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# Estimates of global terrestrial isoprene emissions using MEGAN (Model of Emissions of Gases and Aerosols from Nature)

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## Abstract

Reactive gases and aerosols are produced by terrestrial ecosystems, processed within plant canopies, and can then be emitted into the above-canopy atmosphere. Estimates of the above-canopy fluxes are needed for quantitative earth system studies and assessments of past, present and future air quality and climate. The Model of Emissions of Gases and Aerosols from Nature (MEGAN) is described and used to quantify net terrestrial biosphere emission of isoprene into the atmosphere. MEGAN is designed for both global and regional emission modeling and has global coverage with  $\sim 1 \text{ km}^2$  spatial resolution. Field and laboratory investigations of the processes controlling isoprene emission are described and data available for model development and evaluation are summarized. The factors controlling isoprene emissions include biological, physical and chemical driving variables. MEGAN driving variables are derived from models and satellite and ground observations. Broadleaf trees, mostly in the tropics, contribute about half of the estimated global annual isoprene emission due to their relatively high emission factors and because they are often exposed to conditions that are conducive for isoprene emission. The remaining flux is primarily from shrubs which are widespread and dominate at higher latitudes. MEGAN estimates global annual isoprene emissions of  $\sim 600 \text{ Tg}$  isoprene but the results are very sensitive to the driving variables, including temperature, solar radiation, Leaf Area Index, and plant functional type. The annual global emission estimated with MEGAN ranges from about 500 to 750 Tg isoprene depending on the driving variables that are used. Differences in estimated emissions are more than a factor of 3 for specific times and locations. It is difficult to evaluate isoprene emission estimates using the concentration distributions simulated using chemistry and transport models due to the substantial uncertainties in other model components. However, comparison with isoprene emissions estimated from satellite formaldehyde observations indicates reasonable agreement. The sensitivity of isoprene emissions to earth system changes (e.g., climate and landcover) suggests potentially large changes in future emissions. Using temperature distributions

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simulated by global climate models for year 2100, MEGAN estimates that isoprene emissions increase by more than a factor of two. This is considerably greater than previous estimates and additional observations are needed to evaluate and improve the methods used to predict future isoprene emissions.

## 5 1. Introduction

Chemicals produced by the biosphere include volatile compounds that are emitted into the air where they can have a substantial impact on the chemistry of the atmosphere. These compounds are dominated by volatile organic compounds (VOCs) both in total mass and number of compounds. The impact of biogenic VOCs on global chemistry and climate has been investigated using global models (e.g., Houweling et al., 1998; Guenther et al., 1999a; Granier et al., 2000; Poisson et al., 2000; Collins et al., 2002; Sanderson et al., 2003) while regional air quality models have included biogenic VOC emissions in efforts to develop pollution control strategies (e.g., Pierce et al., 1998). Biogenic VOC emissions were included as inputs to regulatory regional oxidant models in the mid 1980s (Pierce and Waldruff, 1991) and by the 1990s were routinely included in chemical transport models, but typically as off-line, static emission inventories. There is increasing demand for biogenic emission algorithms that can be integrated into regional and global models. This would facilitate studies of chemical and physical feedbacks to biogenic emissions and other earth system components and to ensure consistency in the landcover and weather variables.

Although hundreds of biogenic VOC have been identified, two compounds dominate the annual global flux to the atmosphere: methane and isoprene. Microbes are the major source of biogenic methane, while over 90% of all isoprene is emitted from terrestrial plant foliage. Minor sources of isoprene include microbes, animals (including humans) and aquatic organisms (Wagner et al., 1999). Methane and isoprene each comprises about a third of the annual global VOC emission from all natural and anthropogenic sources. The remaining third is the sum of hundreds of compounds. Methane is a

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long-lived (years) compound with a well mixed distribution throughout the atmosphere while isoprene is short-lived (minutes to hours) with atmospheric concentrations that vary several orders of magnitude over a time scale of less than one day and over spatial scales of less than a few km. As a result, we can be relatively certain of the annual global emission of methane, based on estimates of the global atmospheric burden and the average lifetime; however, the annual global isoprene emission is much less well constrained. Satellite-derived global distributions of isoprene oxidation products (e.g., formaldehyde and carbon monoxide) are beginning to provide constraints on global isoprene emission rates but they too are associated with significant uncertainties and they cannot provide estimates of past (pre-satellite era) and future emissions. There remains a need for models that can estimate past, current and future isoprene emissions.

In the early 1990s, the International Global Atmospheric Chemistry (IGAC) Global Emissions Inventory Activity (GEIA) initiated working groups to develop global emission inventories on a 1 degree by 1 degree grid for use in global chemistry and transport models (Graedel et al., 1993). The IGAC-GEIA natural VOC working group developed a model of emissions of isoprene and other VOC (Guenther et al., 1995). A regional biogenic emission model, the Biogenic Emissions Inventory System or BEIS (Pierce and Waldruff, 1991), was developed in the mid 1980s and replaced by a second generation model, BEIS2 (Pierce et al., 1998), in the mid 1990s. This manuscript describes the Model of Emissions of Gases and Aerosols from Nature (MEGAN) which was developed to replace both the Guenther et al. (1995) global emission model and the BEIS/BEIS2/BEIS3 regional emission models. We focus in this paper on isoprene emissions and will describe MEGAN procedures for simulating emissions of other gases and aerosols elsewhere. Field and laboratory investigations of the processes controlling isoprene emission are described in this manuscript and data available for model development and evaluation are summarized. The model procedures are described and predicted emissions and the associated uncertainties are discussed and compared to top down emission estimates. Model simulations of the response of iso-

prene emissions to earth system changes (e.g., climate, chemistry and landcover) are presented and used to identify major uncertainties.

