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Quantifying regional, seasonal and interannual contributions of environmental factors on isoprene and monoterpene emissions estimates over eastern Texas

Ling Huang, Gary McGaughey*, Elena McDonald-Buller, Yosuke Kimura, David T. Allen

Center for Energy and Environmental Resources, The University of Texas at Austin, Austin, TX, USA

HIGHLIGHTS

- Eastern Texas has diverse land cover and climatology with recent severe drought.
- Temperature was a primary driver of variations in predicted biogenic emissions.
- The response of biogenic emissions to soil water stress is a source of uncertainty.

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ABSTRACT

Recent years have brought renewed attention to the effects of drought on emissions of biogenic volatile organic compounds. Variability in environmental inputs that influence isoprene and monoterpene emissions within eastern Texas was quantified by examining seasonal and interannual changes in activity factors intrinsic to the Model of Emissions of Gases and Aerosols from Nature (MEGAN) during years that included average-to-wet conditions (2007) and extreme drought and heat (2006 and 2011). Activity factors are used in MEGAN to multiplicatively adjust emissions rates from an assumed set of standard conditions for temperature, light, leaf area index (LAI), and soil moisture. Temperature was found to be the primary driver of seasonal and interannual variations of isoprene and monoterpene emissions; during drought years, reductions in LAI were dominated by predicted emissions increases caused by much warmer temperatures. The response of biogenic emissions to soil water stress is a major source of uncertainty. Dependent on the specific soil moisture database employed, predicted reductions in isoprene emissions ranged from minimal to −70% during the summer of 2011, a period characterized by all-time record drought in the South Central U.S.

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1. Introduction

Isoprene (2-methyl-1, 3-butadiene, C_5H_8) and monoterpenes (a class of terpenes composed of two isoprene units) have been widely recognized for their key roles in atmospheric chemistry and climate, including contributions as precursors for tropospheric ozone (Atkinson, 2000) and secondary organic aerosol (SOA) formation (Tsigaridis and Kanakidou, 2003; Claeys et al., 2004). Globally, isoprene and monoterpenes are estimated to comprise 70% and 11%, respectively, of total annual biogenic volatile organic compounds (BVOCs) emitted from vegetation (Sindelarova et al., 2014). Average Texas statewide VOC emissions reported in the EPA 2011 National Emission Inventory (Version 1) were ranked first within the continental United States at approximately 11,650 and 4600 tons per day for biogenic and anthropogenic emissions, respectively.

The Model of Emissions of Gases and Aerosols from Nature (MEGAN) has been utilized extensively for the estimation of BVOC emissions on global and regional scales (Müller et al., 2008; Arneth et al., 2011; Sindelarova et al., 2014; Guenther et al., 2006, 2012; Ferreira et al., 2010; Potosnak et al., 2014; Han et al., 2013) as well as to investigate the impacts of biogenic emissions on atmospheric chemistry (Heald et al., 2008; Fu and Liao, 2012; Geng et al., 2011). Isoprene and monoterpene emissions are controlled by various environmental factors, including temperature and light (Petron et al., 2001; Tingey et al., 1980; Sharkey et al., 1996), soil moisture (Pegoraro et al., 2004; Ormeno et al., 2007), atmospheric CO_2 concentration (Rosenstiel et al., 2003; Wilkinson et al., 2009),

* Corresponding author.
E-mail address: garym@mail.utexas.edu (G. McGaughey).

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and phenology (Kuhn et al., 2004; Fischbach et al., 2002).

Previous studies have investigated the sensitivities of biogenic emissions (primarily isoprene) estimated by MEGAN to the driving meteorology, basal emission rate, vegetation distribution, and leaf area index (LAI) (Guenther et al., 2006; Wiedinmyer et al., 2001; Müller et al., 2008; Smiatek and Bogacki, 2005). Temperature has an important influence on estimates of emissions of isoprene and monoterpenes and their interannual variations (Stavrakou et al., 2014; Tawfik et al., 2012; Guenther et al., 2006). Solar radiation is an essential driving variable for light-dependent isoprene emissions; recent studies have suggested that solar radiation contributes negligibly to summer variations in sub-regions of the U.S. (Tawfik et al., 2012) but is a primary influence on interannual variations in East Asia (Stavrakou et al., 2014). The emission of de novo biosynthesized monoterpenes is controlled by light on a daily basis and is modeled in a similar way as for isoprene (Guenther et al., 2012).

A limited number of observational studies have suggested that soil water deficits are associated with an overall decline in leaf-level isoprene and monoterpene emissions (Lusebrink et al., 2011; Rodríguez-Calcerrada et al., 2013). The impact of modeled variations of soil moisture on biogenic emissions has been inconsistent and is likely sensitive to the specific soil moisture and wilting point data being employed (Müller et al., 2008; Tawfik et al., 2012; Sindelarova et al., 2014; Potosnak et al., 2014). Modeled impacts of LAI variability on isoprene emissions have shown a wide range (Huang et al., 2014; Gulden et al., 2007; Tawfik et al., 2012; Müller et al., 2008). With respect to uncertainty, recent MEGAN studies that have compared the impact of variability in environmental inputs on predicted emissions have shown greater sensitivity (suggesting potentially larger uncertainty) for temperature, Photosynthetically Active Radiation (PAR), and soil moisture compared to other environmental inputs such as LAI (e.g., Holm et al., 2014; Situ et al., 2014; Stravrakou et al., 2014).

Many of the aforementioned studies have utilized MEGAN in support of sensitivity analyses of emissions estimates via perturbations of environmental inputs or climate/vegetation scenarios (e.g., Lathiere et al., 2010; Sindelarova et al., 2014; Chen et al., 2009; Arneth et al., 2011; Guenther et al., 2006, 2012). In MEGANv2.1, activity factors are used to multiplicatively adjust emissions from a standardized set of environmental conditions (Guenther et al., 2012). In order to track the relative changes in these activity factors internal to the MEGAN estimations, we modified the model source codes to enable the examination of individual activity factors for temperature, light, LAI, and soil moisture. The objective of this study is to quantify and interpret the differences in these environmental activity factors between years that had above average rainfall and average temperatures (2007) to years with substantially warmer and drier conditions (2006 and 2011) to assess the influence on isoprene and monoterpene emissions estimates in MEGAN.

