrm{PAR}^2\right)^{0.05}} \right] \quad (3)$$

$$\gamma_T = E_{opt} \times \left[\frac{C_{T2} \times \exp\left(C_{T1} \times x\right)}{C_{T2} - C_{T1} \times \left(1 - \exp\left(C_{T2} \times x\right)\right)} \right] \quad (4)$$

The light activity factor, γ_P (Eq. 3) accounting for solar radiation follows the algorithms described in Eqs. (6) and (7) of Guenther et al. (2006). New developments in MEGAN 2.1 include emission activity factors that are determined for each compound class, including a light dependent fraction and a remaining light independent fraction, and Eq. (3) is applied separately for sunlit and shaded leaves. The temperature activity factor, γ_T (Eq. 4) follows the algorithms described in Eqs. (8) and (9) of Guenther et al. (2006). Eq. (8) in Guenther et al. (2006) solves for the temperature optimum coefficient (T_{opt}) as a function of average leaf temperature over the past 240 h, and additional coefficients based on observations. Similar to the light activity factor, the temperature activity factor also takes into account the light dependent and light independent fraction of the canopy. This temperature activity factor algorithm has been used in many BVOC model studies. However, it has been found that BVOC emissions are highly sensitive to changes in leaf temperature (Tingey et al., 1991; Penuelas and Llusia, 2003; Pacifico et al., 2009), and could lead to large uncertainties in tropical emission estimates. Parameter descriptions and values for the parameters found in each emissions activity factor (γ_P, γ_T, γ_L, γ_C), which determine the overall emissions activity factor (γ, normalized ratio) can be found in Table 1. These algorithms have been used extensively, but uncertainties still remain. A goal of this paper is to investigate the biophysical processes controlling ecosystem emission variations as predicted by Eq. (1) in MEGAN and CLM.

ACPD
14, 23995–24041, 2014

2.1.2 Community Land Model (CLM)

The Community Land Model (CLM) is the land component of the Community Earth System Model (CESM) (Collins et al., 2006; Gent et al., 2011) that models global climate and earth systems. In this study we used the stand-alone version of CLM 4.0 and CLM 4.5. In both versions of CLM we used a data atmosphere model, a "stub" ocean, a "stub" sea-ice model, and we utilized the carbon-nitrogen (CN) or biogeochemistry (BGC) option. Detailed descriptions of updates to version 4.0, algorithms used, and the general structure of CLM can be found in the CLM 4.0 Technical Description (http://www.cesm.ucar.edu/models/cesm1.0/clm/CLM4_Tech_Note.pdf; Oleson et al., 2010; and Lawrence et al., 2011). In this study for CLM 4.0 we used the present day, 2000 control CLM-CN case, using Qian atmospheric forcing data (Qian et al., 2006). For CLM 4.5 we used the present day, 2000 control CLM-BGC case, using CRUNCEP reanalysis atmospheric forcing data (Piao et al., 2012). For model comparisons against observed field data, we used CLM results from a single gridcell located at 2°35′ S, 60° W, located in the Central Amazon.

MEGAN 2.1 comprises the BVOC submodel that has been embedded in CESM/CLM (Guenther et al., 2012), and estimates emissions for 19 compound classes, which can be broken into 147 individual compounds. This version uses vegetation emission factors for each of the compound classes, and for each plant functional type (PFT) using the PFT scheme followed in CLM (Lawrence et al., 2011). Emission factors that are regional and site specific can be adopted in MEGAN, however generic PFT vegetation categories are used while running MEGAN in CESM. This categorization allows for global modeling that is intended to represent the global average for each PFT but cannot capture the considerable regional variability within a PFT. The CLM PFT scheme includes fifteen PFTs plus bare ground in CLM 4.0 and updates to CLM 4.5 include an additional crop PFT if the irrigation model is active, and six additional PFTs if the crop model is active. This study is focused on the sensitivities and variation of BVOC emissions from tropical forests as reported by MEGAN-CLM. Currently, only the broadleaf

ACPD
14, 23995–24041, 2014

evergreen tropical tree PFT covers the CLM gridcell for the locale of interest. Vegetation VOC emission can vary widely between species, and regarding isoprene specifically, some species are emitters while others are non-emitters. Therefore, a single isoprene emission factor for a PFT cannot represent the actual variability and will be unsatisfactory for simulations that require an accurate representation of regional variability. In order to account for observed variability in emissions, MEGAN2.1 includes a land-cover base with more than 2000 ecoregions and PFT emissions that can differ for each ecoregion (Guenther et al., 2012). Including ecoregions in tropical forests improves the representation of variability in PFT emission factors and while there are some indirect and direct above-canopy flux measurements that were available for assigning these factors, there are relatively very few observations for tropical forests.

2.2 Model analysis

The emission activity factor, Eq. (1), for each PFT in CLM is specified by 19 parameters (Table 2). We conducted a sensitivity analysis to help determine which parameters were most and least influential in terms of isoprene emissions from tropical plants. We define sensitivity analysis here as the study of how uncertainty in the output of the model can be apportioned to different sources of uncertainty in the model input, as defined by Saltelli et al. (2008). It is then intended that the sensitivity analysis will influence and prioritize observational data. Simple linear regression analysis was conducted to explore the relationship between the emission activity factor for a Central Amazon tropical forest and 14 out of the 19 explanatory variables in Eq. (1), reporting the coefficient of determination (R^2) for each of the 14 variables. We would like to infer how well the emission activity factor can be predicted, and to what degree by model variables such as leaf temperature (T_{leaf}), PAR on sunlit and shaded leafs (PAR_{sun} and PAR_{shade}), LAI, intracellular leaf CO_2 (Ci_{sun} and Ci_{shade}), or sunlit fraction of canopy (f_{sun}). Results from the correlation between the biophysical variables and the emission activity factor were compared for a Central Amazon forest and a temperate forest

ACPD
14, 23995–24041, 2014

located in North American, the dominant studied forest type for estimated emission factors and emission activity.

A Monte Carlo simulation analysis has been used to determine model parameter output uncertainty, and gauge which parameter leads to the largest variation and uncertainty in BVOC emission in tropical forests. We define uncertainty analysis here as a type of sensitivity analyses which focuses rather on quantifying uncertainty in model output. Probability density functions (PDFs) for each of the model parameters in the Monte Carlo simulation have been estimated based on variability seen over eight decades of model simulations by an offline CLM present-day control run. A random sample was chosen from the PDF of each parameter, and then solved deterministically. A Monte Carlo simulation was conducted for varying all 14 of the non-constant uncertain parameters used in MEGAN-CLM for a combined output uncertainty. Next, additional Monte Carlo simulations were conducted which varied each of the 19 parameters one-at-a-time, while all other parameters were held constant. A total of 5000 simulations were conducted for each of the 20 Monte Carlo simulations.

2.3 Field data and sampling

2.4 In situ Amazon leaf temperature measurements

Leaf temperatures from upper canopy leaves in a primary rainforest in the central Amazon were collected from the ZF2 field station in Brazil (02°38′ S 60°09′ W), during 2003. Leaf temperature data during the daytime hours (10:00–16:00 AMT) were analyzed from the TN-S and T14 towers. Leaf temperatures were monitored every minute, using 25 thermocouples (copper-constant, 0.08 mm, AWG40, Omega Engineering, Stanford, CT, USA). Equipment failure did occur intermediately, resulting in periodic lack of sampling over the one-year period. The largest amount of equipment failure occurred during the rainy season, over the months of December, January, and February. The thermocouples were kept in contact with the leaves using a micro-porous surgical tape (1538-0 3M^{TM}Company, USA), and placed on leaves that were fully expanded. A leaf

ACPD
14, 23995–24041, 2014

temperature > 50.0 °C was categorized as an outlier and removed from the dataset. To account for potential measurement error or non-transpiring leaves, maximum leaf temperature for a given seasonal period was estimated as an average of the upper 5 % of the maximum individual leaf temperature. Leaf temperatures were collected from 16 different species in order to capture a wide representation of the forest canopy (*Peltogine excelsa*, *Inga* sp., *Brosimum parinarioides*, *Jacaranda copaia*, *Protiumapiculatum*, *Protium* sp., *Guarea* sp., *Abuta cf. panurensis*, *Macherium* sp., *Tetracera amazonica*, *Zygia racemosa*, *Micropholisguyanensis*, *Pouteriaanomala*, *Pouteriawilliamii*, *Licaniaoctandra* and *Eschweilera wachenheimii*).

2.5 In situ Amazon isoprene emission measurements

Field measurements of isoprene and other BVOC emissions in tropical forests are lacking. Reported values include indirect flux estimates based on inverse modeling of ambient concentrations, direct above-canopy fluxes estimates, and leaf level flux measurements. Many of these data are focused on characterizing species level diversity and do not examine biophysical variability. Measurements are usually taken over a few days and/or on few trees. For example, Harley et al. (2004) reports a large summary of isoprene emission across the Large Scale Biosphere–Atmosphere Experiment (LBA) including 125 species but rates for most species are based on only a few measurements. In the tropics isoprene emissions dominate over monoterpene emissions (Guenther et al., 1995; Rinne et al., 2002), so in this study we are going to focus on the response of isoprene emission to varying parameters in MEGAN-CLM. We are using field measurements of isoprene from previous studies located in four Amazonia sites (Kesselmeier et al., 2002; Greenberg et al., 2004; Harley et al., 2004; Rinne et al., 2002; Alves et al., 2014), each using multiple measurement techniques and covering 10 months of the year (Table 1, Fig. 1). In situ measurements of isoprene were collected during the months of January, February, June, and July from Floresta Nacional do Tapajos, Para, Brazil (02°51′ S 54°58′ W) at primary terra firme, closed canopy sites using eddy flux techniques (Rinne et al., 2002), ambient concentrations measured us-

ACPD
14, 23995–24041, 2014

ing a tethered balloon and inverse boundary layer chemistry and dynamics modeling (Greenberg et al., 2004), or from leaf level measurements using both controlled and uncontrolled leaf enclosures (Harley et al., 2004). Additional in situ measurements of isoprene for the months of November and December were collected at sites north of Manaus, Brazil at Reserva Biologica do Cuieiras (02°36′ S 60°12′ W), a primary rainforest using leaf measurements on a single tree species (Alves et al., 2014), and measured in the afternoon by a relaxed eddy accumulation technique (Kesselmeier et al., 2002). In situ measurements for the month of September and October were collected at Reserva Biologica Jaru, also a primary rainforest in Rondonia, Brazil (10°08′ S 62°54′ W), using leaf and branch enclosures on three tree species. This site is furthest in distance from the other sites and from the ZF2 field station where leaf temperature measurements where collected. Lastly, estimates of emissions for the month of March were collected at Balbina, Amazonas (01°59′ S 59°12′ W) in a moist forest, based on tethered balloon measurements of boundary layer concentrations and an inverse model (Greenberg et al., 2004).

3 Results

3.1 MEGAN-CLM isoprene emission results

The MEGAN-CLM 4.0 model predicted annual isoprene emissions from a Central Amazon tropical forest to be 5.7 mg m^{-2} h^{-1}, with an average standard deviation of 8.0 mg m^{-2} h^{-1} across the seasonal variation (Fig. 1). The time of the year with the lowest modeled isoprene emission was June, right at the on-set of the dry season. From July through October isoprene emissions steadily increased to a peak in October of 6.9 mg m^{-2} h^{-1} ± 1.0 (SD). Isoprene emissions during the wet season were on average less than the dry season for the Central Amazon forest as predicted by MEGAN-CLM 4.0. All driving variables, apart from the prescribed emission factor ε for

ACPD
14, 23995–24041, 2014

each PFT and compound, were determined from the functionalities and processes in the CLM biogeochemical, land surface model.