## 2. Isoprene observations

Enclosure methods were first used to study biogenic VOC emissions in the late 1920s (Isidorov, 1990). In the following 75 years, investigators enclosed thousands of leaves, branches and whole plants in bags, jars, and cuvettes to characterize fluxes of isoprene and other VOCs. The earliest studies focused on monoterpenes (see Went, 1960; Isidorov, 1990) but the co-discovery of abundant emissions of isoprene from some plant species by Rasmussen and Went (1965) in the U.S. and Sanadze (1957) in the former Soviet Union led to considerable interest in emissions of this compound. Wiedinmyer et al. (2004) reviewed the scientific literature describing enclosure measurements of foliar emissions of isoprene and other biogenic VOC (BVOC) and have compiled this information into an online searchable database (see <http://bvoc.acd.ucar.edu>). The database includes the results of more than 160 studies that have characterized isoprene emissions from hundreds of plant species using enclosure measurement systems.

Rasmussen and Went (1965) extrapolated a few biogenic VOC enclosure observations to the global scale by simply multiplying a typical emission rate by the global area covered by vegetation and the fraction of the year that plants are growing. The resulting annual total (isoprene plus all other non-methane biogenic VOC) flux estimate of 438 Tg ( $10^{12}$  g) is about a factor of three lower than the estimate of Guenther et al. (1995). A simple approach like this can be used to establish an upper bound global isoprene emission estimate. The highest leaf-level isoprene emission rates are  $\sim 150 \mu\text{g g}^{-1} \text{h}^{-1}$ . If all leaves emitted continuously at this rate, the global annual isoprene emission would exceed 25 Gt ( $10^{15}$  g). However, the actual global annual isoprene emission is about 2% of this rate due to environmental conditions that are not optimal for isoprene emission and because not all plants have the ability to emit substantial amounts of isoprene.

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5 Guenther et al. (1995) relied primarily on enclosure measurement studies to assign  
leaf level isoprene emission factors to 72 global ecosystems. The emission factors  
for about half of these ecosystems were assigned based on observations reported in  
twenty publications and the remaining ecosystems were assigned default values. Only  
10 three of the twenty publications included studies from tropical regions even though the  
tropics were estimated to contribute about 80% of the global annual isoprene emis-  
sions. Furthermore, the emission activity algorithms that describe the response of  
isoprene to temperature and light were based on investigations of temperate plants  
growing in temperate weather conditions and had not been evaluated by any measure-  
15 ments in the tropics.

Thousands of isoprene emission rate measurements have been made using enclo-  
sure techniques in the decade since the Guenther et al. (1995) model was developed.  
Many of these measurements have been incorporated into the isoprene emission fac-  
tors used for MEGAN. Recent studies have also shown that much of the observed  
15 isoprene variability among plant species with significant emission rates (e.g., *Quercus*,  
*Liquidambar*, *Nyssa*, *Populus*, *Salix*, and *Robinia* species) can be attributed to weather,  
plant physiology and the location of a leaf within the canopy rather than genetics (Geron  
et al., 2000). Other studies have characterized how emissions respond to various fac-  
tors including leaf age (Monson et al., 1994; Petron et al., 2001), nutrient availability  
20 (Harley et al., 1994), weather (Sharkey et al., 2000) and the chemical composition of  
the atmosphere (Velikova et al., 2005; Rosentiel et al., 2003). Of particular impor-  
tance for global modeling, many more enclosure measurements have been conducted  
in tropical landscapes (Keller and Lerdau, 1999; Guenther et al., 1999a; Kesselmeier  
et al., 2000; Klinger et al., 2002; Kuhn et al., 2002; Harley et al., 2004). Accompanying  
25 these emission measurements have been efforts to process tree inventory data into a  
format suitable for characterizing regional isoprene emission distributions.

Enclosure measurements of isoprene emission rates can be extrapolated to the  
whole canopy scale using canopy environment models. The resulting canopy emission  
rate estimates are associated with substantial uncertainties due to 1) a limited under-

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standing of chemical sinks and deposition losses within vegetation canopies, 2) artificially disturbed emission rates due to the enclosure, 3) differences between the functioning of individual ecosystem components (e.g. leaves) and the entire ecosystem, and 4) limited sample size within the enclosure (relative to the whole landscape), as well as uncertainties associated with canopy microclimate models themselves. Direct measurements of above canopy fluxes are suitable for characterizing whole canopy net emission rates and are fortunately becoming increasingly available to parameterize key global ecosystems. Above canopy isoprene flux measurement systems continue to become more reliable and widespread than in the past. Isoprene fluxes can now be measured routinely using eddy flux techniques such as relaxed eddy accumulation (e.g., Guenther et al., 1996) and eddy covariance (Guenther and Hills, 1998). In addition to these direct flux measurement methods, inverse modeling and gradient approaches use isoprene concentrations obtained from aircraft and tethered balloon sampling platforms to characterize isoprene emissions across spatial scales of tens to hundreds of km<sup>2</sup> (e.g., Greenberg et al., 1999). The geographical distribution of the >80 studies used to assign the isoprene emission factor distributions described in this manuscript is illustrated in Fig. 1. More than 80 laboratory studies were also incorporated into the development of model algorithms and emission factors.