2. Methodology

2.1. Description of MEGANv2.1

The latest version of MEGAN (MEGANv2.1) is described in detail by Guenther et al. (2012). The emissions rate (F) of isoprene/monoterpenes from terrestrial landscapes in units of flux (μg m^{-2} ground area h^{-1}) is calculated as:

$$F = \gamma \sum \varepsilon_j \chi_j \tag{1}$$

where ε is the basal emission factor for vegetation type j with fractional coverage χ_j; it represents the emission rate under standard environmental conditions defined in Guenther et al. (2006, 2012) including an air temperature of 303 K, solar angle of 60°, photosynthetic photon flux density (PPFD) transmission of 0.6, LAI of 5 m^2/m^2 consisting of 80% mature, 10% growing and 10% old foliage, and volumetric soil moisture of 0.3 m^3/m^3. γ is the overall emissions activity factor that accounts for variations in environmental conditions, and is constructed differently for isoprene and monoterpenes. For isoprene, emissions are light-dependent with a light dependent fraction (LDF) assigned as unity; the overall activity factor is calculated as:

$$\gamma = \gamma_{age} \cdot \gamma_{SM} \cdot \gamma_{CE} \tag{2}$$

with each of the individual gammas calculated as below (detailed descriptions of all activity factor variables are provided in Supplemental Information, Table S1):

$$\text{leaf age}: \ \gamma_{age} = A_{new}F_{new} + A_{gro}F_{gro} + A_{mat}F_{mat} + A_{old}F_{old} \tag{3}$$

$$\text{soil moisture}: \ \gamma_{SM} = \sum_{i=1}^{4} f_{root}^{i} \max\left(0, \min\left(1, \left(\theta^{i} - \theta_{wilt}\right) \Big/ 0.04\right)\right) \tag{4}$$

$$\text{canopy environment}: \ \gamma_{CE} = 0.56 \cdot \sum_{i=1}^{5} \left[\left(\gamma_T^i\right)_{sun} \left(\gamma_P^i\right)_{sun} f_{sun}^i + \left(\gamma_T^i\right)_{shade} \left(\gamma_P^i\right)_{shade} f_{shade}^i\right] \cdot LAI^i \tag{5}$$

The default MEGAN configuration sets the relative emissions rates based on mature leaves. γ_{age} accounts for differences in basal emission rates among four leaf stages – new, growing, mature and old foliage. Emission rates for each leaf stage are assigned based on experimental observations (Guenther et al., 2006) and the distribution of leaf ages is determined by changes in LAI between the current and previous time steps; a positive difference increases the amount of new and growing leaves and vice versa.

For monoterpenes, the soil moisture effect is not considered (γ_{SM}=1); a LDF of either 0.4 (for β-pinene, limonene, 3-carene, *t*-β-ocimene) or 0.6 (for α-pinene, myrcene, sabinene) is assigned. The overall activity factor is calculated as:

$$\gamma = \gamma_{age} \cdot \left[(1 - LDF) \cdot \gamma_{T_LIF} \cdot \gamma_{LAI} + LDF \cdot \gamma_{CE}\right] \tag{6}$$

with light independent fraction (LIF) related factors calculated as:

$$\text{temperature}: \ \gamma_{T_LIF} = \sum_{i=1}^{5} \left[\left(\gamma_{T_LIF}^i\right)_{sun} f_{sun}^i + \left(\gamma_{T_LIF}^i\right)_{shade} f_{shade}^i\right] \tag{7}$$

$$\text{leaf area index}: \ \gamma_{LAI} = 0.49LAI \Big/ \left(1 + 0.2LAI^2\right)^{0.5} \tag{8}$$

The canopy environment model within MEGANv2.1 consists of five canopy layers. For each layer, temperature (γ_T, γ_{T_LIF}) and light (γ_P) activity factors are calculated for both sun and shaded leaves based on layer-specific temperature and PPFD, and then summed based on the sun/shaded fractions (*f*) for each layer. LAI is distributed between the layers using a Gaussian distribution. The sum of the product of γ_T, γ_P and LAI over the five layers provides the canopy environment activity factor (γ_{CE}). The parameters are further described in Supplementary Table S1 and Guenther et al. (2012).

2.2. MEGAN configuration

MEGAN was run at a 1-km horizontal spatial resolution and configured according to the approach of Huang et al. (2014). Utilized datasets included a regional land cover database with high spatial resolution (~30 m, obtained from the Texas Commission on Environmental Quality) consisting of 36 Land Classification System classes that were mapped to MEGAN's 16 default Plant Functional Types (PFTs), MODIS (Moderate Resolution Imaging Spectroradiometer) 4-day LAI product (MCD15A3, 1-km), National Centers for Environmental Predictions - North American Regional Reanalysis (NCEP – NARR, 32-km) meteorological data, and Photosynthetic Active Radiation (PAR, 4-km) produced by University of Alabama Huntsville from the Geostationary Operational Environmental Satellites (GOES).

The soil moisture datasets employed in our study were driven by North American Land Data Assimilation System Phase 2 (NLDAS-2) meteorological forcings, which provide hourly temporal and 1/8th degree spatial resolution; the NLDAS-2 nonprecipitation fields are provided by NCEP – NARR while the precipitation data are derived from gaged daily rainfall from NCEP/Climate Prediction Center (Cai et al., 2014a). The original NLDAS testbed, which was designed to provide land surface states to coupled weather/climate models (Mitchell et al., 2004), consists of four land surface models (LSMs): the community Noah LSM (Noah) (Ek et al., 2003), the Mosaic LSM (Mosaic) (Koster and Suarez, 1996), the Sacramento Soil Moisture Accounting model (SAC-SMA) (Burnash et al., 1973), and the Variable Infiltration Capacity (VIC) model (Liang et al., 1994). These original NLDAS LSMs do not yet include recent developments in the land model community such as improved physics and new functionalities (e.g., prognostic leaf models, dynamic groundwater, multilayer snow) that have been incorporated into the Community Land Model version 4 (CLM4) (Lawrence et al., 2011) and the multi-parameterization options version of the Noah model (Noah-MP) (Niu et al., 2011). Because Noah-MP has been shown to have good performance for soil moisture in Texas (Cai et al., 2014b), Noah-MP was the primary soil moisture dataset used for our study. Additionally, soil moisture predictions from the Mosaic LSM were used for sensitivity simulations to investigate the impact of soil moisture uncertainty on estimates of isoprene emissions. As stressed by Müller et al. (2008) and Guenther et al. (2012), wilting point values for a given MEGAN simulation were those provided by the specific land surface model employed.

In addition to the default overall activity factor (γ), MEGAN source codes were modified to output each of the individual activity factors (e.g., γ_{age}, γ_{SM}, γ_{CE}, γ_{LAI}, etc.). MEGAN simulations were conducted over eastern Texas (ref. Fig. 1) for March–October during 2006, 2007 and 2011. As shown by the drought indices as well as annual precipitation distributions anomalies (Supplementary Fig. S1), 2007 was a relatively wet year with greater than average annual precipitation; in contrast, year 2006 and 2011 were characterized by extreme to exceptional drought. Hourly individual activity factors for each 1-km grid cell were averaged by season (spring: March-April-May or MAM; summer: June-July-August or JJA; fall: September–October or SO), eastern Texas climate region (North Central Texas, South Central Texas, East Texas and Upper Coast) and year to generate area- and season-averaged values. Grid cells designated as water by the land cover database were ignored. For isoprene, only hours with non-zero PAR values (i.e. daytime) were considered.