In contrast MEGAN-CLM 4.5, which has been updated with a new belowground biogeochemistry scheme and uses the CRUNCEP reanalysis atmospheric forcing data (Oleson et al., 2013; Piao et al., 2012) predicts the annual isoprene emissions for the same Central Amazon tropical forest at a lower flux of 3.8 mg m^{-2} h^{-1}, with an average standard deviation of 3.9 mg m^{-2} h^{-1} across the seasonal variation (Fig. 1). The changes made to CLM 4.5 lead to a 33 % decrease in landscape scale isoprene emissions compared to CLM 4.0, but with no difference in seasonal pattern. The annual average isoprene flux predicted by MEGAN-CLM 4.5 was similar, within ~ 7 %, to the observational emission rate averaged from four Brazilian Amazon sites: 3.6 mg m^{-2} h^{-1} (Fig. 1). The month-to-month variability in the observational dataset showed an unclear pattern and could be attributed to either seasonal variability and/or differences among the four sites. It is typical to have high variance in biogenic emission estimates from field measurements taken from the same ecoregion (Harley et al., 2004), usually but not limited to differences in measurement techniques, measurements only taken during a short time period and weather anomalies that year, species composition, and regional-site differences. For example, the higher isoprene emissions observed in September and October appear to match the peak predicted by MEGAN-CLM (Fig. 1), but this could be coincidental due to a bias in site location for those measurements. Measurements for September and October were collected from Rondonia, Brazil, which is further to the west and south than the other four locations used in this study, and the modeled MEGAN-CLM plot (Table 1). This coincidence in seasonal peak could be a consequence of only having data from a single time period, and single site located further away that has differences in meteorology and species composition. Therefore it is beneficial to have multiple emission estimates when comparing at the landscape scale used in models.

ACPD
14, 23995–24041, 2014

3.2 Linear regression analysis

The relationship between the response variable, the emissions activity factor (γ), and the 14 explanatory variables were separately estimated through scatterplots and a simple linear regression. Linear regression of the modeled data found that the explanatory variables related to T_{leaf} exhibit the strongest predictive relationship, with R^2 equal to 0.889, 0.887, and 0.810 for hourly T_{leaf}, T_{leaf_24}, and T_{leaf_240} respectively (Fig. 2). The next explanatory variables that had a strong influence on emissions activity factor was PAR on sunlit leaves (i.e., PAR_{sun}, PAR_{24_sun}, PAR_{240_sun}) followed by PAR on shaded leaves (i.e., PAR_{shade}, PAR_{24_shade}, PAR_{240_shade}), however the spread of the relationship is narrow with R^2 ranging from 0.720 to 0.759 across the six variables. The last five variables tested here: LAI, atmospheric pressure ($forc_{pbot}$), Ci_{sun}, Ci_{shade}, F_{SUN}, showed a weak relationship with the emissions activity factor. For a tropical forest the model predicts that these five variables remain relatively constant over time, thus lacking statistical predictability.

The relationship between the emission activity factor, γ, and modeled explanatory variables were also compared for a North American northeastern temperate forest. The simple linear regression from this region also found that T_{leaf} and the related two variables, T_{leaf_24} and T_{leaf_240}, displayed a strong correlation (R^2 ranging 0.943 to 0.966). For the temperate forest 13 out of the 14 variables were found to have strong correlations with the emission activity factor, the exception being $forc_{pbot}$, and all had R^2 greater than 0.647. While in the tropical forest only 9 of the explanatory variables had a strong correlation. Due to seasonal patterns of leaf growth and senescence in deciduous trees in temperate forests, there is an expected strong relationship between isoprene emission and LAI, $R^2 = 0.807$. The absolute value of LAI has been known to have a strong effect on isoprene emissions, as it is a main driving parameter in Eq. (2) and influencing the modeled canopy environment, but the relatively constant LAI in tropical forests does not lead to a strong correlation with emission activity.

ACPD
14, 23995–24041, 2014

3.3 Monte Carlo uncertainty simulations

The distribution of the emissions activity factor, one of the two major components required for modeling biogenic emissions from terrestrial ecosystems, for the Central Amazon rainforest can be seen in Fig. 3. The top left panel was based on the intra-annual variation seen over eight decades of CLM simulations (with constant CO_2; present day control run); the remaining panels were based on 5000 Monte Carlo simulations. The mean simulated output as a result of CLM intra-annual variation (pre-Monte Carlo simulation) was 0.82 ± 0.15 (SD) with a normal distribution, but with a longer tail in the higher emissions activity range. The top center panel in Fig. 3 represents the uncertainty analysis that varied all 14 non-constant parameters listed in Table 2 at once, in the same uncertainty analysis. The mean simulated output value was 0.87 ± 0.09 (SD), range of 0.5, and the variance was 0.01. The remaining panels in Fig. 3 account for the top 10 parameters, out of 19, that contributed the most to emission variability and uncertainty. The simulated mean, standard variation, range, and contribution to isoprene uncertainty of all 19 parameters can be found in Table 3.

More than 28 % of the output variability was determined by the uncertainty found in T_{leaf}, and by varying this one input parameter a mean simulated output of 0.87 ± 0.08 (SD) was predicted. The mean and SD from varying only T_{leaf} are very similar to the outputs from varying all parameters, however the spread was more narrow from the uncertainty attributed by T_{leaf}. Four out of the top five variables that contributed the most to uncertainty were related to leaf temperature: T_{leaf}, T_{leaf_24}, CT1, and CT2. CT1 (= 95) and CT2 (= 230) are empirical coefficients that are found in γ_T (Eq. 4).

More than 61 % of the output variability was determined by the uncertainty in five parameters related to leaf temperature and found in γ_T (Eq. 4). In contrast 15 % of the output variability was determined by the uncertainty in eight parameters related to PAR and found in γ_P (Eq. 3). A parameter related to PAR was not seen until the 6th ranking in the uncertainty analysis (Table 3), and contributed to 7 % of the output variability. The PAR related to shaded leaves were consistently ranked higher in contributing to

ACPD
14, 23995–24041, 2014

output variability compared to their counterparts of PAR related to sunlit leaves, with the one exception of PAR_{24_sun} vs. PAR_{24_shade}. The last five parameters that were not related to γ_T or γ_P accounted for only 6 % of the variability in emissions activity output, with Ci_{SUN} and $forc_{pbot}$ being the two lowest ranking parameters (Table 3).

3.4 CLM driving variables compared to observational data

The uncertainty analysis produced distributions of simulated emissions activity factor, γ as predicted by each of parameters that influence and control biogenic emissions. The spread and shape of the distributions are beneficial in quantifying model uncertainty, but how well can the model represent these functionalities compared to empirical data? T_{leaf}, which could contribute up to 61 % of the variability in emissions estimates, was compared to in situ leaf temperature measurements from ZF2 field station, for each of the four seasons (Fig. 4, Table 4). Comparisons of modeled and observational seasonal T_{leaf} gave root-mean-square errors (RMSE) of 1.26 to 1.59 °C. Multiple differences emerge between the modeled vs. observed data, with a major discrepancy being (1) the T_{leaf} range was narrow in CLM compared to field measurements, and (2) high T_{leaf} values were not reached in CLM. For example, in situ measurements found maximum T_{leaf} to reach 43.5 to 45.9 °C across the seasons, but only 31.5 to 33.5 °C in CLM (Table 4). The lower T_{leaf} observed at the end of the wet season; March, April, May (MAM), were not well replicated in CLM. In addition the shape of the T_{leaf} curves showed different patterns between the modeled and observed, with CLM being bimodal in some months, and in situ measurement displaying more uni-modal with the potential for longer tails. However the mean T_{leaf} were very consistent between the in situ measurements and CLM simulations, with no significant difference between the means (two sample t test, $t_{(6,1.94)} = 1.15$, $p = 0.2934$).

Similar to the high T_{leaf} not being reached in CLM, the same occurred with respect to PAR. In situ measurements found PAR reaching up to 2500 µmol m^{-2} s^{-1}. However as modeled by CLM, PAR only reached an upper threshold of ∼ 1600 µmol m^{-2} s^{-1} for the modeled Central Amazon tropical forests (Fig. 5). Up to 17 % of the in situ

ACPD
14, 23995–24041, 2014

PAR measurements were greater than 1600 µmol m^{-2} s^{-1}. CLM lacked at capturing the higher midday PAR values. The peak in PAR averaged over the beginning of the dry season was 1136 µmol m^{-2} s^{-1} in CLM, while in situ data was 25 % higher at 1523 µmol m^{-2} s^{-1}, a difference of 387 µmol m^{-2} s^{-1}.

A further look (Fig. 6) examined isoprene emission, net photosynthesis on sunlit leaves, and GPP in response to changes in PAR and T_{leaf} as predicted by CLM for the Central Amazon forest. Model simulations predicted that at the landscape level, isoprene emission increased linearly with increasing PAR (R^2 = 0.924), and at the higher range of PAR, > 1000 µmol m^{-2} s^{-1}, photosynthesis and isoprene became uncoupled (Fig. 6a). Instead, experimental studies have found a strong coupling between photosynthesis and isoprene emissions in that they both increase in parallel and have a hyperbolic response with a tight correlation existing between these processes (Harley et al., 1996; Lerdau and Keller, 1997; Keller and Lerdau, 1999). There was also a strong linear correlation with isoprene emissions and T_{leaf} (R^2 = 0.889, Fig. 6b) predicted by CLM, while net photosynthesis and GPP were not strongly correlated with T_{leaf} (R^2 = 0.233 and R^2 = 0.299 respectively). Daily peak photosynthesis and related GPP in CLM were found across a wide range of leaf temperatures. As leaf temperature increased MEGAN-CLM did not show any signs of increasing isoprene emissions past the growth temperature optimum for net photosynthesis (A_{max}) as has been found in experimental studies (Lerdau and Keller, 1997; Keller and Lerdau, 1999; Jardine et al., 2014), potentially because high temperatures were never reached in the model.

3.5 MEGAN-CLM 4.5 modifications for the Central Amazon

CLM 4.5 improved estimates of GPP, NPP, and LAI for tropical regions (Bonan et al., 2011; Oleson et al., 2013) compared to the high predictions in CLM 4.0 (Beer et al., 2010; Lawrence et al., 2011), but overall tropical forest biomass was still overestimated for a Central Amazon forest in CLM 4.5 (Holm et al., 2014). The decrease in LAI from 8.85 to 6.39 in CLM 4.5 (Table 2), a 28 % decrease, was likely the sole driver

ACPD
14, 23995–24041, 2014

that lowered isoprene estimates from 5.7 mg m^{-2} h^{-1} to a more accurate estimate of 3.8 mg m^{-2} h^{-1} (Figs. 1 and 7a vs. Fig. 7b). The closer estimate of LAI in CLM 4.5 to observed data had the strongest impact on γ (Eq. 1) by directly impacting γ_L (Eq. 2). On average MEGAN-CLM 4.5 showed a 33 % decrease in γ_L throughout the entire Amazon Basin (Fig. 7d) compared to MEGAN-CLM 4.0. This led to a matching average decrease of 34 % in the total emissions activity factor, γ. The biophysical variable T_{leaf} predicted by CLM 4.5 led to both an increase of up to 0.2 and decrease by 0.1 in γ_T (Eq. 4) in the Amazon Basin compared to CLM 4.0 (Fig. 7e). South of the Amazon Basin in the cerrado and Atlantic Forest areas new predictions of higher T_{leaf} led to a strong increase in γ_T. The difference in γ_P between CLM 4.5 and CLM 4.0 was minimal, leading to a slight decrease in $\gamma > 0.1$ (Fig. 7f).