### 3. MEGAN model description

MEGAN estimates the net emission rate (mg compound m<sup>-2</sup> earth surface h<sup>-1</sup>) of isoprene and other trace gases and aerosols from terrestrial ecosystems into the atmosphere at a specific location and time as

$$\text{Emission} = \varepsilon \cdot \gamma \cdot \rho \quad (1)$$

where  $\varepsilon$  (mg m<sup>-2</sup> h<sup>-1</sup>) is an emission factor which represents the net above-canopy emission rate expected at standard conditions,  $\gamma$  (normalized ratio) is an emission

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activity factor that accounts for emission changes due to deviations from standard conditions and  $\rho$  (normalized ratio) is a factor that accounts for chemical production and loss within plant canopies. The MEGAN canopy-scale emission factor differs from most other biogenic emission models which use a leaf-scale emission factor. The standard conditions for landcover characteristics include a leaf area index, LAI, of 5 and a canopy with 92% mature leaves; current environmental conditions include a solar angle (degrees from horizon to sun) of 60 degrees, a photosynthetic photon flux density (PPFD) transmission (ratio of PPFD at the top of the canopy to PPFD at the top of the atmosphere) of 0.6, air temperature=303 K, humidity=14 g kg<sup>-1</sup>, wind speed=3 m s<sup>-1</sup>, and soil moisture=0.3 m<sup>3</sup> m<sup>-3</sup>; average canopy environmental conditions of the past 24 to 240 h include leaf temperature=297 K and PPFD=200  $\mu\text{mol m}^{-2} \text{s}^{-1}$  for sun leaves and 50  $\mu\text{mol m}^{-2} \text{s}^{-1}$  for shade leaves. The factor  $\gamma$  is equal to unity at these standard conditions. Note that a solar angle of 60 degrees and a PPFD transmission of 0.6 results in a PPFD of  $\sim 1500 \mu\text{mol m}^{-2} \text{s}^{-1}$ . Emissions are calculated separately for each plant functional type (PFT) that occurs within a grid cell. The emission from each PFT is summed to estimate the total emission. MEGAN is a global scale model with a base resolution of  $\sim 1 \text{ km}^2$  (30 s latitude by 30 s longitude) enabling both regional scale and global scale simulations. The MEGAN emission factors, algorithms and driving variables can be accessed through a public data portal (see <http://bai.acd.ucar.edu>) at the base and lower resolutions for specific years. Methods for estimating each of the factors in Eq. (1) are described in the following sections.

### 3.1. Emission factor, $\varepsilon$

Isoprene is emitted by soil bacteria, algae, and in the breath of animals (including humans) as well as plants (Wagner et al., 1999). Only vegetation emissions have been shown to occur at levels that can influence atmospheric composition although relatively little is known about soil bacteria. The isoprene emission rates of different plant species range from  $<0.1$  to  $>100 \mu\text{g g}^{-1} \text{h}^{-1}$ . Very low and very high emitters often occur within a given plant family and even within some globally important plant genera

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including *Quercus* (oaks), *Picea* (spruce), *Abies* (firs) and *Acacia*. The large taxonomic variability makes the characterization of isoprene emission factor distributions a challenging task. The MEGAN landcover approach divides each grid cell into vegetated and non-vegetated earth surface, and places all vegetation into one of six PFTs.

5 These include three tree categories (broadleaf, fineleaf evergreen and fineleaf deciduous), categories for shrubs and crops, and a category for all other vegetation (i.e., grasses, sedges, forbs, and mosses). In contrast to the ecosystem approach, in which each location or model grid cell is characterized by a single ecosystem type, the PFT approach covers each grid cell with a variable fraction of each PFT. MEGAN accounts  
10 for regional  $\varepsilon$  variations using geographically gridded databases of isoprene emission factors for each PFT. A unique isoprene emission factor for a given PFT, for example, broadleaf trees, can be assigned to each grid cell, depending on the measured or assumed isoprene emission characteristics of the broadleaf tree species found in that cell.