3. Results

3.1. Isoprene and monoterpene emissions estimates

Consistent with other studies for the South Central U.S. (Lamb et al., 1993; Kleindienst et al., 2007), Huang et al. (2014) demonstrated that biogenic emissions peak during summer. Table 1 shows the 2006–2011 season-averaged isoprene and monoterpene emissions and their variability for the four eastern Texas climate

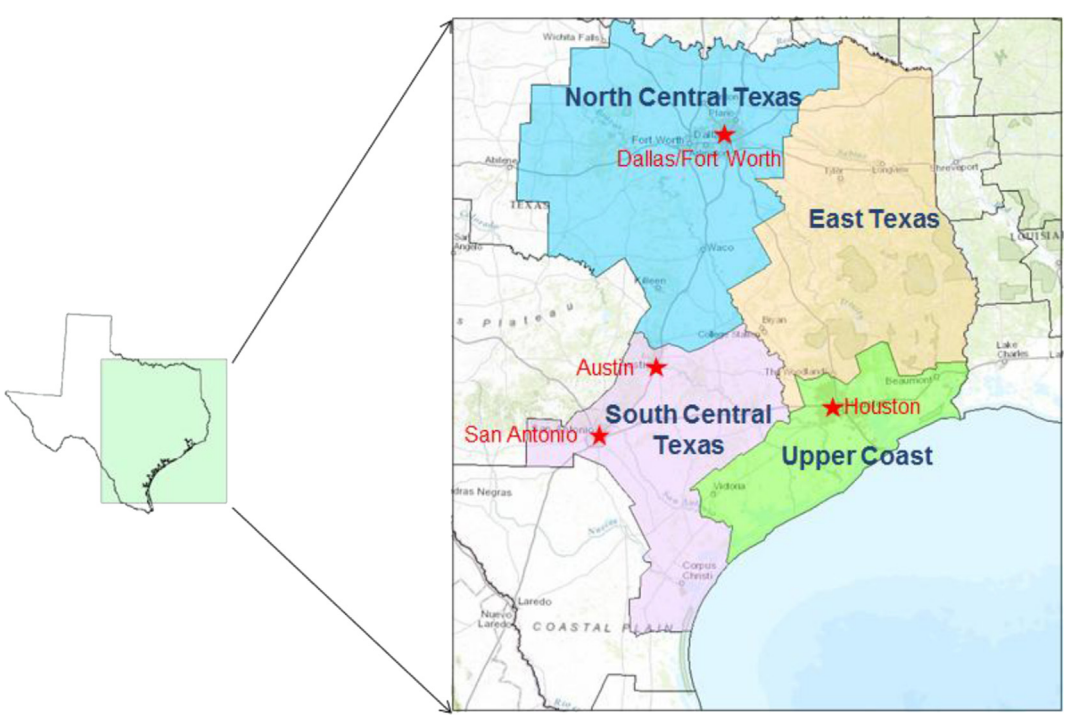

Fig. 1. The MEGAN domain over eastern Texas including the four eastern Texas climate regions – North Central Texas, South Central Texas, East Texas and Upper Coast (Source: National Oceanic and Atmospheric Administration). The centers of major metropolitan areas are shown by red stars. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

regions from Huang et al. (2014). East Texas exhibits the highest emissions among the four climate regions, primarily due to its densely forested areas; by region, summer emissions can be more than three times greater compared to spring/fall. Isoprene interannual variations ranged from 13.9% during summer in South Central Texas to 24.6% during spring in North Central Texas; monoterpenes exhibited weaker interannual variations by season.

3.2. Canopy-level comparisons

3.2.1. Isoprene

Fig. 2 shows the canopy-level activity factors for isoprene during 2006, 2007 and 2011 averaged by season for the North Central (predominantly grassland) and East (predominantly forested) regions; analogous results for South Central and Upper Coast are provided in Supplementary Fig. S2. As expected, the overall activity factors (γ_{tot}) exhibit strong seasonal patterns with highest values during summer regardless of region and year. Because the basal emission factor (ε) and vegetation distributions (χ_j) are assumed constant, the seasonal pattern of the absolute emissions is solely controlled by changes in the overall activity factor.

Across all regions and seasons the leaf age activity factors (γ_{age}) typically range from 0.85 to 0.94 (with a low of 0.8 during spring 2007 for South Central Texas) and exhibit negligible interannual or seasonal variations. Mature and older leaves have higher isoprene emissions than new and growing leaves; therefore, the leaf age factor is always below unity. As shown in Fig. 2, the leaf age activity factor during the generally wet year (2007) is always slightly lower than the drought years (i.e. 2006 and 2011) related to the more rapid changes and variations in LAI during 2007.

The soil moisture activity factors also demonstrate low seasonal and interannual variations (<5%). As shown in Fig. 2, the soil moisture activity factor for 2007 is essentially constant near unity; during the drought years (2006 and 2011), the soil moisture activity factor primarily ranges between 0.94 and 0.99. During 2011, a year that had conditions of the all-time record drought throughout most of Texas, the minimum soil moisture activity factor is 0.90 during the North Central Texas summer. The impact of drought on isoprene emissions as currently characterized by MEGANv2.1 may have substantial uncertainty; for example, a recent study by Potosnak et al. (2014) observed a time-dependent response of field isoprene emissions to drought where an initial increase of emissions (about a week) was followed by a subsequent decrease and concluded that the MEGAN time-independent soil moisture algorithm was not able to capture the relevant response of isoprene emissions to drought. Nonetheless, soil moisture represents a primary mechanism by which drought effects are manifested in MEGAN isoprene estimates.

Fig. 2 illustrates that the majority of changes in the overall activity factor is captured by differences in the canopy environmental factor (γ_{CE}). Seasonal variations are greater than inter-annual variations; year-to-year differences in γ_{CE} diminished in the fall, particularly in East Texas (and Upper Coast shown in Fig. S2). As an example, the seasonal values of γ_{CE} for East Texas during 2011 ranged from 0.53 during the fall to 1.85 during the summer, differing by a factor of 3.5. In contrast, summer γ_{CE} values for 2006 and 2007 are 1.27 and 0.94, respectively.

3.2.2. Monoterpenes

Fig. 3 (North Central and East) and (South Central and Upper Coast) show the canopy-level activity factors for monoterpenes during 2006, 2007 and 2011 averaged by season and climate region. In contrast to the methodology used for isoprene, the hourly-generated activity factors are averaged over the entire period instead of daylight hours because monoterpenes have both light-dependent and light-independent fractions; thus there are two additional activity factors (γ_{T_LIF}, γ_{LAI}) related to light-independent emissions. The use of different light-dependent fractions causes negligible differences in the overall activity factor; thus the seven classes of monoterpenes are considered as one monoterpene class for the purposes of this study.

As shown in Fig. 3, the light-independent temperature (γ_{T_LIF}) and canopy environment activity (γ_{CE}) factors have substantial seasonal variations. The seasonal variations of the light-independent LAI activity factor (γ_{LAI}) are generally low and reach a maximum value of 14.8% in North Central Texas during 2011; interannual variations are strong in the two central regions during summer and fall (>15%) but less (<10%) in East Texas; this is consistent with the substantial LAI reductions associated with drought in the central regions as demonstrated by Huang et al. (2014).

In contrast to isoprene, new and growing leaves emit more monoterpenes than mature and old leaves. Thus, the leaf age activity factor for monoterpenes is always above unity and had slightly greater values during the wetter than normal year (2007) compared to the drought years, with a maximum value of 1.2 in spring 2007. Similar to isoprene, leaf age is not a significant contributor to seasonal or interannual monoterpene variations. The soil moisture algorithm is not applied to monoterpenes in MEGAN.