In Sect. 3.5, in situ measurements show that daytime T_{leaf} exceeds the maximum values predicted by CLM, up to 14 °C higher in individual leaves. Additional model simulations were conducted with adjustments to the γ_T algorithm to increase T_{leaf} in CLM 4.5 by 1.0 °C and decreasing T_{opt} to 40 °C (or 313.15 K). Prior to adjustment, T_{opt} was 42.4 °C (or 315.6 K) in MEGAN-CLM, which is a higher T_{opt} compared to the estimates predicted by other studies of ~ 40.0 °C (Lerdau and Keller, 1997; Harley et al., 2004). In accordance with Guenther et al. (2006) when T_{opt} is adjusted the C_{CE} coefficient must also be modified so that the emissions activity factor γ is equal to unity at the standard conditions. Therefore C_{CE} was lowered to 0.22. An increase of 1.0 °C was chosen because it was the difference between the in situ annual average T_{leaf} (29.6 °C) and modeled annual average T_{leaf} (28.9 °C), rounded up. The T_{leaf} adjustment was conducted in CLM 4.5, due to improved LAI predictions in version 4.5 over version 4.0. Using CLM 4.5 as a more accurate base to modify T_{leaf} to values closer to observational estimates, new model runs found isoprene emissions to increase up to 4.8 mg m^{-2} h^{-1} (Fig. 7c). This slight modification in T_{leaf} resulted in an ~ 24 % increase in isoprene emissions. The lowering of T_{opt} to a value found in previous tropical studies resulted in isoprene emissions to decrease to 3.5 mg m^{-2} h^{-1}, and 9 % decrease from non-modified runs. Lowering the T_{opt} alone will increase isoprene emissions, but the required adjustment

ACPD
14, 23995–24041, 2014

of C_{CE}, to 0.22, outweighed the response due to lowering T_{opt}. When the two adjustments (i.e., T_{leaf} and T_{opt}) are combined they canceled each other out and isoprene emissions were 4.3 mg m^{-2} h^{-1}, and within 12 % of non-modified MEGAN-CLM 4.5.

4 Discussion

MEGAN-CLM is particularly useful for evaluating future scenarios of BVOC emissions under changing climates, transient CO_2 estimates, changing land-use and land-cover, and altered meteorology due to the coupling in CESM. However, there is still uncertainty concerning the complex relationships among the ecophysiological functioning of trees, changes in environmental conditions, phylogenetic associations, and corresponding tropical forest BVOC emissions, all of which needs improvement in MEGAN-CLM. This study narrowed that uncertainty by predicting which biophysical variables in CLM have the strongest control and contributes to the most variability on landscape scale tropical forest BVOC emissions. Annual isoprene emissions were found to vary by 33 % between different versions of MEGAN-CLM (4.0 vs. 4.5) due almost completely to changes in LAI, and the latest version MEGAN-CLM 4.5 matched the regional observational average. For a Central Amazon forest simulated by MEGAN-CLM, T_{leaf} was the largest contributor to uncertainty in isoprene emissions, contributing up to 61 % of emission uncertainty. Increasing T_{leaf} by 1.0 °C resulted in a 24 % increase in tropical forest isoprene emissions.

4.1 Model comparison

Many global isoprene emission models use the same emissions algorithms, typically based on the G95 light and temperature algorithms (Arneth et al., 2008). Some comparisons of global emission models have found that simulated isoprene emissions are in close agreement with each other and converging near 500 ± 100 Tg C. Additionally, interannual variability is small, ranging from 5–10 % around the mean (Arneth et al.,

ACPD
14, 23995–24041, 2014

2008, 2011). For example, in a review of four modeling studies, each of which used a different ecosystem/land surface model to produce the driving variables, but all used similar biogenic emission algorithms based off of G95, global isoprene emissions varied from 454 to 559 Tg C (Wang and Shallcross, 2000; Potter et al., 2001; Levis et al., 2003; Naik et al., 2004). A larger synthesis of 15 studies found global isoprene emissions ranged from 412 Tg C using LPJ-GUESS emission algorithms based on photosynthetic supply (Arneth et al., 2007) to 601 Tg C using 13 global land cover classifications and G95 algorithms (Tao and Jain, 2005).

A sensitivity test using three global terrestrial isoprene emission models that differ in core processes (i.e., MEGAN, LPJ-GUESS, BVOCEM) quantified the variability due to climate and representation of vegetation with no change to the "standard" model setup. Variability in climate and vegetation yielded increased or decreased annual emissions by at least 30 % and up to 200 % (Arneth et al., 2011). The combined effect of switching climate and vegetation between MEGAN and LPJ-GUESS resulted in reduced emissions of 70 % in MEGAN, and increasing emissions by 200 % in LPJ-GUESS. When compared to MEGAN predictions, the Integrated Biospheric Simulator (IBIS), using G95 algorithms, predicted global annual isoprene emissions to be only 10 % lower (454 vs. 503 Tg C) (Naik et al., 2004). This reduced prediction was based on differences in canopy variables and processes, LAI, climatology, and using MOSES2-TRIFFID vegetation physiological scheme.

In a regional BVOC study in the Amazon Basin, Karl et al. (2007) found that MEGAN (G06) estimated fluxes were lower than observations but within airborne measurement uncertainty, and could describe observed variations associated with land-use change for that region. Karl et al. (2007) corrected MEGAN for environmental conditions consistent with the measurement conditions (i.e., T = 34 °C and 1260 PAR), which could have contributed to improved accuracy for the tropical forest. Compared to measurements at the Z14 tower 60 km NW of Manaus using mixed layer variance (MLV) techniques, MEGAN isoprene emission estimates were 40 % lower (Karl et al., 2007). Here we found that MEGAN-CLM 4.0 over-predicted isoprene estimates similar to other model-

ACPD
14, 23995–24041, 2014

ing studies (Harley et al., 2004; Hewitt et al., 2011) by 60 %, however MEGAN-CLM 4.5 estimates were in close agreement and only 7 % higher than the observational datasets used in this study from Brazil.

In summary, debate continues on whether the assemblages of emission models are in general agreement with each other or whether differences in biophysical environmental variables, vegetation cover, or climate as determined within each model can lead to unrealistic ranges of BVOC estimates. Synthesis of model inter-comparisons are showing the latter, in that differences in driving biophysical parameters are larger than the differences in emission activity algorithms, and in order to get accurate emissions it is necessary to have accurate predictions of driving parameters. In particular, we found that a slight variation in T_{leaf} can produce large shifts in isoprene emissions.

Improving modeling estimates of biogenic emissions remains a challenge due to the lack of observations for quantifying emissions from tropical forests, and we have limited understanding of how canopy and leaf-level processes affect emission rates. Studies have found a large spread in daytime isoprene emission rates over the Amazon Basin, ranging from 1.5 to 9.8 mg m^{-2} h^{-1} (Barkley et al., 2008). This large range is attributed to differences between wet and dry season, regional location, interannual variability, and/or measurement techniques. For example, isoprene emissions from the Ducke Forest Reserve, 10 km north of Manaus Brazil, ranged from 1.6 to 3.6 mg m^{-2} h^{-1} (Jacob and Wofsy, 1988; Davis et al., 1994), while another nearby site 60 km northwest of Manaus (tower Z14 and K34) ranged from 2.4 to 7.8 mg m^{-2} h^{-1} (Karl et al., 2007; Kuhn et al., 2007). In addition, regional variation is also prominent across the Amazon Basin. For example a primary rainforest west of Iquitos, Peru can reach up to 8.2 mg m^{-2} h^{-1} (Helmig et al., 1998), and Reserva Biologica do Jaru, in the southwestern region of Brazil can reach up to 9.8 mg m^{-2} h^{-1} (Greenberg et al., 2004).

4.2 Leaf temperature in tropical plants and BVOC emissions

BVOC emissions are known to be temperature sensitive in that higher temperatures will increase chemical reaction rates in plants and increase the vapor pressures of volatile

ACPD
14, 23995–24041, 2014

compounds (Tingey et al., 1991). Global BVOC emission rates could increase by 25–45 % as a result of elevated mean global air temperatures by 2–3 °C (Penuelas and Llusia, 2003). This study found that a 1 °C increase in T_{leaf} in the temperature-dependent G95 algorithm resulted in a 24 % increase in isoprene emissions for a tropical forest. To improve flux estimates, a better understanding of the detailed relationship between isoprene emissions and T_{leaf} is required; especially when data has shown that algorithm prediction was not satisfactory for temperatures > 40 °C for a common tropical tree (Alves et al., 2014). Some have suggested that at high vegetation temperatures (> 40 °C) isoprene emissions dramatically decline, but this assumption has been challenged (Monson et al., 1992; Sharkey et al., 1996; Alves et al., 2014; Jardine et al., 2014). Monson et al. (1992) showed that plants growing in warm temperatures (i.e., 34 °C) had a temperature optimum for isoprene emission rate that shifted to 45 °C compared to plants growing in cooler temperatures (i.e., 26 °C) which had a temperature optimum of 40 °C. The relationship between high temperatures and isoprene emissions in tropical evergreen leaves should be explored in more detail.

In general higher variability has been attributed to isoprene emission response to leaf temperature compared to PPFD (Penuelas and Llusia, 2003; Pacifico et al., 2009; Alves et al., 2014). Isoprene emissions follow a clear trend of leveling off at high values of PPFD with normalized isoprene emission having little variation, ranging from 1.0–1.2. However, stronger uncertainties existed in isoprene emissions at high temperatures (> 35 °C) across multiple tree species ranging from ~ 1.4–4.5 normalized isoprene emission (Pacifico et al., 2009). High temperatures, > 34 °C, were not experienced in CLM. The lack of reproducing high temperatures that are found in empirical measurements (Fig. 4) by CLM, led to a lack of generating higher isoprene emissions. MEGAN-CLM 4.5 predicted a close match in isoprene emission flux for a Central Amazon forest, with only a slight over-prediction occurring. However if higher leaf temperatures were replicated in CLM the over-estimation of isoprene flux would become stronger. It is suggested that additional in situ measurements of tropical leaf temperatures is required to gain a better understanding of current changes due to varying

ACPD
14, 23995–24041, 2014

environmental conditions, extremes, and seasonality. A more up-to-date and extensive field campaign to capture current trends in T_{leaf} could greatly improve modeling capacity and predictability. The consensus from the CMIP5 analysis using the Representative Concentration Pathways (RCPs), is that temperature will increase over the next century by 1.0–4.0 °C (IPCC 2007; Knutti and Sedlacek, 2012). As a result, isoprene emissions will likely increase, and as we have predicted here the uncertainty of predicting the magnitude of emission fluxes from tropical forests resulting from higher temperatures is also likely to increase.