15 Table 1 illustrates the differences in the global average isoprene emission factors for the six PFTs. Broadleaf trees and shrubs have the highest average emission factor. The average fineleaf evergreen tree isoprene emission factor is ~84% lower than the average broadleaf tree emission factor. The fineleaf deciduous tree and grass/other PFTs have average emission factors that are about a factor of 20 lower than the average broadleaf tree emission factor, while the crop isoprene emission factor is about  
20 two orders of magnitude lower. The substantial differences in these global average isoprene emission factors demonstrates the value of the PFT approach but Table 1 also shows that there is considerable variability associated with the isoprene emission factors assigned to a PFT. For example, the isoprene emission factor for broadleaf trees ranges from 0.1 to 30 mg m<sup>-2</sup> h<sup>-1</sup>. Global total isoprene emissions can be approximated using the PFT-average emission factors shown in Table 1 but this will introduce  
25 significant errors due to correlations between  $\varepsilon$  and  $\gamma$  distributions. For example, the broadleaf trees that grow in montane and boreal regions often have high isoprene emission factors but low isoprene emission activity factors. Furthermore, there will be

substantial errors in estimates for any location where  $\varepsilon$  deviates significantly from the PFT average  $\varepsilon$ .

Isoprene emission factor distributions for each PFT were estimated by combining the isoprene observations described in Sect. 2 with landcover information that includes ground measurement inventories, satellite based inventories, and ecoregion descriptions. The available landcover and isoprene observations differ considerably for the 6 PFTs and also differ for geographic regions. In some cases, vegetation inventories were combined with satellite observations to generate high resolution ( $\sim 1 \text{ km}^2$ ) species composition distributions, while in other cases general descriptions were used to characterize global ecoregions. A description of the methods used for each PFT is given below.

Since geographical distributions of PFTs and PFT-specific isoprene emission factors change with time, the distributions used to estimate emissions should be representative of the time period being simulated. Climate-driven changes in species composition can substantially modify both PFT and  $\varepsilon$  values on a time scale of decades to centuries (e.g., Turner et al., 1991; Martin and Guenther, 1995) while changes associated with land management can occur on time scales of years (e.g., Guenther et al., 1999b; Schaab et al., 2000). Global PFT and  $\varepsilon$  databases are needed on time scales of 50 to 100 years for simulating global earth system changes. A considerably shorter time step for PFT and  $\varepsilon$  inputs is required for regional studies investigating the impacts of land cover change.

### 3.1.1. Trees

Trees have been the focus of most isoprene emission rate measurement studies and there is a relatively large database for assigning tree emission factors. Trees are also economically valuable which has led to the compilation of high resolution geographically referenced tree inventories in Europe (e.g., France, Germany), Asia (e.g. Japan, China, Russia), North America (e.g., U.S., Canada), Australia and New Zealand. Biogenic emission inventories have been developed using summaries (i.e., county,

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province, national totals) based on this information (e.g. Geron et al., 1994; Klinger et al., 2002; Simpson et al., 1999). The current version of MEGAN uses these regional summaries but we have initiated efforts to use plot level data for some regions which will improve the local accuracy of future estimates.

5 Isoprene emission factors for trees in sub-Saharan Africa are estimated using an approach that combines highly spatially resolved ecoregions, species composition measurements for representative sites, and enclosure measurements of dominant tree species. The approaches used for southern Africa (Otter et al., 2003) and central Africa (Guenther et al., 1999a) are described in more detail elsewhere.

10 Our default approach for assigning tree isoprene emission factors uses the 867 ecoregions in the digital terrestrial ecoregion database developed by Olson et al. (2001) and illustrated in Fig. 1. The assigned  $\varepsilon$  are based on ecoregion descriptions of common plant species and available isoprene emissions measurements. A default value, based on the global average for other regions, was assigned if no measurements were  
15 available for characterizing trees in the ecoregion. This scheme provides global coverage using an approach that contains sufficient resolution to simulate biogeographical units with similar isoprene emission characteristics. The Olson et al. (2001) database is the product of over 1000 biogeographers, taxonomists, conservation biologists and ecologists from around the world. Most ecoregions include a fairly detailed description of the dominant plant species found within the region. Uncertainties associated with  $\varepsilon$  distributions for tropical broadleaf trees are a major component of the overall  
20 uncertainty in global isoprene emission estimates.

25 Figure 2 illustrates the global distribution of isoprene emission factors for each PFT. Broadleaf tree isoprene emission factors are close to the PFT global average of  $12.6 \text{ mg m}^{-2} \text{ h}^{-1}$  in most regions but are less than  $1 \text{ mg m}^{-2} \text{ h}^{-1}$  and greater than  $20 \text{ mg m}^{-2} \text{ h}^{-1}$  in other regions. The fineleaf evergreen tree  $\varepsilon$  range from  $>4 \text{ mg m}^{-2} \text{ h}^{-1}$  in most of Canada to  $<0.5$  in most of the U.S. and Europe. The isoprene emission factors for fineleaf deciduous trees are very low in regions dominated by larch (*Larix*) species which are the regions with the greatest cover of this PFT type.

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### 3.1.2. Shrubs, grass and other vegetation

The observations described in Sect. 2 include relatively few isoprene emission measurements for plant species other than trees, although at least a few measurements have been reported for some shrub, grass, and other plant species. In addition, there is less quantitative data on distributions of these plants due to their lesser economic importance. However, some countries (e.g., United States, United Kingdom) have land-cover characterization efforts that include shrubs and ground cover. This information has not been incorporated into the current MEGAN emission factors but will be a high priority for future versions.