3.3. Within-canopy comparisons

3.3.1. Isoprene

The detailed results for γ_{CE}, which describes the variations due to temperature, light and LAI within each of the five canopy layers, have been provided as Supplementary Fig. S4. MEGAN uses a

Table 1
Averaged isoprene and monoterpene emissions (kg/km^2/day) and interannual variability[a] (in brackets) during 2006–2011 by season and eastern Texas climate regions from Huang et al. (2014).

Climate region	Isoprene (kg/km^2/day)			Monoterpenes (kg/km^2/day)		
	MAM	JJA	SO	MAM	JJA	SO
North Central Texas	8.1 (24.6%)	33.4 (15.7%)	8.0 (18.5%)	1.5 (10.6%)	4.2 (9.8%)	1.6 (16.8%)
South Central Texas	13.7 (20.4%)	40.6 (13.9%)	13.7 (17.4%)	1.9 (8.3%)	4.1 (8.4%)	2.1 (12.6%)
East Texas	18.7 (23.6%)	69.3 (19.9%)	22.1 (21.1%)	4.5 (10.1%)	11.8 (12.0%)	5.4 (9.8%)
Upper Coast	9.8 (14.5%)	28.7 (14.6%)	11.6 (16.8%)	2.0 (7.6%)	4.5 (7.2%)	2.4 (8.7%)

[a] Interannual variability (IAV) was determined as the average absolute percent departure from the 2006–2011 mean according to the approach of Tawfik et al. (2012):

$$IAV = \frac{1}{n}\sum_{y=1}^{n}\left|\frac{x_{y,seas} - \overline{x_{seas}}}{\overline{x_{seas}}}\right| \times 100\%$$

where $x_{y,seas}$ is the isoprene/monoterpene emissions for year, y, and season, seas; $\overline{x_{seas}}$ is the average seasonal emissions across all years (2006–2011); n is the number of years simulated.

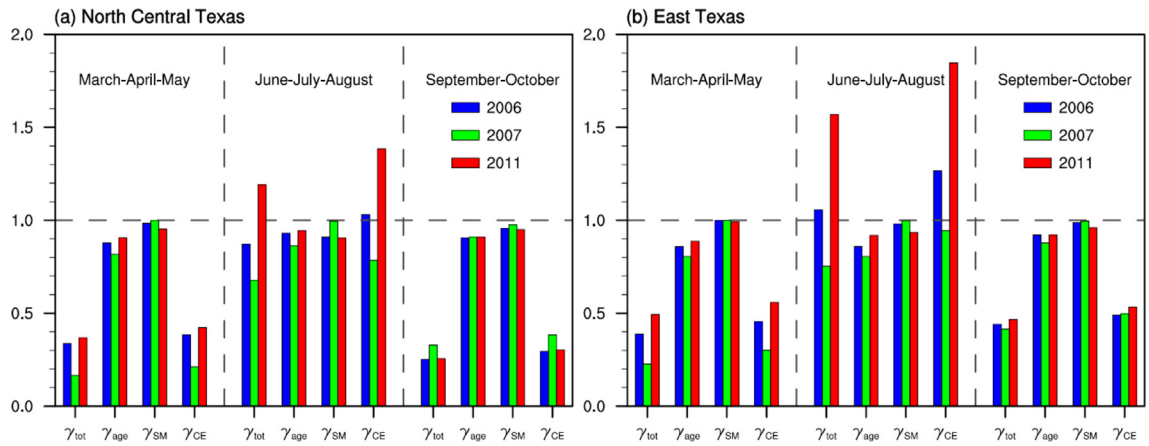

Fig. 2. Area- and season-averaged MEGAN activity factors for isoprene during 2006, 2007, and 2011 in (a) North Central Texas and (b) East Texas. Results for South Central Texas and Upper Coast are shown in Supplementary Fig. S2.

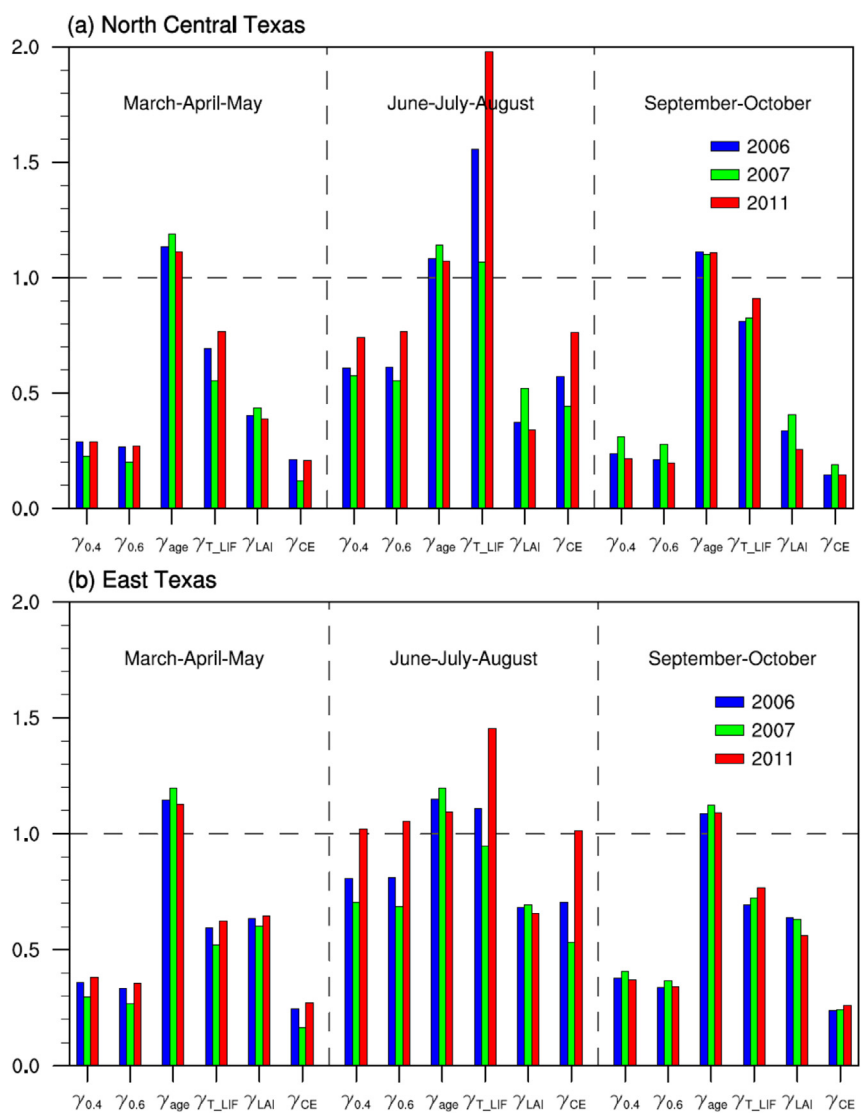

Fig. 3. Area- and season-averaged MEGAN activity factors for monoterpenes during 2006, 2007, and 2011 in (a) North Central Texas and (b) East Texas. $\gamma_{0.4}$and $\gamma_{0.6}$represent the overall activity factor for monoterpene classes with a light dependent fraction of 0.4 and 0.6, respectively. Results for South Central Texas and Upper Coast are shown in Supplementary Fig. S3.