4.3 Additional model parameters and uncertainty

In addition to accounting for the influence of temperature, light, and CO_2, MEGAN 2.1 has the capacity to incorporate processes related to leaf age and soil moisture. However, these two processes are not accounted for when modeling tropical forests, including Amazonia. In the past decade, two severe droughts have occurred in the Amazon Basin, and could increase due to human-induced climate change (Phillips et al., 2009; Allen et al., 2010; Lewis et al., 2011; Anderegg et al., 2013). During a drought scenario in the Biosphere 2 tropical rainforest GPP was significantly reduced by 32 %, when soil water content reached its minimum. This led to fixed carbon from photosynthesis as isoprene production to increase by 100 %, from 1 % to 2 %, but otherwise isoprene production was not largely affected as a result of the water stress treatment (Pegoraro et al., 2006). Isoprene carbon loss as a fraction of total photosynthesis is an important metric to quantify when trying to account for the total tropical forest carbon sink and "lost" carbon. Leaf age, development status, and senescence have been shown to influence isoprene production in tropical species (Kuhn et al., 2004b; Alves et al., 2014). Over the course of leaf development, isoprene emission capacities of tropical leaves ranged from 0.7 to 111.5 µg C g^{-1} h^{-1} (Kuhn et al., 2004b). In tropical forests, the difference between timing of bud break, leaf senescence, foliar biomass, and specific leaf weight during either the wet or dry season can lead to notable seasonal differences in isoprene and monoterpene emissions, warranting inclusion of leaf development in

ACPD
14, 23995–24041, 2014

emissions algorithms for tropical forests (Kuhn et al., 2004b). In a common Central Amazonian species, *Eschweilera coriacea*, in situ measurements showed that young mature leaves had highest isoprene emissions compared to old mature and senescent leaves (Alves et al., 2014), suggesting that leaf phenology effects should be included in emission algorithms for tropical PFTs.

An additional important metric to consider in global biogenic emission models is that certain tree species are not isoprene emitters. The total number of tropical tree species is very large ($> 1000\,\mathrm{ha}^{-1}$), and while fully comprehensive data is still lacking, it has been estimated that only 38 % of 125 tree species examined in the Brazilian Amazon are isoprene emitters (Harley et al., 2004). Global models assign an average emission factor (ε) to each PFT or vegetation type that accounts for emitters and non-emitters, however these values could be improved. Harley et al. (2004) showed that when using a bottom-up model approach using (1) G95 algorithms, (2) estimates of isoprene-emitted biomass, and (3) site foliar biomass, the canopy flux was still overestimated by ~ 50 % compared to measured data. With tropical trees accounting for ~ 75 % of total isoprene emissions (Guenther et al., 2006), isoprene flux capacity as a function of species composition can dramatically effect global estimates.

5 Summary and concluding remarks

We have estimated that CLM is suboptimal at accurately representing key climate and biophysical processes (i.e., T_{leaf} and PAR) for tropical forest locations that are critical to controlling BVOC emissions. We reported that CLM is not reproducing the higher range of PAR and T_{leaf}, environmental conditions that have been known to increase isoprene emissions as they increase. Specifically, CLM did not capture the upper 10–14 °C range of T_{leaf} (i.e., failed to represent ~ 32 to 46 °C) that can naturally occur during peak temperature episodes in the Central Amazon, nor did CLM capture the upper $900\,\mu\mathrm{mol\,m^{-2}\,s^{-1}}$ range of PAR (i.e., failed to represent ~ 1600 to $2500\,\mu\mathrm{mol\,m^{-2}\,s^{-1}}$). However, MEGAN-CLM is already over-predicting isoprene emis-

ACPD
14, 23995–24041, 2014

sions in tropical forests without reaching potential upper extremes in the biophysical parameters. Allowing MEGAN-CLM to account for higher T_{leaf} (by 1.0 °C) resulted in the model to further over-estimated isoprene emissions compared to field measurements. Air temperatures are predicted to increase over tropical regions over the next century by 2–5 °C (Solomon et al., 2007). Accurately representing vegetation temperature in global land surface models coupled with BVOC emission models is required to represent physiological mechanisms that control BVOC emissions. Attempts to correct the representation of light conditions, radiation, and temperature for tropical forests in CLM are needed, however adjustments to the BVOC algorithms to account for overestimation should also be considered. Results from this study assisted in developing a better understanding of the environmental controls on BVOC emission from tropical forests. This was an important step in evaluating how a changing climate in the tropics will affect BVOC emissions, a critical topic for discerning how short-term forcing and atmospheric constituents contribute to regional and global environmental change.

Acknowledgements. This material is based upon work supported by the US Department of Energy, Office of Science, Office of Biological and Environmental Research under contract No. DE-AC02-05CH11231 as part of the Terrestrial Ecosystem Science (TES) Program. Alex Guenther was supported by the Laboratory Directed Research and Development Program at Pacific Northwest National Laboratory. We would like to thank Niro Higuchi and Cristina Aledi Felsemburgh who helped with leaf temperature data collection, and important logistical help in Brazil. This research used resources of the National Energy Research Scientific Computing Center, which is supported by the Office of Science of the US Department of Energy under contract DE-AC02-05CH11231. We would also like to thank the CESM project, sponsored by the National Science Foundation (NSF) and the US Department of Energy (DOE), and the administration team that is maintained at the National Center for Atmospheric Research (NCAR).

ACPD
14, 23995–24041, 2014

References

Ahlström, A., Schurgers, G., Arneth, A., and Smith, B.: Robustness and uncertainty in terrestrial ecosystem carbon response to CMIP5 climate change projections, Environ. Res. Lett., 7, 044008, doi:10.1088/1748-9326/7/4/044008, 2012.

Allen, C. D., Macalady, A. K., Chenchouni, H., Bachelet, D., McDowell, N., Vennetier, M., Kitzberger, T., Rigling, A., Breshears, D. D., Hogg, E. H., Gonzalez, P., Fensham, R., Zhang, Z., Castro, J., Demidova, N., Lim, J- H., Allard, G., Running, S. W., Semerci, A., and Cobb, N.: A global overview of drought and heat-induced tree mortality reveals emerging climate change risks for forests, Forest Ecol. Manag., 259, 660–684, 2010.

Alton, P. B., North, P. R., and Los, S. O.: The impact of diffuse sunlight on canopy light-use efficiency, gross photosynthetic product and net ecosystem exchange in three forest biomes, Glob. Change Biol., 13, 776–787, 2007.

Alves, E. G., Harley, P., Goncalves, J. F. de C., Moura, C. E. da S., and Jardine, K.: Effects of light and temperature on isoprene emission at different leaf development stages of *Eschweilera coriacea* in Central Amazon, Acta Amaz., 44, 9–18, 2014.

Anderegg, W. R. L., Kane, J. M., and Anderegg, L. D. L.: Consequences of widespread tree mortality triggered by drought and temperature stress, Nature Clim. Change, 3, 30–36, 2013.

Arneth, A., Niinemets, Ü., Pressley, S., Bäck, J., Hari, P., Karl, T., Noe, S., Prentice, I. C., Serça, D., Hickler, T., Wolf, A., and Smith, B.: Process-based estimates of terrestrial ecosystem isoprene emissions: incorporating the effects of a direct CO_2-isoprene interaction, Atmos. Chem. Phys., 7, 31–53, doi:10.5194/acp-7-31-2007, 2007.

Arneth, A., Monson, R. K., Schurgers, G., Niinemets, Ü., and Palmer, P. I.: Why are estimates of global terrestrial isoprene emissions so similar (and why is this not so for monoterpenes)?, Atmos. Chem. Phys., 8, 4605–4620, doi:10.5194/acp-8-4605-2008, 2008.

Arneth, A., Schurgers, G., Lathiere, J., Duhl, T., Beerling, D. J., Hewitt, C. N., Martin, M., and Guenther, A.: Global terrestrial isoprene emission models: sensitivity to variability in climate and vegetation, Atmos. Chem. Phys., 11, 8037–8052, doi:10.5194/acp-11-8037-2011, 2011.

Atkinson, R. and Arey, J.: Gas-phase tropospheric chemistry of biogenic volatile organic compounds: a review, Atmos. Environ., 37, S197–S219, 2003.

Baker, B., Bai, J., Johnson, C., Cai, Z., Li, Q., Wang, Y., Guenther, A., Greenberg, J., Klinger, L., Geron, C., and Rasmussen, R.: Wet and dry season ecosystem level fluxes of isoprene and

ACPD
14, 23995–24041, 2014

monoterpenes from a southeast Asian secondary forest and rubber tree plantation, Atmos. Environ., 39, 381–390, 2005.
Baker, K.: Peak 8-hr Ozone Model Performance when using Biogenic VOC estimated by MEGAN and BIOME (BEIS), in: 6th Annual CMAS Conference, Chapel Hill, NC, 1–3 October 2007, 2007.
Barkley, M. P., Palmer, P. I., Kuhn, U., Kesselmeier, J., Chance, K., Kurosu, T. P., Martin, R. V., Helmig, D., and Guenther, A.: Net ecosystem fluxes of isoprene over tropical South America inferred from GOME observations of HCHO columns, J. Geophys. Res., 113, D20304, doi:10.1029/2008JD009863, 2008.
Beer, C., Reichstein, M., Tomelleri, E., Ciais, P., Jung, M., Carvalhais, N., Rödenbeck, C., Altaf Arain, M., Baldocchi, D., Bonan, G. B., Bondeau, A., Cescatti, A., Lasslop, G., Lindroth, A., Lomas, M., Luyssaert, S., Margolis, H., Oleson, K. W., Roupsard, O., Veenendaal, E., Viovy, N., Williams, C., Woodward, I. F., and Papale, D.: Terrestrial gross carbon dioxide uptake: global distribution and covariation with climate, Science, 329, 834–838, doi:10.1126/science.1184984, 2010.
Bonan, G. B., Lawrence, P. J., Oleson, K. W., Levis, S., Jung, M., Reichstein, M., Lawrence, D. M., and Swenson, S. C.: Improving canopy processes in the Community Land Model version 4 (CLM4) using global flux fields empirically inferred from FLUXNET data, J. Geophys. Res., 116, G02014, doi:10.1029/2010JG001593, 2011.
Choudbury, B.: Estimating gross photosynthesis using satellite and ancillary data: approach and preliminary results, Remote Sens. Environ., 75, 1–21, 2001.
Collins, W. D., Bitz, C. M., Blackmon, M. L., Bonan, G. B., Bretherton, C. S., Carton, J. A., Chang, P., Doney, S. C., Hack, J. J., Henderson, T. B., Kiehl, J. T., Large, W. G., McKenna, D. S., Santer, B. D., and Smith, R. D.: The Community Climate System Model version 3 (CCSM3), J. Climate, 19, 2122–2143, 2006.
Cox, P. M., Pearson, D., Booth, B. B., Friedlingstein, P., Huntingford, C., Jones, C. D., and Luke, C. M.: Sensitivity of tropical carbon to climate change constrained by carbon dioxide variability, Nature, 494, 341–344, 2013.
Davis, K. J., Lenschow, D. H., and Zimmerman, P. R.: Biogenic nonmethane hydrocarbon emissions estimated from tethered balloon observations, J. Geophys. Res., 99, 25587–25598, doi:10.1029/94JD02009, 1994.