Since some plant species occur in both tree and shrub form, MEGAN estimates of shrub isoprene  $\varepsilon$  in forest dominated regions are based on tree isoprene emission factors. Emission factors for shrub dominated regions are based on available shrub emission measurements and available descriptions of shrub species distributions within each ecoregion. The resulting emission factor distribution is illustrated in Fig. 2. The relatively large uncertainty associated with shrub emission factors and the substantial global emission results in a large contribution to the overall uncertainty in global isoprene emission estimates.

Isoprene emission is rarely observed from plants that are entirely “non-woody”. A rare example is the spider-lily, *Hymenocallis americana*. However, there are a number of isoprene-emitting plants that fall within the MEGAN PFT for grass and other vegetation. Some of the important isoprene emitting genera in this category include *Phragmites* (a reed), *Carex* (a sedge), *Stipa* (a grass) and *Sphagnum* (a moss). Reported isoprene emission factors for herbaceous cover range from  $\sim 0.004 \text{ mg m}^{-2} \text{ h}^{-1}$  for grasslands in Australia (Kirstine et al., 1998) and central U.S. (Fukui and Doskey, 1998) to  $\sim 0.4 \text{ mg m}^{-2} \text{ h}^{-1}$  for a grassland in China (Bai et al., 2005<sup>1</sup>) and  $\sim 1.2 \text{ mg m}^{-2} \text{ h}^{-1}$  for forests and wetlands in southern U.S. (Zimmerman, 1979), northern U.S. (Isebrands

<sup>1</sup>Bai, J., Baker, B., Liang, B., Greenberg, J., and Guenther, A.: Isoprene and monoterpene emissions from an Inner Mongolia grassland, Atmos. Environ., submitted, 2005.

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et al., 1999), Canada (Klinger et al., 1994) and Scandinavia (Janson et al., 1999). We assigned one of these three values to the grass and other vegetation PFT in each of the 867 ecoregions to develop the emission factor distribution shown in Fig. 2.

### 3.1.3. Crops

At least one enclosure measurement has characterized each of the 25 globally dominant crop genera and none have been found to emit isoprene (see <http://bvoc.acd.ucar.edu>). However, agricultural landscapes are isoprene sources in at least some regions. Plantations of isoprene-emitting trees (e.g., poplar, eucalyptus, oil palms) are classified as crops by some PFT schemes. In addition, isoprene-emitting plants are introduced into croplands to increase nitrogen availability and to provide windbreaks. Nitrogen fixing plants grown in croplands to provide “green manure” include Velvet bean (*Mucuna pruriens*, a legume) in cornfields and *Azolla*, an aquatic fern, in rice paddies. Both of these plants produce substantial amounts of isoprene (Silver and Fall, 1995). While the use of Velvet bean is relatively limited, *Azolla* is widely used in the major rice producing regions (Clark, 1980). Tropical kudzu (*Pueraria phaseoloides*) is the most widely used “green manure” plant in tropical agricultural lands. Although there are no reported isoprene emission measurements for tropical kudzu, all other examined *Pueraria* species have been identified as isoprene emitters (e.g. Guenther et al., 1996). We have used the global crop distribution database of Leff et al. (2004) to identify agricultural landscapes (oil palm and rice) where isoprene emissions are likely higher than in other agricultural regions. An isoprene  $\varepsilon$  of  $1 \text{ mg m}^{-2} \text{ h}^{-1}$  was assigned to crop PFT in these landscapes and a value of  $0.01 \text{ mg m}^{-2} \text{ h}^{-1}$  was assigned to all other regions.

### 3.2. Emission activity factor ( $\gamma$ )

Experimental evidence over the past two decades has implicated a number of physical and biological factors in modifying the capacity of a leaf to emit isoprene. Among these factors are incident PPFD and leaf temperature, which control emissions on short

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(seconds to minutes) time scales (Guenther et al., 1993), but which also influence the isoprene emission capacity of a leaf over longer (hours to weeks) time scales (Monson et al., 1994; Sharkey et al., 2000; Geron et al., 2000; Petron et al., 2001). A leaf's ability to emit isoprene is clearly influenced by leaf phenology; generally speaking, very young leaves of isoprene-emitting species emit no isoprene, mature leaves emit maximally, and as leaves senesce, emission capacity gradually declines. Although studies indicate that isoprene emission is less sensitive than photosynthesis to decreasing soil moisture (Pegoraro et al., 2004), increasing drought appears to have direct effects on isoprene emission (as well as indirect effects mediated through changes in leaf temperature). Finally, there is growing evidence that changes in the composition of the atmosphere, e.g., increased CO<sub>2</sub> (Rosenstiel et al., 2003) and episodic increases in O<sub>3</sub> (Velikova et al., 2005), may affect isoprene emission capacity. Some of these controls over isoprene emission are much less well understood than others, but we have attempted below to incorporate what is currently known about these influences in the emission activity factor,  $\gamma$ .