Gaussian distribution to distribute LAI between the layers such that the middle layer has the largest LAI values. Temperature variability, as demonstrated by the temperature activity factor (γ_T), is relatively low and varies as much as 7% between the top and bottom layers. There is often a substantial change in the light activity factor (γ_P) with top to bottom differences of 10–30%; larger LAI values produce greater attenuation as light passes through the canopy. For example, in North Central Texas during 2011, summer γ_P values decrease from 0.97 at the canopy top to 0.64 at the bottom (a factor of 1.5 attenuation); during the wetter-than-normal year (2007) with relatively larger LAI, γ_P is reduced from 0.85 to 0.45 (a factor of 1.9 attenuation). As shown in Supplementary Fig. S4, East Texas has the greatest values of LAI as well as the largest layer-to-layer differences in γ_P compared to the other regions.

In order to investigate the seasonal and interannual variations in canopy activity factors, layer-averaged values for LAI, temperature and light activity are shown in Fig. 4 and Supplementary Fig. S5. The temperature activity factor has much greater seasonal variation compared to LAI and light for all regions, indicating that temperature is the primary driver of the seasonal variations of the canopy environment activity factor and, thus, isoprene emissions. Seasonal variations of the temperature activity factor were 20–55% with the greatest variation during 2011 in North Central Texas. Interannually, the variability of the LAI activity factor is sometimes comparable to that for temperature. Within seasons, the temperature activity factor varies substantially between years during spring and summer but shows minimal changes (<6%) during fall. LAI has substantial interannual differences during summer and fall in the central regions comparable to (or even greater than) the variations in the temperature activity factor but relatively small year-to-year changes for the East Texas and Upper Coast regions. As noted by Huang et al. (2014), the different regional response in LAI interannual variability is likely related to the dominant land cover types by region; East Texas and the Upper Coast are dominated by broadleaf and needleleaf forest versus low-growing vegetation (e.g., grasses) in the central regions. Sunlight controls isoprene emissions on a daily basis; however, it is not a significant contributor to seasonal or interannual variations in isoprene emissions.

3.3.2. Monoterpenes

The by-layer activity factors for monoterpenes (Supplementary Fig. S6) demonstrate that the relative directional variations in light/temperature activity factors are similar to those for isoprene. Fig. 5 and Supplementary Fig. S7 demonstrates that the layer-averaged temperature activity (γ_T) has the greatest seasonal variations and reaches a maximum value of 60% during 2011 in North Central Texas. LAI and light activity factors also show some seasonal variations with values ranging between 10 and 20% for LAI and 10–15% for light.

Overall, the relative importance of factors that contribute to interannual monoterpene variations are similar to those for isoprene: in central regions, the LAI and temperature activity factors dominate interannual variations while in East Texas and Upper Coast, LAI exhibits relatively smaller interannual changes (<10%). As for isoprene, the contribution of the light activity factor to interannual variations of monoterpene emissions is minimal.

3.4. Uncertainty of isoprene emissions to soil moisture

In order to test the sensitivity of isoprene predictions during drought to the specific soil moisture database employed, MEGAN simulations were conducted for North Central and East Texas using the Mosaic soil moisture database in place of the Noah MP database. As demonstrated in Table 2, the Mosaic simulations for the all-time record drought year 2011 predicted dramatically lower isoprene emissions compared to those for the basecase (i.e., impact of soil moisture not considered) and Noah MP runs. Maximum reductions were −69% for the North Central summer compared to −12% for Noah MP. An investigation of upper-level soil moisture values revealed that Mosaic tends to predict lower moisture availability compared to Noah MP; crucially, the Mosaic wilting point values are almost a factor of two greater than those for Noah MP. The difference in the wilting points between the NLDAS-2 databases is significant because θ_{wilt} is a threshold value below which γ_{SM} is set to zero (ref. Eq. (4)).

During 2011, in-situ measurements of volumetric soil moisture within the root zone were available at three locations in eastern Texas; a comparison between these limited observations and the NLDAS-2 datasets showed that Mosaic and especially Noah MP tended to be too wet in the near-surface layer and too dry at deeper depths compared to observations. The evaluation and validation of simulated soil moisture datasets is important; however, the current spatial coverage of in-situ root-zone measurements is sparse for most of the U.S. (e.g., Ochsner, et al., 2013). In addition to uncertainties in the accurate simulation of soil moisture within land surface models, substantial errors can also be introduced when sharing data between applications because outputs are often highly model-dependent (e.g., Koster et al., 2009). Previous MEGAN studies have typically employed a single soil moisture database; predicted impacts on isoprene emissions have ranged from minimal (e.g., Guenther, et al., 2006; Potosnak et al., 2014) to substantial (e.g., global isoprene reductions of 20–50% for Müller et al., 2008;

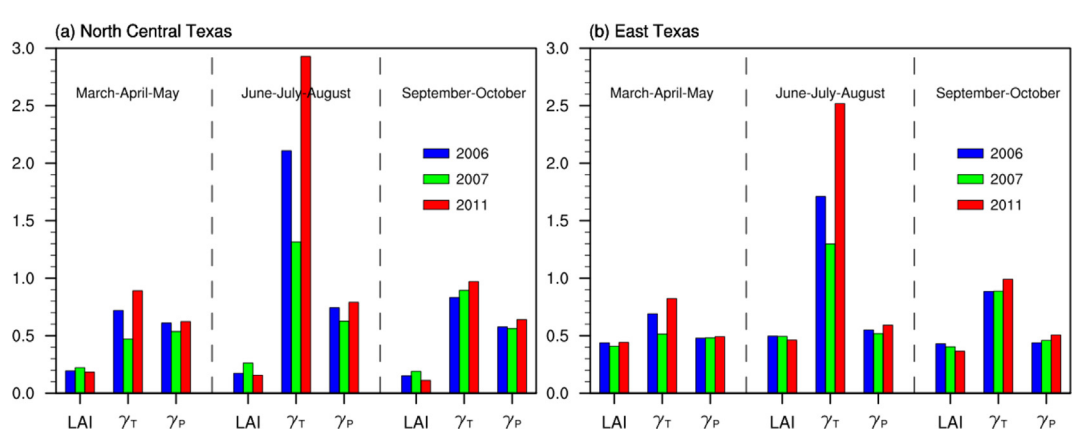

Fig. 4. Layer-averaged LAI, temperature and light activity factors for isoprene during 2006, 2007, and 2011 by season and region – (a) North Central Texas and (b) East Texas. Results for South Central Texas and Upper Coast are shown in Supplementary Fig. S5.