ACPD
14, 23995–24041, 2014

Doughty, C. E., Flanner, M. G., and Goulden, M. L.: Effect of smoke on subcanopy shaded light, canopy temperature, and carbon dioxide uptake in an Amazon rainforest, Global Biogeochem. Cy., 24, GB3015, doi:10.1029/2009GB003670, 2010.

Friedlingstein, P., Cox, P., Betts, R., Bopp, L., von Bloh, W., Brovkin, V., Doney, S., Eby, M., Fung, I., Bala, G., John, J., Jones, C., Joos, F., Kato, T., Kawamiya, M., Knorr, W., Lindsay, K., Matthews, H. D., Raddatz, T., Rayner, P., Reick, C., Roeckner, E., Schnitzler, K.-G., Schnur, R., Strassmann, K., Weaver, A. J., Yoshikawa, C., and Zeng, N.: Climate-carbon cycle feedback analysis: results from the C4MIP model intercomparison, J. Climate, 19, 3337–3353, doi:10.1175/JCLI3800.1, 2006.

Forster, P., Ramaswamy, V., Artaxo, P., Berntsen, T., Betts, R., Fahey, D. W., Haywood, J., Lean, J., Lowe, D. C., Myhre, G., Nganga, J., Prinn, R., Raga, G., Schulz, M., and Van Dorland, R.: Changes in atmospheric constituents and in radiative forcing, in: Climate Change 2007: The Physical Science Basis. Contribution of Working Group I to the Fourth Assessment Report of the Intergovernmental Panel on Climate Change, edited by: Solomon, S., Qin, D., Manning, M., Chen, Z., Marquis, M., Averyt, K. B., Tignor, M., and Miller, H. L., Cambridge University Press, Cambridge, UK and New York, NY, USA, 130–234, 2007.

Gent, P. R., Danabasoglu, G., Donner, L. J., Holland, M. M., Hunke, E. C., Jayne, S. R., Lawrence, D. M., Neale, R. B., Rasch, P. J., Vertenstein, M., Worley, P. H., Yang, Z.-L., and Zhang, M.: The Community Climate System Model version 4, J. Climate, 24, 4973–4991, 2011.

Goldstein, A. H. and Galbally, I. E.: Known and unexplored organic constituents in the Earth's atmosphere, Environ. Sci. Technol., 41, 1514–1521, 2007.

Greenberg, J. P., Guenther, A. B., Peìtron, G., Wiedinmyer, C., Vega, O., Gatti, L. V., Tota, J., and Fisch, G.: Biogenic VOC emissions from forested Amazonian landscapes, Glob. Change Biol., 10, 651–662, 2004.

Guenther, A.: Seasonal and spatial variations in natural volatile organic compound emissions, Ecol. Appl., 7, 34–45, 1997.

Guenther, A. B., Zimmerman, P. R., Harley, P. C., Monson, R. K., and Fall, R.: Isoprene and monoterpene emission rate variability – model evaluations and sensitivity analyses, J. Geophys. Res.-Atmos., 98, 12609–12617, 1993.

Guenther, A., Hewitt, C. N., Erickson, D., Fall, R., Geron, C., Graedel, T., Harley, P., Klinger, L., Lerdau, M., McKay, W. A., Pierce, T., Scholes, B., Steinbrecher, R., Tallamraju, R., Taylor, J.,

ACPD
14, 23995–24041, 2014

and Zimmerman, P.: A global model of natural volatile organic compound emissions, J. Geophys. Res.-Atmos., 100, 8873–8892, 1995.
Guenther, A., Karl, T., Harley, P., Wiedinmyer, C., Palmer, P. I., and Geron, C.: Estimates of global terrestrial isoprene emissions using MEGAN (Model of Emissions of Gases and Aerosols from Nature), Atmos. Chem. Phys., 6, 3181–3210, doi:10.5194/acp-6-3181-2006, 2006.
Guenther, A. B., Jiang, X., Heald, C. L., Sakulyanontvittaya, T., Duhl, T., Emmons, L. K., and Wang, X.: The Model of Emissions of Gases and Aerosols from Nature version 2.1 (MEGAN2.1): an extended and updated framework for modeling biogenic emissions, Geosci. Model Dev., 5, 1471–1492, doi:10.5194/gmd-5-1471-2012, 2012.
Harley, P., Guenther, A., and Zimmerman, P.: Effects of light, temperature and canopy position on net photosynthesis and isoprene emission from sweetgum (*Liquidambar styraciflua*) leaves, Tree Physiol., 16, 25–32, 1996.
Harley, P., Vasconcellos, P., Vierling, L., Pinheiro, C., Greenberg, J., Guenther, A., Klinger, L., Almeida, S., Neill, D., Baker, T., Phillips, O., and Malhi, Y.: Variation in potential for isoprene emissions among Neotropical forest sites, Glob. Change Biol., 10, 630–650, 2004.
Helmig, D., Balsley, B., Davis, K., Kuck, L. R., Jensen, M., Bognar, J., Smith, T. Jr., Vasquez Arrieta, R., Rodriquez, R., and Birks, J. W.: Vertical profiling and determination of landscape fluxes of biogenic non-methane hydrocarbons within the planetary boundary layer in the Peruvian Amazon, J. Geophys. Res., 103, 25519–25532, doi:10.1029/98JD01023, 1998.
Hewitt, C. N., Ashworth, K., Boynard, A., Guenther, A., Langford, B., MacKenzie, A. R., Misztal, P. K., Nemitz, E., Owen, S. M., Possell, M., Pugh, T. A. M., Ryan, A. C., and Wild, O.: Ground-level ozone influenced by circadian control of isoprene emissions, Nat. Geosci., 4, 671–674, 2011.
Holm, J. A., Chambers, J. Q., Collins, W. D., and Higuchi, N.: Forest response to increased disturbance in the Central Amazon and comparison to Western Amazonian forests, Biogeosciences Discuss., 11, 7721–7773, doi:10.5194/bgd-11-7721-2014, 2014.
IPCC: Climate Change 2007: The Physical Scientific Basis, Summary For Policymakers, IPCC Secretariat, Geneva, 2007.
Jacob, D. J. and Wofsy, S. C.: Photochemistry of biogenic emissions over the Amazon Forest, J. Geophys. Res., 93, 1477–1486, doi:10.1029/JD093iD02p01477, 1988.
Jardine, K., Vickers, C. E., Nielsen, L. K., Alves, E. G., Garcia, S., Holm, J., Higuchi, N., Manzi, A., Fuentes, J. D., Torn, M., and Chambers, J.: Dynamic balancing of isoprene carbon

ACPD
14, 23995–24041, 2014

sources reflects photosynthetic and photorespiratory responses to environmental change, Plant Cell Environ., submitted, 2014.
Karl, T., Guenther, A., Yokelson, R. J., Greenberg, J., Potosnak, M., Blake, D. R., and Artaxo, P.: The tropical forest and fire emissions experiment: emission, chemistry, and transport of biogenic volatile organic compounds in the lower atmosphere over Amazonia, J. Geophys. Res.-Atmos., 112, D18302, doi:10.1029/2007JD008539, 2007.
Keller, M. and Lerdau, M.: Isoprene emission from tropical forest canopy leaves, Global Biogeochem. Cy., 13, 19–29, 1999.
Kesselmeier, J., Ciccioli, P., Kuhn, U., Stefani, P., Biesenthal, T., Rottenberger, S., Wolf, A., Vitullo, M., Valentini, R., Nobre, A., Kabat, P., and Andreae, M. O.: Volatile organic compound emissions in relation to plant carbon fixation and the terrestrial carbon budget, Global Biogeochem. Cy., 16, 1126, doi:10.1029/2001GB001813, 2002.
Knutti, R. and Sedlacek, J.: Robustness and uncertainties in the new CMIP5 climate model projections, Nature Clim. Change, 3, 369–373, 2012.
Kulmala, M., Nieminen, T., Chellapermal, R., Makkonen, R., Back, J., and Kerminen, V.-M.: Climate feedbacks linking the increasing atmospheric CO_2 concentration, BVOC emissions, aerosols and cloud in forest ecosystems, in: Biology, Controls and Models of Tree Volatile Organic Compound Emissions, Tree Physiology, 5, edited by: Niinemets, U. and Monson, R. K., Springer, the Netherlands, 489–508, doi:10.1007/978-94-007-6606-8_17, 2013.
Kuhn, U., Rottenberger, S., Biesenthal, T., Wolf, A., Schebeske, G., Cicciolo, P., Brancaleoni, E., Frattoni, M., Tavares, T. M., and Kesselmeier, J.: Seasonal differences in isoprene and light-dependent monoterpene emission by Amazonian tree species, Glob. Change Biol., 10, 663–682, doi:10.1111/j.1529-8817.2003.00771.x, 2004a.
Kuhn, U., Rottenberger, S., Biesenthal, T., Wolf, A., Schebeske, G., Cicciolo, P., and Kesselmeier, J.: Strong correlation between isoprene emission and gross photosynthetic capacity during leaf phenology of the tropical tree species *Hymenaea courbaril* with fundamental changes in volatile organic compounds emission composition during early leaf development, Plant Cell Environ., 27, 1469–1485, 2004b.
Kuhn, U., Andreae, M. O., Ammann, C., Araújo, A. C., Brancaleoni, E., Ciccioli, P., Dindorf, T., Frattoni, M., Gatti, L. V., Ganzeveld, L., Kruijt, B., Lelieveld, J., Lloyd, J., Meixner, F. X., Nobre, A. D., Pöschl, U., Spirig, C., Stefani, P., Thielmann, A., Valentini, R., and Kesselmeier, J.: Isoprene and monoterpene fluxes from Central Amazonian rainforest inferred from tower-based and airborne measurements, and implications on the atmospheric chemistry and

ACPD
14, 23995–24041, 2014

the local carbon budget, Atmos. Chem. Phys., 7, 2855–2879, doi:10.5194/acp-7-2855-2007, 2007.
Lamb, B., Gay, D., Westberg, H., and Pierce, T.: A biogenic hydrocarbon emission inventory for the USA using a simple forest canopy model, Atmos. Environ., 27, 1673–1690, 1993.
Lawrence, D. M., Oleson, K. W., Flanner, M. G., Thornton, P. E., Swenson, S. C., Lawrence, P. J., Zeng, X., Yang, Z.-L., Levis, S., Sakaguchi, K., Bonan, G. B., and Slater, A. G.: Parameterization improvements and functional and structural advances in version 4 of the Community Land Model, J. Adv. Model. Earth Syst., 3, 27 pp., doi:10.1029/2011MS000045, 2011.
Lerdau, M. and Keller, M.: Controls on isoprene emissions from trees in a subtropical dry forest, Plant Cell Environ., 20, 569–578, 1997.
Levis, S., Wiedinmyer, C., Bonan, G. B., and Guenther, A.: Simulating biogenic volatile organic compound emissions in the Community Climate System Model, J. Geophys. Res., 108, 4659, doi:10.1029/2002JD003203, 2003.
Lewis, S. L., Brando, P. M., Phillips, O. L., van der Heijden, G. M. F., and Nepstad, D.: The 2010 Amazon drought, Science, 331, 554, 2011.
Loreto, F., Ciccioli, P., Cecinato, A., Brancaleoni, E., Frattoni, M., Fabozzi, C., and Tricoli, D.: Evidence of the photosynthetic origin of monoterpenes emitted by *Quercus ilex* L. leaves by ^{13}C labeling, Plant Physiol., 110, 1317–1322, 1996.
Monson, R. K. and Fall, R.: Isoprene emission from Aspen leaves – influence of environment and relation to photosynthesis and photorespiration, Plant Physiol., 90, 267–274, 1989.
Monson, R. K., Jaeger, C. H., Adams III, W. W., Driggers, E. M., Silver, G. M., and Fall, R.: Relationships among isoprene emission rate, photosynthesis, and isoprene synthase activity as influenced by temperature, Plant Physiol., 98, 1175–1180, 1992.
Naik, V., Delire, C., and Wuebbles, D. J.: Sensitivity of global biogenic isoprenoid emissions to climate variability and atmospheric CO_2, J. Geophys. Res., 109, D06301, doi:10.1029/2003JD004236, 2004.
Nguyen, T. B., Roach, P. J., Laskin, J., Laskin, A., and Nizkorodov, S. A.: Effect of humidity on the composition of isoprene photooxidation secondary organic aerosol, Atmos. Chem. Phys., 11, 6931–6944, doi:10.5194/acp-11-6931-2011, 2011.
Oleson, K. W., Lawrence, D. M., Bonan, G. B., Flanner, M. G., Kluzek, E., Lawrence, P. J., Levis, S., Swenson, S. C., and Thornton, P. E.: Technical Description of Version 4.0 of the