The emission activity factor describes variations due to the physiological and phenological processes that drive isoprene emission rate changes. The total emission activity factor is the product of a set of non-dimensional emission activity factors that are each equal to unity at standard conditions,

$$\gamma = \gamma_{CE} \cdot \gamma_{age} \cdot \gamma_{SM} \quad (2)$$

where  $\gamma_{CE}$  describes variation due to light, temperature, humidity and wind conditions within the canopy environment,  $\gamma_{age}$  makes adjustments for effects of leaf age, and  $\gamma_{SM}$  accounts for direct changes in  $\gamma$  due to changes in soil moisture. Descriptions of the methods used to estimate each of the activity factors included in Eq. (2) are given below.

### 3.2.1. Canopy environment ( $\gamma_{CE}$ )

Isoprene emissions are strongly dependent on leaf level PPFD and temperature (Guenther et al., 1993). The PPFD and temperature of leaves within a canopy can differ substantially from above canopy conditions but can be estimated for sun and shade leaves in each layer using a canopy environment model. The canopy average influence of leaf PPFD and temperature,  $\gamma_{CE}$ , is estimated as

$$\gamma_{CE} = C_{CE} \cdot \gamma_{PT} \cdot LAI \quad (3)$$

where  $C_{CE}$  (=0.57 for the MEGAN canopy model) is a factor that sets the emission activity to unity at standard conditions,  $\gamma_{PT}$  is the weighted average, for all leaves, of the product of a temperature emission activity factor ( $\gamma_T$ ) and a PPFD emission activity factor ( $\gamma_P$ ), and LAI is leaf area index.

Leaves in direct sunlight often experience temperatures that are a degree or more higher than ambient air while shaded leaves are often cooler than ambient air temperature. PPFD can be very low on shaded leaves in dense canopies and the PPFD of sun leaves depends on the angle between the sun and the leaf. Guenther et al. (1995) used a relatively simple canopy environment model to estimate PPFD on sun and shade leaves at several canopy depths and assumed that leaf temperature was equal to air temperature. The non-linear relationships between isoprene emission and environmental conditions, coupled with the strong correlation between PPFD and temperature, will result in a significant underestimation of isoprene emissions if canopy or daily average PPFD and temperature are used (rather than calculating emissions for each canopy level and each hour of the day). Guenther et al. (1999a) used a more detailed canopy radiation model and added a leaf energy balance model that predicts leaf temperature based on the solar radiation, air temperature, wind speed, and humidity at each canopy depth. Lamb et al. (1996) evaluated the use of several canopy environment models for predicting whole canopy isoprene fluxes and found that the results from both simple and complex canopy models were within the uncertainty range of observed isoprene fluxes. Although detailed canopy environment models may not

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always substantially improve isoprene emission estimates, these models may be better for investigating how changes in environmental conditions will perturb isoprene emission rates. The integration of MEGAN within the land surface model component of an earth system model will allow investigations of interactions between isoprene emissions and environmental conditions. The standard MEGAN canopy environment model is based on the methods described by Guenther et al. (1999). Other canopy environment models can be used with MEGAN by setting  $C_{CE}$  so that  $\gamma_{CE}$  is equal to unity for the MEGAN standard conditions.

The algorithms described by Guenther et al. (1993) and modified by Guenther et al. (1999a) have been used extensively to simulate the response of isoprene emission to changes in light and temperature on a time scale of seconds to minutes. The algorithms simulate emission variations as

$$\gamma_P = C_P [(\alpha \cdot \text{PPFD}) / ((1 + \alpha^2 \cdot \text{PPFD}^2)^{0.5})] \quad (4)$$

$$\gamma_T = E_{opt} \cdot [C_{T2} \cdot \text{Exp}(C_{T1} \cdot x) / (C_{T2} - C_{T1} \cdot (1 - \text{Exp}(C_{T2} \cdot x)))] \quad (5)$$

where PPFD is the photosynthetic photon flux density ( $\mu\text{mol m}^{-2} \text{s}^{-1}$ ),  $x = [(1/T_{opt}) - (1/T)] / 0.00831$ ,  $T$  is leaf temperature (K),  $C_{T1}$  (=95) and  $C_{T2}$  (=230) are empirical coefficients, and  $C_P$ ,  $\alpha$ ,  $E_{opt}$ , and  $T_{opt}$  are estimated using Eq. (6) through (9). The simulated behavior reflects the activity of the enzyme isoprene synthase (Fall and Wildermuth, 1998). MEGAN extends these algorithms to account for past temperature and PPFD conditions which are not considered by the Guenther et al. (1993) algorithms. The substantial deviations from the Guenther et al. (1993) algorithms that have been observed over longer time scales could be due to changes in production of the isoprene substrate, dimethylallyl pyrophosphate (DMAPP), or variations in the activity of isoprene synthase, the enzyme that converts DMAPP to isoprene, or to both of these factors. Variations in DMAPP supply could be due to changes in production, either availability of the carbon precursor (pyruvate) or adenosine triphosphate (ATP) used for phosphorylation, or changes in DMAPP consumption. Variations in isoprene synthase activity