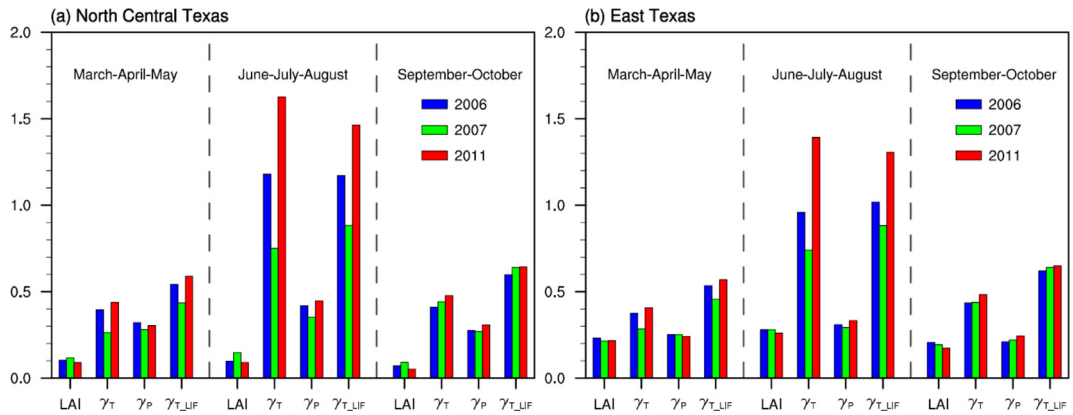

Fig. 5. Layer-averaged LAI, temperature and light activity factors for monoterpenes during 2006, 2007 and 2011 by season and region – (a) North Central Texas and (b) East Texas. Results for South Central Texas and Upper Coast are shown in Supplementary Fig. S7.

Tawfik et al., 2012; Sindelarova et al., 2014) suggesting that γ_{SM} is characterized by substantial uncertainty. The high sensitivity of predicted isoprene emissions to soil moisture inputs suggests a continued need for investigations to evaluate and improve the drought stress parameterizations and/or representations in models such as MEGAN (e.g., Potosnak, et al., 2014).

4. Discussion

Drought evolves through a complex interaction of land/atmosphere processes; typical components of drought include reductions in volumetric soil moisture and increases in land/atmospheric temperatures. Table 3 presents the percentage change in summer activity factors between 2007, which had average-to-wet conditions, and 2011, a year characterized by all-time record drought and heat throughout Texas. The relative change in summer emissions between 2007 and 2011 is also shown. For isoprene, the γ_{SM} and emissions ratio results are provided based on both the Noah MP and Mosaic soil moisture databases.

For all climate regions, higher temperatures between 2007 and 2011 drive a nonlinear increase in the temperature activity factors (γ_T, γ_{T_LIF}) producing a nonlinear increase in the overall activity factors; for example, the 2011 γ_T in North Central Texas is more than a factor of two greater compared to that for 2007. The light activity factors are also greater during 2011 compared to 2007, while the LAI activity factors (LAI, γ_{LAI}) show decreases. In the two central regions, drought-induced summer LAI reductions are greater than 40%, suggesting a strong negative effect of drought on summer isoprene and monoterpene emissions.

For the isoprene simulation with Noah MP, the combined negative impacts of LAI and soil moisture are dominated by emissions increases associated with leaf age, PAR and, especially, temperature. In East Texas, LAI shows a small decrease between 2007 and 2011; consequently, summer isoprene emissions increase by a factor of 2.2 compared to factors of 1.8 and 1.5 for North and South Central Texas, respectively. Significantly, if the soil moisture results from the Mosaic simulation better represent actual conditions compared to those that used Noah MP, the substantially larger decreases in isoprene emissions associated with reduced soil moisture availability would overwhelm the increases in emissions caused by warmer temperatures across most regions. The negative impacts of soil moisture and LAI reduce summer emissions by 50% in South Central and Upper Coast for the Mosaic simulation; in East Texas, relatively lower magnitude reductions associated with LAI and soil moisture results in an emissions increase of 30% for 2011 relative to 2007.

For monoterpenes, the percentage increases in summer emissions between 2007 and 2011 are less than those for isoprene. This attenuated response can be attributed to the differential methodology used by MEGAN to estimate emissions for the two compounds. First, isoprene has a steeper temperature response than monoterpenes (Guenther et al., 2012); thus, a given temperature increase produces a greater percentage change in isoprene compared to monoterpenes. Second, the impact of leaf age on monoterpene emissions is slightly negative compared to slightly positive for isoprene. During the fall, the relative contribution of temperature on both isoprene and monoterpene emissions diminishes substantially; thus, fall isoprene emissions would range from only slightly greater during 2011 compared to 2007 for the Noah MP simulation to substantially lower during 2011 for Mosaic, while monoterpene emissions have slightly greater emissions during 2007 compared to 2011.

Table 2
Season-averaged isoprene emissions for the North Central and East Texas climate regions during 2011 for three MEGAN simulations: (1) basecase (impact of soil moisture not considered), (2) basecase utilizing the Noah MP soil moisture database (Noah MP), and (3) basecase utilizing the Mosaic soil moisture database (Mosaic).

Climate Region	Months during 2011	Area-averaged daily total isoprene emissions (kg/km^2/day)			Percentage change relative to basecase	
		Basecase	Noah MP	Mosaic	Noah MP	Mosaic
North Central Texas	Apr/May	15.1	14.0	6.7	−7%	−56%
	Jun/Jul/Aug	43.9	38.8	13.5	−12%	−69%
	Sep/Oct	8.5	7.7	2.7	−10%	−68%
East Texas	Apr/May	35.4	35.0	25.0	−1%	−29%
	Jun/Jul/Aug	104.1	96.5	59.6	−7%	−43%
	Sep/Oct	26.9	25.4	16.2	−6%	−40%

5. Conclusions

During recent years, the importance of biogenic emissions to air quality and climate has brought renewed attention to the effects of drought on isoprene and monoterpene emissions rates. Drought is a recurring phenomenon in Texas; similar to most of the central and western U.S., the frequency and intensity of Texas droughts are expected to increase over the coming decades (Melillo et al., 2014). This work quantified the variability of environmental inputs on isoprene and monoterpene emissions in eastern Texas by tracking seasonal and interannual changes in activity factors intrinsic to MEGAN; this methodology maintains an environmentally consistent (i.e., "real-world") set of model inputs. Comparisons of results

Table 3
Percentage change[a] in MEGAN activity factors and emissions of isoprene and monoterpenes by climate division between the summers of 2007 and 2011. Two soil moisture datasets were considered for isoprene emission estimates.

Isoprene	γ_{age}	LAI	γ_T	γ_P	Noah MP		Mosaic	
					γ_{SM}	Emissions	γ_{SM}	Emissions
North Central Texas	9%	−40%	123%	26%	−9%	83%	−70%	−30%
South Central Texas	10%	−44%	66%	30%	−8%	51%	−66%	−45%
East Texas	14%	−7%	94%	14%	−6%	117%	−44%	34%
Upper Coast	11%	−15%	46%	18%	−3%	74%	−71%	−46%
Monoterpenes	γ_{age}	LAI	γ_T	γ_P	γ_{T_LIF}	γ_{LAI}	γ_{SM}	Emissions
North Central Texas	−6%	−40%	112%	27%	85%	−34%	Na	34%
South Central Texas	−6%	−44%	52%	30%	51%	−37%	Na	7%
East Texas	−9%	−6%	78%	14%	54%	−5%	Na	54%
Upper Coast	−7%	−15%	33%	18%	28%	−13%	Na	23%

[a] Calculated as $\frac{\gamma_{2011}-\gamma_{2007}}{\gamma_{2007}} \times 100\%$. Note that "na" means not applicable.

between drought and non-drought years reinforced the importance of temperature on predicted emissions. Decreases in emissions associated with reduced LAI during periods of drought were dominated by emission increases caused by much warmer temperatures. MEGAN sensitivity simulations using two different soil moisture datasets demonstrated that the soil moisture activity factor is subject to large uncertainty; dependent on the soil moisture database employed, predicted reductions in isoprene emissions ranged from nearly negligible to almost −70% during the summer of 2011, a time period characterized by all-time record drought in Texas.