ACPD
14, 23995–24041, 2014

Community Land Model (CLM), NCAR Tech. Note NCAR/TN-478+STR, National Center for Atmospheric Research, Boulder, CO, 257 pp., doi:10.5065/D6FB50WZ, 2010.
Oleson, K. W., Lawrence, D. M., Bonan, G. B., Drewniak, B., Huang, M., Koven, C. D., Levis, S., Li, F., Riley, W. J., Subin, Z. M., Swenson, S. C., Thornton, P. E., Bozbiyik, A., Fisher, R., Kluzek, E., Lamarque, J.-F., Lawrence, P. J., Leung, R. L., Lipscomb, W., Muszala, S., Ricciuto, D. M., Sacks, W., Sun, Y., Tang, J., and Yang, Z.-L.: Technical Description of version 4.5 of the Community Land Model (CLM), NCAR Technical Note NCAR/TN-503+STR, National Center for Atmospheric Research, Boulder, CO, pp. 422, doi:10.5065/D6RR1W7M, 2013.
Pacifico, F., Harrison, S. P., Jones, C. D., and Sitch, S.: Isoprene emissions and climate, Atmos. Environ., 43, 6121–6135, 2009.
Pegoraro, E., Rey, A., Abrell, L., Haren, J., and Lin, G.: Drought effect on isoprene production and consumption in Biosphere 2 tropical rainforest, Glob. Change Biol., 12, 456–469, doi:10.1111/j.1365-2486.2006.01112.x, 2006.
Peñuelas, J. and Llusià J.: BVOCs: plant defense against climate warming?, Trends Plant Sci., 8, 105–109, 2003.
Penuelas, J. and Staudt, M.: BVOCs and global change, Trends Plant Sci., 15, 133–144, 2010.
Phillips, O. L., Aragão, L. E. O. C., Lewis, S. L., Fisher, J. B., Lloyd, J., López-González, G., Malhi, Y., Monteagudo, A., Peacock, J., Quesada, C. A., van der Heijden, G., Almeida, S., Amaral, I., Arroyo, L., Aymard, G., Baker, T. R., Ba'nki, O., Blanc, L., Bonal, D., Brando, P., Chave, J., Alves de Oliveira, A'. C., Dávila Cardozo, N., Czimczik, C. I., Feldpausch, T. R., Freitas, M. A., Gloor, E., Higuchi, N., Jiménez, E., Lloyd, G., Meir, P., Mendoza, C., Morel, A., Neill, D. A., Nepstad, D., Patiño, S., Peñuela, M. C., Prieto, A., Ramrez, F., Schwarz, M., Silva, J., Silveira, M., Sota Thomas, A., ter Steege, H., Stropp, J., Vásquez, R., Zelazowski, P., Alvarez Dávila, E., Andelman, S., Andrade, A., Chao, K., Erwin, T., Di Fiore, A., Honorio, C., Keeling, E., Killeen, H., Laurance, T. J., Peñ a Cruz, W. F., Pitman, A., Núñez Vargas, N. C. A., Ramrez-Angulo, P., Rudas, H., Salamão, A., Silva, R., Terborgh, N., and Torres-Lezama, J. A.: Drought sensitivity of the Amazon rainforest, Science, 323, 1344–1347, 2009.
Pöschl, U., Martin, S. T., Sinha, B., Chen, Q., Gunthe, S. S., Huffman, J. A., Borrmann, S., Farmer, D. K., Garland, R. M., Helas, G., Jimenez, J. L., King, S. M., Manzi, A., Mikhailov, E., Pauliquevis, T., Petters, M. D., Prenni, A. J., Roldin, P., Rose, D., Schneider, J., Su, H., Zorn, S. R., Artaxo, P., and Andreae, M. O.: Rainforest aerosols as biogenic nuclei of clouds and precipitation in the Amazon, Science, 329, 1513–1516, 2010.

ACPD
14, 23995–24041, 2014

Potter, C. S., Alexander, S. E., Coughlan, J. C., and Klooster, S. A.: Modeling biogenic isoprene: exploration of model drivers, climate control algorithms, and use of global satellite observations, Atmos. Environ., 35, 6151–6165, 2001.

Pouliot, G. and Pierce, T. E.: Integration of the Model of Emissions of Gases and Aerosols from Nature (MEGAN) into the CMAQ Modeling System, 18th International Emission Inventory Conference, Baltimore, Maryland, 14–17 April 2009.

Piao, S. L., Ito, A., Li, S. G., Huang, Y., Ciais, P., Wang, X. H., Peng, S. S., Nan, H. J., Zhao, C., Ahlström, A., Andres, R. J., Chevallier, F., Fang, J. Y., Hartmann, J., Huntingford, C., Jeong, S., Levis, S., Levy, P. E., Li, J. S., Lomas, M. R., Mao, J. F., Mayorga, E., Mohammat, A., Muraoka, H., Peng, C. H., Peylin, P., Poulter, B., Shen, Z. H., Shi, X., Sitch, S., Tao, S., Tian, H. Q., Wu, X. P., Xu, M., Yu, G. R., Viovy, N., Zaehle, S., Zeng, N., and Zhu, B.: The carbon budget of terrestrial ecosystems in East Asia over the last two decades, Biogeosciences, 9, 3571–3586, doi:10.5194/bg-9-3571-2012, 2012.

Prather, M., Ehhalt, D., Dentener, F. J., Derwent, R., Dlugokencky, E. J., Holland, E., Isaksen, I., Katima, J., Kirchhoff, V., Matson, P., Midgley, P., and Wang, M.: Atmospheric chemistry and greenhouse gases, in: Climate Change 2001, The Scientific Basis, Contribution of Working Group I to the Third Assessment Report of the Intergovernmental Panel on Climate Change, edited by: Houghton, J. T., Ding, Y., Griggs, D. J., Noguer, M., van der Linden, P. J., Dai, X., Maskell, K., and Johnson, C. A., University Press, Cambridge, 238–287, 2001.

Qian, T., Dai, A., Trenberth, K. E., and Oleson, K. W.: Simulation of global land surface conditions from 1948 to 2004, Part I: forcing data and evaluations, J. Hydrometeorol., 7, 953–975, 2006.

Rinne, H. J. I., Guenther, A. B., Greenberg, J. P., and Harley, P. C.: Isoprene and monoterpene fluxes measured above Amazonian rainforest and their dependence on light and temperature, Atmos. Environ., 36, 2421–2426, 2002.

Saltelli, A., Ratto, M., Andres, T., Campolongo, F., Cariboni, J., Gatelli, D., Saisana, M., and Tarantola, S.: Global Sensitivity Analysis: The Primer, Wiley, New York, NY, 2008.

Sharkey, T. D., Singsaas, E. L., Vanderveer, P. J., and Geron, C.: Field measurements of isoprene emission from trees in response to temperature and light, Tree Physiol., 16, 649–654, 1996.

Solomon, S., Qin, D., Manning, M., Chen, Z., Marquis, M., Averyt, K. B., Tignor, M., and Miller, H. L.: Climate Change 2007: The Physical Science Basis: Contribution of Work-

ACPD
14, 23995–24041, 2014

ing Group I to the Fourth Assessment Report of the Intergovernmental Panel on Climate Change, Cambridge University Press, Cambridge, UK and New York, 2007.

Tao, Z. and Jain, A. K.: Modeling of global biogenic emissions for key indirect greenhouse gases and their response to atmospheric CO_2 increases and changes in land cover and climate, J. Geophys. Res., 110, D21309, doi:10.1029/2005JD005874, 2005.

Tingey, D. T., Turner, D. P., and Weber, J. A.: Factors controlling the emissions of monoterpenes and other volatile compounds, in: Trace Gas Emissions From Plants, edited by: Sharkey, T. D., Holland, E. A., and Mooney, H. A., Academic Press Inc., San Diego, California, 93–119, 1991.

von Kuhlmann, R., Lawrence, M. G., Pöschl, U., and Crutzen, P. J.: Sensitivities in global scale modeling of isoprene, Atmos. Chem. Phys., 4, 1–17, doi:10.5194/acp-4-1-2004, 2004.

Wang, K.-Y. and Shallcross, D. E.: Modeling terrestrial biogenic isoprene fluxes and their potential impact on global chemical species using a coupled LSM-CTM model, Atmos. Environ., 34, 2909–2925, 2000.

Wang, X., Situ, S., Guenther, A. B., Chen, F., Wu, Z., and Xia, B.: Spatiotemporal variability of biogenic terpenoid emissions in Pearl River Delta, China, with high-resolution land-cover and meteorological data, Tellus B, 63, 241–254, 2011.

Warneke, C., de Gouw, J. A., Del Negro, L., Brioude, J., McKeen, S., Stark, H., Kuster, W. C., Goldan, P. D., Trainer, M., Fehsenfeld, F. C., Wiedinmyer, C., Guenther, A. B., Hansel, A., Wisthaler, A., Atlas, E., Holloway, J. S., Ryerson, T. B., Peischl, J., Huey, L. G., and Hanks, A. T. C.: Biogenic emission measurement and inventories determination of biogenic emissions in the eastern United States and Texas and comparison with biogenic emission inventories, J. Geophys. Res., 115, D00F18, doi:10.1029/2009JD012445, 2010.

Went, F. W.: Blue hazes in the atmosphere, Nature, 187, 641–643, 1960.

World Meteorological Organization: Scientific Assessment of Ozone Depletion: 1994, Global Ozone Research and Monitoring Project, WMO/UNEP Report No. 37, Geneva, Switzerland, 1994.

Zare, A., Christensen, J. H., Irannejad, P., and Brandt, J.: Evaluation of two isoprene emission models for use in a long-range air pollution model, Atmos. Chem. Phys., 12, 7399–7412, doi:10.5194/acp-12-7399-2012, 2012.

ACPD
14, 23995–24041, 2014

Table 1. Estimated and direct measurements of isoprene emission flux, using different measurements techniques from tropical rainforest sites located in Brazil.