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and DMAPP have been observed but are not well characterized (Bruggemann et al., 2002; Wolfertz et al., 2003). Isoprene emission rates, measured at standard light and temperature conditions, are higher when warm sunny conditions have occurred during the previous day(s) and are lower if there were cool shady conditions (Sharkey et al., 2000). Petron et al. (2001) found that exposure to high or low temperatures can influence isoprene emission for several weeks. The time required to reach a new, lower, steady-state isoprene emission capacity following a step decrease in temperature was longer than that required to reach a new, higher, equilibrium following an increase in temperature, indicating that down regulation of isoprene emission is a slower process than up regulation. The factors controlling these variations presumably operate over a continuous range of time scales but for modeling purposes MEGAN currently considers only 24 and 240 h. The average PPFD of the past 24 h ( $P_{24}$ ) and past 240 h ( $P_{240}$ ) influence the estimated emission activity by adjusting the coefficients in Eq. (4) as follows,

$$\alpha = 0.004 - 0.0005 \ln(P_{240}) \quad (6)$$

$$C_P = 0.0468 \cdot \exp(0.0005 \cdot [P_{24} - P_0]) \cdot [P_{240}]^{0.6} \quad (7)$$

where  $P_0$  represents the standard conditions for PPFD averaged over the past 24 h and is equal to  $200 \mu\text{mol m}^{-2} \text{s}^{-1}$  for sun leaves and  $50 \mu\text{mol m}^{-2} \text{s}^{-1}$  for shade leaves.

MEGAN estimates the coefficients in Eq. (5) as a function of the average leaf temperature over the past 24 ( $T_{24}$ ) and 240 ( $T_{240}$ ) h, as follows,

$$T_{\text{opt}} = 313 + (0.6 \cdot (T_{240} - T_0)) \quad (8)$$

$$E_{\text{opt}} = 2.038 \cdot \exp(0.05 \cdot (T_{24} - T_0)) \cdot \exp(0.05 \cdot (T_{240} - T_0)) \quad (9)$$

where  $T_0$  (=297 K) is the standard condition for leaf temperature averaged over both the past 24 and 240 h. The coefficients used for Eqs. (6–9) are based on observations reported by Petron et al. (2001), Monson et al. (1994), Sharkey et al. (2000), Geron

et al. (2000), and Hanson and Sharkey (2001). Although these five studies report results that are qualitatively similar, there remain significant uncertainties associated with these algorithms.

Figure 3 shows the response of  $\gamma_{CE}$  estimates to variations in LAI, solar angle and transmission, and temperature. Isoprene emission increases exponentially with temperature up to a maximum that is dependent on the average temperature that the canopy has experienced during the past 240 h. Both the magnitude of the emissions and the temperature at which the maximum occurs are dependent on the past temperature. The result is that MEGAN predicts lower (higher) isoprene emissions in cool (warm) climates than would be simulated by the Guenther et al. (1993) algorithms. However, MEGAN predictions of the isoprene emission response to short term (<24 h) temperature variations is often less than that predicted by models that do not calculate leaf temperature, e.g., BEIS2/BEIS3 or Guenther et al. (1995). This is because leaf transpiration tends to result in leaf temperature increases that are less than ambient temperature increases.

Above canopy PPFD is determined by solar angle and transmission. MEGAN estimates of  $\gamma_{CE}$  increase nearly linearly with PPFD transmission for canopies that have experienced high PPFD levels (e.g., 24 h average of  $600 \mu\text{mol m}^{-2} \text{s}^{-1}$  for sun leaves) during the past day. The emission increase begins to saturate at high PPFD transmission for low solar angles or if the average PPFD has been low during the previous day.

Figure 3 shows that estimated isoprene emission increases nearly linearly with LAI until LAI exceeds  $\sim 1.5$  and is nearly constant for  $\text{LAI} > 5$ . The relationship between LAI and  $\gamma_{CE}$  depends on solar angle and on canopy characteristics, which differ with PFT type. Isoprene emissions from canopies with clumped leaves increase relatively slowly with increasing LAI for  $\text{LAI} < 3$  in contrast to canopies with horizontal leaves that exhibit a stronger LAI dependence for  $\text{LAI} < 3$ . Figure 3 also shows that MEGAN predicts a stronger initial increase with LAI, and a lack of increase with higher LAI, for low solar angles (e.g.,  $< 30$  degrees).

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### 3.2.2. Leaf age

Leaves begin to photosynthesize soon after budbreak but isoprene is not emitted in substantial quantities for days after the onset of photosynthesis (Guenther et al., 1991). In addition, old leaves eventually lose their ability to photosynthesize and produce isoprene. Guenther et al. (1999a) developed a simple algorithm to simulate the reduced emissions expected for young and old leaves based on the observed change in foliar mass over a month. An increase in foliage was assumed to imply a higher proportion of young leaves while decreasing foliage was associated with the presence of older leaves. This algorithm required a time step of one month, assumed that young leaves and old leaves had the same emission rate, and included variables that could not easily be quantified. The following procedures to account for leaf age effects on isoprene emission estimates reduce these deficiencies.