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Appendix A. Supplementary data

Supplementary data related to this article can be found at http://dx.doi.org/10.1016/j.atmosenv.2015.01.072.

References

Arneth, A., Schurgers, G., Lathiere, J., Duhl, T., Beerling, D.J., Hewitt, C.N., Martin, M., Guenther, A., 2011. Global terrestrial isoprene emission models: sensitivity to variability in climate and vegetation. Atmos. Chem. Phys. 11 (15), 8037–8052.
Atkinson, R., 2000. Atmospheric chemistry of VOCs and NO_x. Atmos. Environ. 34 (12), 2063–2101.
Burnash, R.J.C., Ferral, R.L., McGuire, R.A., 1973. A Generalized Streamflow Simulation System: Conceptual Models for Digital Computer (Technical report, joint Federal-State River Forecast Center, Sacramento, Calif.).
Cai, X., Yang, Z.L., David, C.H., Niu, G.Y., Rodell, M., 2014a. Hydrological evaluation of the Noah-MP land surface model for the Mississippi River Basin. J. Geophys. Res. Atmos. 119 (1), 23–38.
Cai, X., Yang, Z.-L., Xia, Y., Huang, M., Wei, H., Leung, L.R., Ek, M.B., 2014b. Assessment of simulated water balance from Noah, Noah-MP, CLM, and VIC over CONUS using the NLDAS test bed. J. Geophys. Res. Atmos. 119.
Chen, J., Avise, J., Guenther, A., Wiedinmyer, C., Salathe, E., Jackson, R.B., Lamb, B., 2009. Future land use and land cover influences on regional biogenic emissions and air quality in the United States. Atmos. Environ. 43 (36), 5771–5780.
Claeys, M., Graham, B., Vas, G., Wang, W., Vermeylen, R., Pashynska, V., Cafmeyer, J., Guyon, P., Andreae, M.O., Artaxo, P., Maenhaut, W., 2004. Formation of secondary organic aerosols through photooxidation of isoprene. Science 303 (5661), 1173–1176.
Ek, M.B., Mitchell, K.E., Lin, Y., Rogers, E., Grunmann, P., Koren, V., Gayno, G., Tarpley, J.D., 2003. Implementation of Noah land surface model advances in the national centers for environmental prediction operational mesoscale eta model. J. Geophys. Res. 108 (D22).
Ferreira, J., Reeves, C.E., Murphy, J.G., Garcia-Carreras, L., Parker, D.J., Oram, D.E., 2010. Isoprene emissions modelling for West Africa: MEGAN model evaluation and sensitivity analysis. Atmos. Chem. Phys. 10 (17), 8453–8467.
Fischbach, R.J., Staudt, M., Zimmer, I., Rambal, S., Schnitzler, J.P., 2002. Seasonal pattern of monoterpene synthase activities in leaves of the evergreen tree Quercus ilex. Physiol. Plant. 114 (3), 354–360.
Fu, Y., Liao, H., 2012. Simulation of the interannual variations of biogenic emissions of volatile organic compounds in China: impacts on tropospheric ozone and secondary organic aerosol. Atmos. Environ. 59, 170–185.
Geng, F., Tie, X., Guenther, A., Li, G., Cao, J., Harley, P., 2011. Effect of isoprene emissions from major forests on ozone formation in the city of Shanghai, China. Atmos. Chem. Phys. 11 (20), 10449–10459.
Guenther, A.B., Jiang, X., Heald, C.L., Sakulyanontvittaya, T., Duhl, T., Emmons, L.K., Wang, X., 2012. 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. Discuss. 5, 1503–1560.
Guenther, A., Karl, T., Harley, P., Wiedinmyer, C., Palmer, P.I., Geron, C., 2006. Estimates of global terrestrial isoprene emissions using MEGAN (Model of emissions of gases and aerosols from Nature). Atmos. Chem. Phys. 6 (11), 3181–3210.
Gulden, L.E., Yang, Z.L., Niu, G.Y., 2007. Interannual variation in biogenic emissions on a regional scale. J. Geophys. Res. Atmos. (1984–2012) 112 (D14).
Han, K.M., Park, R.S., Kim, H.K., Woo, J.H., Kim, J., Song, C.H., 2013. Uncertainty in biogenic isoprene emissions and its impacts on tropospheric chemistry in East Asia. Sci. Total Environ. 463, 754–771.
Heald, C.L., Henze, D.K., Horowitz, L.W., Feddema, J., Lamarque, J.F., Guenther, A., Hess, P.G., Vitt, F., Seinfeld, J.H., Goldstein, A.H., Fung, I., 2008. Predicted change in global secondary organic aerosol concentrations in response to future climate, emissions, and land use change. J. Geophys. Res. Atmos. (1984–2012) 113 (D5).
Holm, J.A., Jardine, K., Guenther, A.B., Chambers, J.Q., Tribuzy, E., 2014. Evaluation of MEGAN-CLM parameter sensitivity to predictions of isoprene emissions from an Amazonian rainforest. Atmos. Chem. Phys. Discuss. 14, 23995–24041.
Huang, L., McDonald-Buller, E.C., McGaughey, G., Kimura, Y., Allen, D.T., 2014. Annual variability in leaf area index and isoprene and monoterpene emissions during drought years in Texas. Atmos. Environ. 92, 240–249.
Kleindienst, T.E., Jaoui, M., Lewandowski, M., Offenberg, J.H., Lewis, C.W., Bhave, P.V., Edney, E.O., 2007. Estimates of the contributions of biogenic and anthropogenic hydrocarbons to secondary organic aerosol at a southeastern US location. Atmos. Environ. 41 (37), 8288–8300.
Koster, R.D., Guo, Z., Yang, R., Dirmeyer, P.A., Mitchell, K., Puma, M.J., 2009. On the nature of soil moisture in land surface models. J. Clim. 22, 4322–4335.
Koster, R., Suarez, M., 1996. Energy and water balance calculations in the Mosaic LSM. NASA technical memorandum. NASA TM-104606 9, 60 pp.
Kuhn, U., Rottenberger, S., Biesenthal, T., Wolf, A., Schebeske, G., Ciccioli, P., Kesselmeier, J., 2004. 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 (12), 1469–1485.
Lamb, B., Gay, D., Westberg, H., Pierce, T., 1993. A biogenic hydrocarbon emission inventory for the USA using a simple forest canopy model. Atmos. Environ. Part A. General Top. 27 (11), 1673–1690.
Lathiere, J., Hewitt, C.N., Beerling, D.J., 2010. Sensitivity of isoprene emissions from the terrestrial biosphere to 20th century changes in atmospheric CO_2 concentration, climate, and land use. Glob. Biogeochem. Cycles 24 (1).