Month	Site	Location	Ecosystem	Isoprene Flux ($mg\,m^{-2}\,h^{-1}$)	Reference
Jan	FLONA Tapajo's, Km 83, PA Brazil	02°51′ S 54°58′ W	Primary, upland terra firme	2.2	Greenberg et al. (2004)
Feb	FLONA Tapajo's, Km 83, PA Brazil	02°51′ S 54°58′ W	Primary, upland terra firme	2.2	Greenberg et al. (2004)
Mar	Balbina, AM, Brazil	01°59′ S 59°12′ W	Upland, moist forest	5.3	Greenberg et al. (2004)
Apr	FLONA Tapajo's, Km 67, PA Brazil	02°51′ S 54°58′ W	Primary, upland terra firme	3.2	Harley et al. (2004)
Jun	FLONA Tapajo's, Km 67, PA Brazil	02°51′ S 54°58′ W	Primary, upland terra firme	3.2	Harley et al. (2004)
Jul	FLONA Tapajo's, Km 67, PA Brazil	02°51′ S 54°58′ W	Primary, upland terra firme	2.4	Rinne et al. (2002)
Sep	Reserva Biologica Jaru (RBJ), RO, Brazil	10°08′ S 62°54′ W	Primary forest	6.3	Kuhn et al. (2004a)
Oct	Reserva Biologica Jaru (RBJ), RO, Brazil	10°08′ S 62°54′ W	Primary forest	6.3	Kuhn et al. (2004a)
Nov	Reserva Biologica do Cuieiras, AM, Brazil	02°36′ S 60°12′ W	Primary forest	1.7	Alves et al. (2014)
Dec	Reserva Biologica do Cuieiras, AM, Brazil	02°36′ S 60°12′ W	Primary forest	3.2	Kesselmeier et al. (2002)

ACPD
14, 23995–24041, 2014

Table 2. Parameter name, description, sub-equation assignment, and mean ± SD estimated by CLM 4.0 and CLM 4.5 for a Central Amazon forest for all variables in the emission activity factor (γ, Ep. 1). NA = not a standard output in model version.

Parameter	Parameter Description	Sub-Equation	CLM4.0 (± SD)	CLM4.5 (± SD)	Units
T_{leaf}	Leaf temperature	γT	301.25 (0.78)	300.63 (0.74)	K
T_{leaf_24}	Leaf temperature in the last 24 h	γT	301.25 (0.77)	300.49 (0.79)	K
T_{leaf_240}	Leaf temperature in the last 240 h	γT	301.25 (0.72)	300.49 (0.69)	K
CT1	Empirical coefficient	γT	95	95	Constant
CT2	Empirical coefficient	γT	230	230	Constant
PAR_{SUN}	Sunlit PAR	γP	353.99 (34.24)	343.83 (34.84)	$\mu mol\, m^{-2}\, s^{-1}$
PAR_{24_SUN}	Sunlit PAR in last 24 h	γP	341.47 (33.59)	327.02 (29.84)	$\mu mol\, m^{-2}\, s^{-1}$
PAR_{240_SUN}	Sunlit PAR in last 240 h	γP	341.20 (32.29)	326.59 (23.66)	$\mu mol\, m^{-2}\, s^{-1}$
PAR_{SHADE}	Shade PAR	γP	131.85 (4.01)	118.55 (3.98)	$\mu mol\, m^{-2}\, s^{-1}$
PAR_{24_SHADE}	Shade PAR in last 24 h	γP	144.37 (4.39)	135.26 (4.24)	$\mu mol\, m^{-2}\, s^{-1}$
PAR_{240_SHADE}	Shade PAR in last 240 h	γP	144.67 (4.25)	135.64 (3.52)	$\mu mol\, m^{-2}\, s^{-1}$
$P0_{SUN}$	Standard condition for past 24 h for sun leaves	γP	200	200	$\mu mol\, m^{-2}\, s^{-1}$ (Constant)
$P0_{SHADE}$	Standard condition for past 24 h for shade leaves	γP	50	50	$\mu mol\, m^{-2}\, s^{-1}$ (Constant)
C_{CE}	Factor that sets emission activity to unity at standard conditions	γL	0.3	0.3	Empirical Constant
LAI	Leaf area index	γL	8.85 (0.13)	6.39 (0.08)	$m^2\, m^{-2}$
$forc_{pbot}$	Atmospheric pressure	γC	100, 446.24 (105.73)	NA	Pa
Ci_{SUN}	Sunlit leaf intracellular CO_2	γC	−466.87 (19.31)	NA	Pa
Ci_{SHADE}	Shade leaf intracellular CO_2	γC	−466.11 (19.36)	NA	Pa
F_{SUN}	Sunlit fraction of canopy	γC	0.06 (0.002)	0.09 (0.002)	%

ACPD
14, 23995–24041, 2014

Table 3. Ranking of uncertainty. Modeled mean emissions activity factor (γ), standard variation, range, and contribution of uncertainty for each biophysical parameter as predicted by MEGAN-CLM 4.0, or based on Monte Carlo simulation to predict the overall uncertainty of emission activity factor.

Rank	Variables	γ	Stdev.	Range	Contribution to overall uncertainty (%)
NA	MEGAN-CLM 4.0	0.82	0.15	0.87	NA
NA	All parameters	0.87	0.09	0.50	NA
1	T_{leaf}	0.87	0.08	0.28	0.288
2	C_{CE}	0.91	0.05	0.16	0.180
3	T_{leaf_24}	0.84	0.03	0.11	0.108
4	CT1	0.83	0.03	0.10	0.108
5	CT2	0.83	0.02	0.06	0.072
6	PAR_{SHADE}	0.83	0.02	0.06	0.072
7	PAR_{SUN}	0.83	0.01	0.04	0.036
8	T_{leaf_240}	0.83	0.01	0.03	0.036
9	LAI	0.83	0.01	0.03	0.036
10	PAR_{240_SHADE}	0.82	0.005	0.02	0.018
11	F_{SUN}	0.83	0.003	0.01	0.011
12	Ci_{SHADE}	0.82	0.003	0.01	0.011
13	PAR_{24_SUN}	0.82	0.002	0.01	0.007
14	PAR_{240_SUN}	0.83	0.002	0.01	0.007
15	PAR_{24_SHADE}	0.82	0.001	0.004	0.004
16	$P0_{SHADE}$	0.82	0.0006	0.002	0.002
17	$P0_{SUN}$	0.82	0.0005	0.002	0.002
18	Ci_{SUN}	0.82	0.0002	0.00	0.001
19	$forc_{pbot}$	0.82	0.0002	0.00	0.001

ACPD
14, 23995–24041, 2014

Table 4. Leaf temperature (T_{leaf}, °C) averages ± SD for in situ measurements from a Central Amazon mature forest and CLM 4.0, and root-mean-square error (RMSE). In situ maximum temperatures are from individual leaves.

	In situ measurements			CLM 4.0			In Situ vs. CLM
Months	Average ± SD	Range	Max	Average ± SD	Range	Max	RMSE
DJF	29.0 ± 3.1	15.1	45.9	28.9 ± 1.4	5.7	31.8	1.36
MAM	28.5 ± 3.1	16.7	43.5	28.5 ± 1.3	5.6	31.5	1.26
JJA	29.9 ± 2.8	16.5	45.1	28.4 ± 1.6	6.9	32.3	1.59
SON	30.9 ± 2.4	14.2	44.6	29.7 ± 1.6	6.2	33.5	1.59

ACPD
14, 23995–24041, 2014

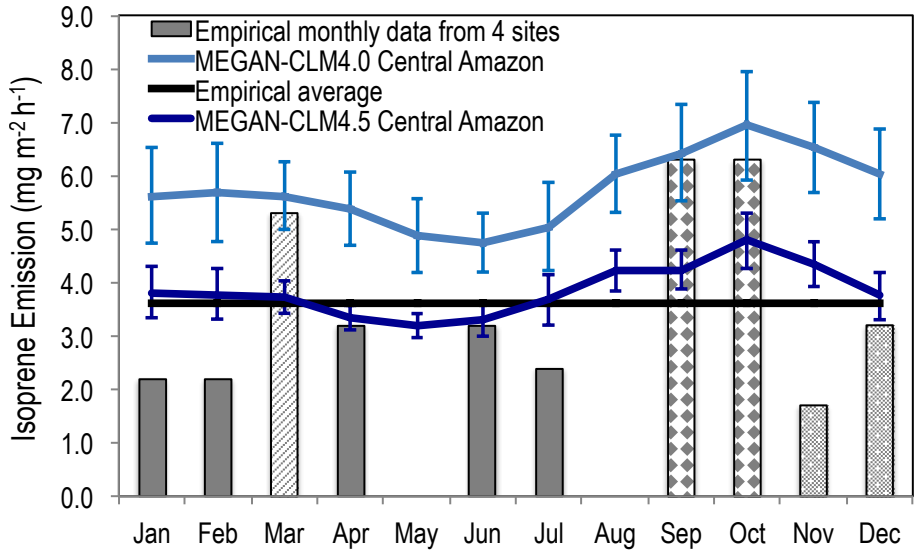


Figure 1. Model predictions of monthly isoprene emissions (mg m^{-2} h^{-1}) ± SD from MEGAN-CLM 4.0 and MEGAN-CLM 4.5 for a Central Amazon forest, compared to in situ datasets from four Brazilian locations (separated by pattern and listed in Table 1). Average annual isoprene emissions from empirical data sets was 3.6 mg m^{-2} h^{-1}. In situ data missing for the months of May and August.

ACPD
14, 23995–24041, 2014

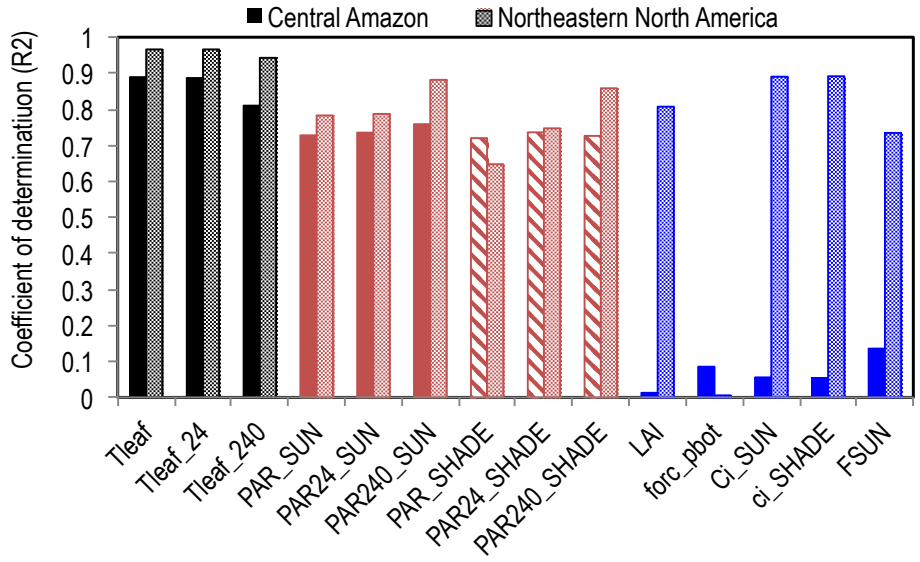


Figure 2. Coefficient of determination, from regression analysis, for 14 out of the 19 variables in Eq. (1) and Table 2, as it relates to the emission activity response, for a Central Amazon forest (i.e., solid color bars) and northeastern temperate forest (i.e., hashed color bars).

ACPD
14, 23995–24041, 2014

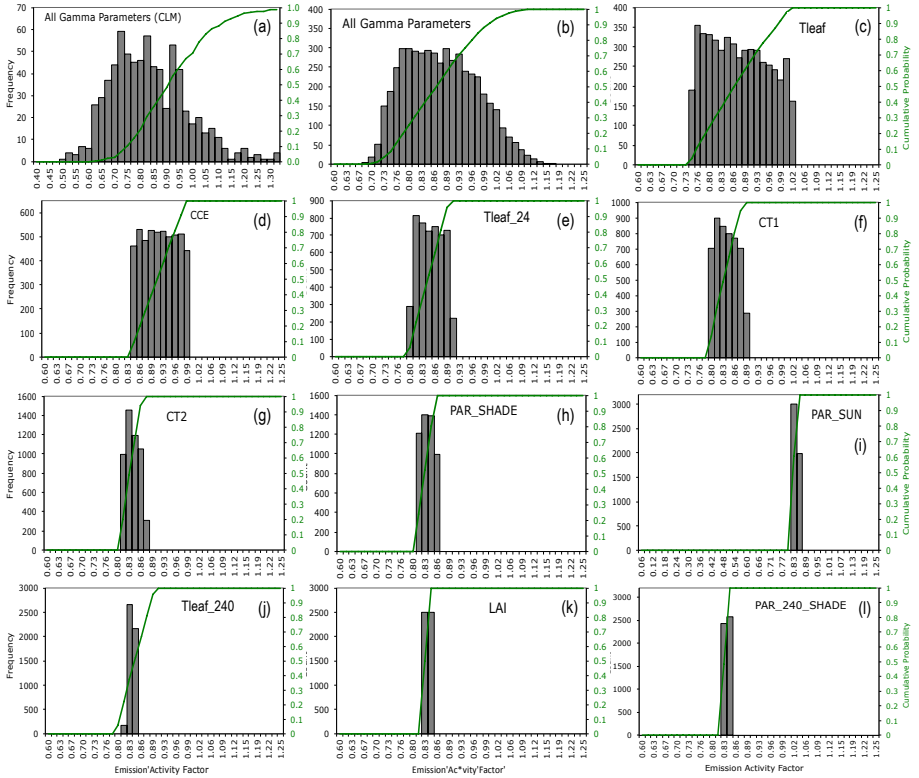
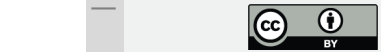


Figure 3. Distribution of the emissions activity factor, γ, using Monte Carlo uncertainty simulations. **(a)** is the predicted distribution based on MEGAN-CLM 4.0 estimates, pre-Monte Carlo simulation. **(b)** was a simulation in which all variables in the emissions activity factor equation were varied, and **(c–l)** are one-at-a-time Monte Carlo simulations. Displaying top 10 variables that contribute the most to variability.

ACPD
14, 23995–24041, 2014



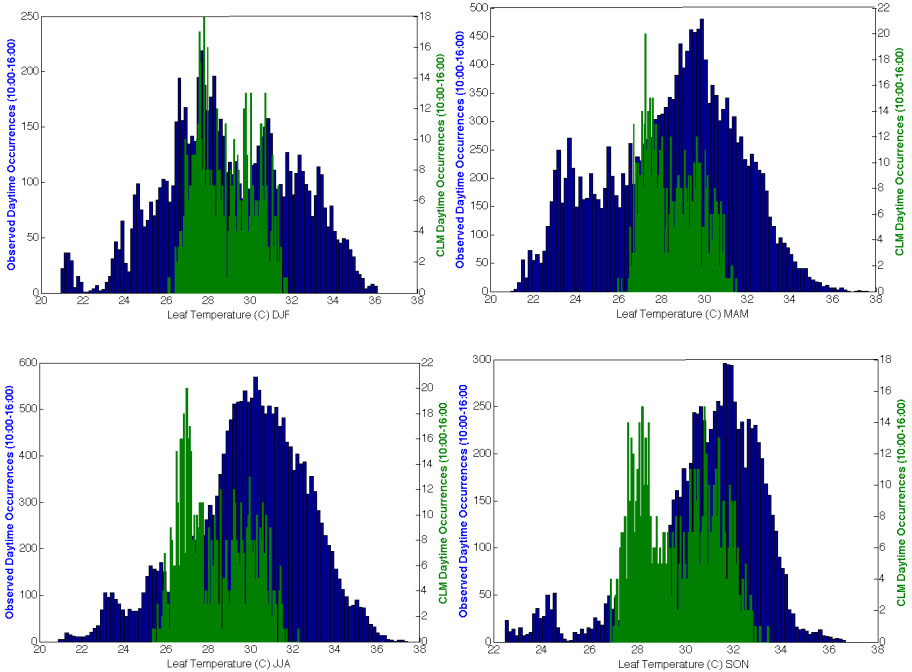


Figure 4. Key: DJF = December, January, February; MAM = March, April, May; JJA = June, July, August; SON = September, October, November. Seasonal leaf temperature (T_{leaf}, ˚C) distribution from in situ measurements, averaged over 25 leaves, recorded every minute, during daytime hours (10:00–16:00 AMT) in blue bars. Seasonal leaf temperature (T_{leaf}, ˚C) distribution from CLM 4.0, averaged over one grid cell, recorded every hour, during daytime hours (10:00–16:00) in green bars.

ACPD
14, 23995–24041, 2014

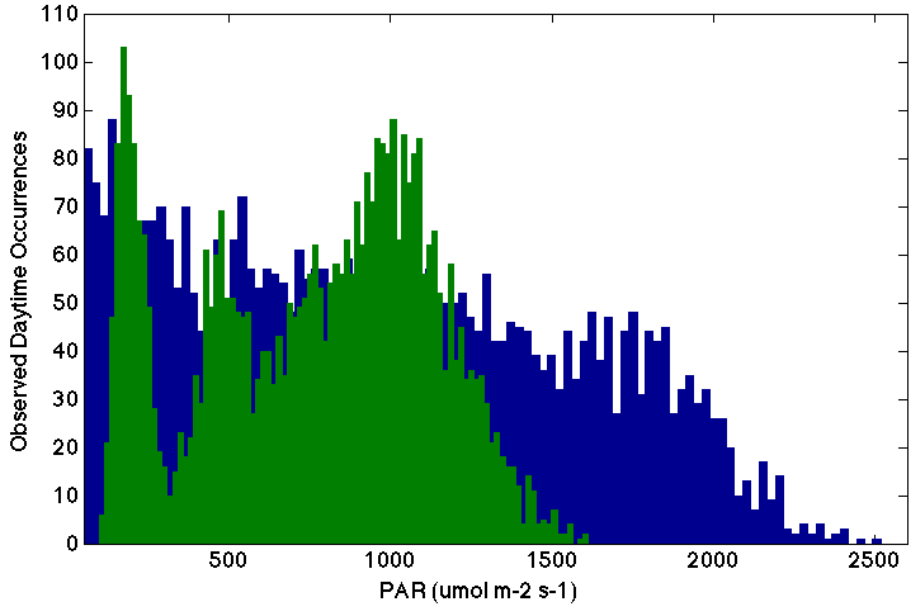


Figure 5. Distribution of annual photosynthetic active radiation (PAR, μmol m^{-2} s^{-1}) from in situ measurements (i.e., blue bars) over daytime hours (10:00–16:00 AMT), and from CLM 4.0 (i.e., green bars) over the twelve-hour daytime period.

ACPD
14, 23995–24041, 2014

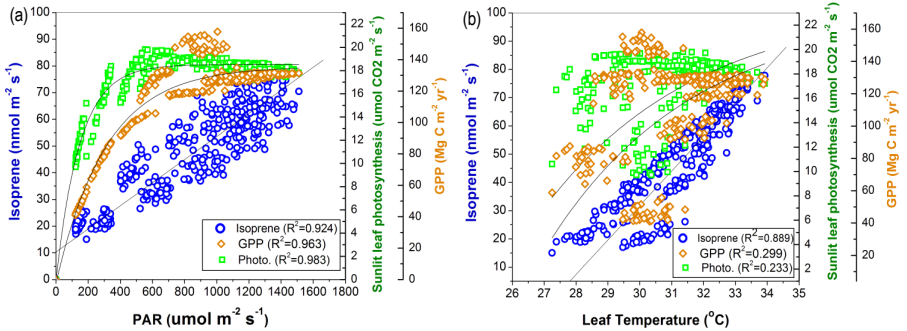


Figure 6. (a) Predicted (i.e., MEGAN-CLM 4.0) isoprene emissions (nmol m^{-2} s^{-1}), sunlit leaf photosynthesis (μmol CO_2 m^{-2} s^{-1}), and gross primary production (GPP, Mg C m^{-2} yr^{-1}) in response to photosynthetic active radiation (PAR, μmol m^{-2} s^{-1}) curves, and **(b)** in response to leaf temperature (°C) curves.

ACPD
14, 23995–24041, 2014

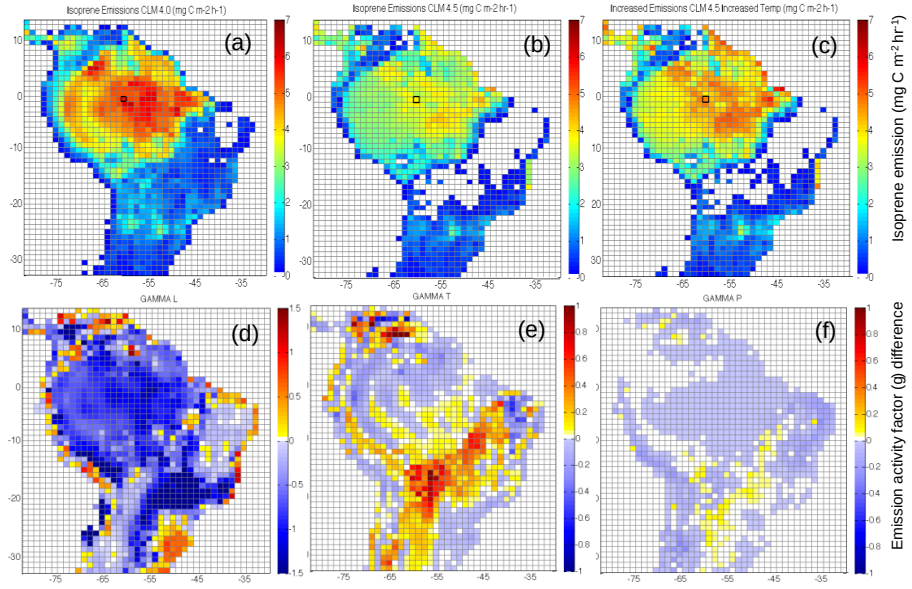


Figure 7. Average annual isoprene emissions (mg C m^{-2} h^{-1}) for South America predicted by **(a)** MEGAN-CLM 4.0, **(b)** MEGAN-CLM 4.5, and **(c)** MEGAN-CLM 4.5 with T_{leaf} increased by 1.0 °C. Difference between MEGAN-CLM 4.5 and MEGAN-CLM 4.0 for the emission activity factor (γ, unitless) predicted by **(d)** the leaf area index algorithm (γL), **(e)** leaf temperature algorithm (γT), and **(f)** light or photosynthetic active radiation (PAR) algorithm (γP).

ACPD
14, 23995–24041, 2014