Lawrence, D., Oleson, K.W., Flanner, M.G., Thornton, P.E., Swenson, S.C., Lawrence, P.J., Zeng, X., Yang, X.-L., Levis, S., Sakaguchi, K., Bonan, G.B., Slater, A.G., 2011. Parameterization improvements and functional and structural advances in version 4 of the community land model. J. Adv. Model. Earth Syst. 3, M03001.

Liang, X., Lettenmaier, D.P., Wood, E.F., Burges, S.J., 1994. A simple hydrologically based model of land surface water and energy fluxes for general circulation models. J. Geophys. Res. 99 (D7), 14415–14428.

Lusebrink, I., Evenden, M.L., Blanchet, F.G., Cooke, J.E., Erbilgin, N., 2011. Effect of water stress and fungal inoculation on monoterpene emission from an historical and a new pine host of the mountain pine beetle. J. Chem. Ecol. 37 (9), 1013–1026.

Melillo, J.M., Richmond, T.C., Yohe, G.W. (Eds.), 2014. Climate Change Impacts in the United States (The Third National Climate Assessment. U.S. Global Change Research Program).

Mitchell, K.E., Lohmann, D., Houser, P.R., Wood, E.F., Schaake, J.C., Robock, A., Cosgrove, B.A., Sheffield, J., Duan, Q., Luo, L., Higgins, R.W., Pinker, R.T., Tarpley, J.D., Lettenmaier, D.P., Marshall, C.H., Entin, J.K., Pan, M., Shi, W., Koren, V., Meng, J., Ramsay, B.H., Bailey, A.A., 2004. The multi-institution North American Land Data Assimilation System (NLDAS): utilizing multiple GCIP products and partners in a continental distributed hydrological modeling system. J. Geophys. Res. 109 (D7).

Müller, J.F., Stavrakou, T., Wallens, S., Smedt, I.D., Roozendael, M.V., Potosnak, M.J., Rinne, J., Munger, B., Goldstein, A., Guenther, A.B., 2008. Global isoprene emissions estimated using MEGAN, ECMWF analyses and a detailed canopy environment model. Atmos. Chem. Phys. 8 (5), 1329–1341.

Niu, G.-Y., Yang, Z.-L., Mitchell, K.E., Chen, F., Ek, M.B., Barlage, M., Kumar, A., Manning, K., Niyogi, D., Rosero, E., Tewari, M., Xia, Y., 2011. The community Noah land surface model with multiparameterization options (Noah-MP): 1. Model description and evaluation with local-scale measurements. J. Geophys. Res. 116.

Ochsner, T.E., Cosh, M.H., Cuenca, R.H., Dorigo, W.A., Draper, C.S., Hagimoto, Y., Kerr, Y.H., Njoku, E.G., Small, E.E., Zreda, M., 2013. State of the art in large-scale soil moisture monitoring. J. Soil Sci. Soc. Am. 77, 1888–1919.

Ormeno, E., Mevy, J.P., Vila, B., Bousquet-Melou, A., Greff, S., Bonin, G., Fernandez, C., 2007. Water deficit stress induces different monoterpene and sesquiterpene emission changes in Mediterranean species. Relationship between terpene emissions and plant water potential. Chemosphere 67 (2), 276–284.

Pegoraro, E., Rey, A., Greenberg, J., Harley, P., Grace, J., Malhi, Y., Guenther, A., 2004. Effect of drought on isoprene emission rates from leaves of *Quercus virginiana* Mill. Atmos. Environ. 38 (36), 6149–6156.

Petron, G., Harley, P., Greenberg, J., Guenther, A., 2001. Seasonal temperature variations influence isoprene emission. Geophys. Res. Lett. 28 (9), 1707–1710.

Potosnak, M.J., LeStourgeon, L., Pallardy, S.G., Hosman, K.P., Gu, L., Karl, T., Geron, C., Guenther, A.B., 2014. Observed and modeled ecosystem isoprene fluxes from an oak-dominated temperate forest and the influence of drought stress. Atmos. Environ. 84, 314–322.

Rodríguez-Calcerrada, J., Buatois, B., Chiche, E., Shahin, O., Staudt, M., 2013. Leaf isoprene emission declines in *Quercus pubescens* seedlings experiencing drought–Any implication of soluble sugars and mitochondrial respiration? Environ. Exp. Bot. 85, 36–42.

Rosenstiel, T.N., Potosnak, M.J., Griffin, K.L., Fall, R., Monson, R.K., 2003. Increased CO_2 uncouples growth from isoprene emission in an agriforest ecosystem. Nature 421 (6920), 256–259.

Sharkey, T.D., Singsaas, E.L., Vanderveer, P.J., Geron, C., 1996. Field measurements of isoprene emission from trees in response to temperature and light. Tree Physiol. 16 (7), 649–654.

Sindelarova, K., Granier, C., Bouarar, I., Guenther, A., Tilmes, S., Stavrakou, T., Müller, J.F., Kuhn, U., Stefani, P., Knorr, W., 2014. Global dataset of biogenic VOC emissions calculated by the MEGAN model over the last 30 years. Atmos. Chem. Phys. Discuss. 14, 10725–10788.

Situ, S., Wang, X., Guenther, A., Zhang, Y., Wang, X., Huang, M., Fan, Q., Xiong, Z., 2014. Uncertainties of isoprene emissions in the MEGAN model estimated for a coniferous and broad-leaved mixed forest in Southern China. Atmos. Environ. 98, 105–110.

Smiatek, G., Bogacki, M., 2005. Uncertainty assessment of potential biogenic volatile organic compound emissions from forests with the Monte carlo method: case study for an episode from 1 to 10 July 2000 in Poland. J. Geophys. Res. Atmos. (1984–2012) 110 (D23).

Stavrakou, T., Müller, J.F., Bauwens, M., De Smedt, I., Van Roozendael, M., Guenther, A., Wild, M., Xia, X., 2014. Isoprene emissions over Asia 1979–2012: impact of climate and land-use changes. Atmos. Chem. Phys. 14 (9), 4587, 4605.

Tawfik, A.B., Stöckli, R., Goldstein, A., Pressley, S., Steiner, A.L., 2012. Quantifying the contribution of environmental factors to isoprene flux interannual variability. Atmos. Environ. 54, 216–224.

Tingey, D.T., Manning, M., Grothaus, L.C., Burns, W.F., 1980. Influence of light and temperature on monoterpene emission rates from slash pine. Plant Physiol. 65 (5), 797–801.

Tsigaridis, K., Kanakidou, M., 2003. Global modelling of secondary organic aerosol in the troposphere: a sensitivity analysis. Atmos. Chem. Phys. 3 (5), 1849–1869.

Wiedinmyer, C., Guenther, A., Estes, M., Strange, I.W., Yarwood, G., Allen, D.T., 2001. A land use database and examples of biogenic isoprene emission estimates for the state of Texas, USA. Atmos. Environ. 35 (36), 6465–6477.

Wilkinson, M.J., Monson, R.K., Trahan, N., Lee, S., Brown, E., Jackson, R.B., Polley, H.W., Fay, P.A., Fall, R., 2009. Leaf isoprene emission rate as a function of atmospheric CO_2 concentration. Glob. Change Biol. 15 (5), 1189–1200.