MEGAN divides the canopy into four fractions: new foliage that emits negligible amounts of isoprene ( $F_{\text{new}}$ ), growing foliage that emits isoprene at less than peak rates ( $F_{\text{gro}}$ ), mature foliage that emits isoprene at peak rates ( $F_{\text{mat}}$ ) and senescing foliage that emits isoprene at reduced rates ( $F_{\text{sen}}$ ). The canopy-weighted average factor is calculated as

$$Y_{\text{age}} = F_{\text{new}}A_{\text{new}} + F_{\text{gro}}A_{\text{gro}} + F_{\text{mat}}A_{\text{mat}} + F_{\text{sen}}A_{\text{sen}} \quad (10)$$

where  $A_{\text{new}}$  (=0.05),  $A_{\text{gro}}$  (=0.5),  $A_{\text{mat}}$  (=1.1), and  $A_{\text{sen}}$  (=0.4) are the relative emission rates assigned to each canopy fraction. The values of these emission factors are based on the observations of Petron et al. (2001), Goldstein et al. (1998), Monson et al. (1994), Guenther et al. (1991) and Karl et al. (2003).

The canopy is divided into leaf age fractions based on the change in LAI between the current time step ( $\text{LAI}_c$ ) and the previous time step ( $\text{LAI}_p$ ). In cases where  $\text{LAI}_c = \text{LAI}_p$  then  $F_{\text{mat}} = 1$  and all other fractions ( $F_{\text{new}}$ ,  $F_{\text{gro}}$ ,  $F_{\text{sen}}$ ) are equal to zero. When  $\text{LAI}_p > \text{LAI}_c$  then  $F_{\text{new}}$  and  $F_{\text{gro}}$  are equal to zero,  $F_{\text{sen}}$  is estimated as  $[(\text{LAI}_p - \text{LAI}_c) / \text{LAI}_p]$  and  $F_{\text{mat}} = 1 - F_{\text{sen}}$ . In the final case, where  $\text{LAI}_p < \text{LAI}_c$ ,  $F_{\text{sen}} = 0$  and the other fractions are

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calculated as

$$F_{\text{new}} = 1 - (\text{LAI}_p/\text{LAI}_c) \quad \text{for } t \leq t_i \quad (11a)$$

$$F_{\text{new}} = [t_i/t][1 - (\text{LAI}_p/\text{LAI}_c)] \quad \text{for } t > t_i \quad (11b)$$

$$F_{\text{gro}} = 0 \quad \text{for } t \leq t_i \quad (11c)$$

$$F_{\text{gro}} = [(t_g - t_i)/t][1 - (\text{LAI}_p/\text{LAI}_c)] \quad \text{for } t > t_i \quad (11d)$$

$$F_{\text{mat}} = (\text{LAI}_p/\text{LAI}_c) \quad \text{for } t \leq t_m \quad (11e)$$

$$F_{\text{mat}} = (\text{LAI}_p/\text{LAI}_c) + [(t - t_m)/t][1 - (\text{LAI}_p/\text{LAI}_c)] \quad \text{for } t > t_m \quad (11f)$$

where  $t$  is the length of the time step (days) between  $\text{LAI}_c$  and  $\text{LAI}_p$ ,  $t_i$  is the number of days between budbreak and the induction of isoprene emission,  $t_m$  is the number of days between budbreak and the initiation of peak isoprene emission rates, and  $t_g = t_m$  for  $t > t_m$  and  $t_g = t$  for  $t \leq t_m$ . The time step,  $t$ , depends on the LAI database that is used but generally is between 7 and 31 days. Petron et al. (2001) grew plants under conditions typical of temperate regions and observed an emission pattern that suggests a  $t_i$  of about 12 days and  $t_m$  of about 28 days. Goldstein et al. (1998) field observations in a temperate forest indicate a similar value for  $t_m$ . Monson et al. (1994) found that  $t_i$  and  $t_m$  are temperature dependent and are considerably less for vegetation growing at high temperatures. These observations suggest that the temperature dependence of these variables can be estimated as

$$t_i = 5 + (0.7 \cdot (300 - T_t)) \quad (12)$$

$$t_m = 2.3 \cdot t_i \quad (13)$$

where  $T_t$  is the average temperature (K) of the preceding time step interval. MEGAN simulations using a constant  $t_i$  and  $t_m$  result in global annual isoprene emissions that

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are ~ 5% lower than estimates based on a variable  $t_i$ . However, the emission rates estimated using variable  $t_i$  and  $t_m$  can be as much as 20% higher in tropical regions and 20% lower in boreal regions when foliage is rapidly expanding. The differences are more pronounced when LAI variations have a higher time resolution (i.e., weekly rather than monthly).

### 3.2.3. Soil moisture

Plants require both carbon dioxide and water for growth. Carbon dioxide is taken up through leaf stomatal openings and water is obtained from the soil. However, large quantities of water are lost through stomata creating a need for adequate soil moisture in order to continue carbon uptake. Field measurements have shown that plants with inadequate soil moisture can have significantly decreased stomatal conductance and photosynthesis, in comparison to well-watered plants, and yet can maintain approximately the same isoprene emission rates (Guenther et al., 1999b). However, isoprene emission does begin to decrease when soil moisture drops below a certain level and eventually becomes negligible when plants are exposed to extended severe drought (Pegoraro et al., 2004). MEGAN simulates the response of isoprene emission to drought through two mechanisms. Isoprene emissions are indirectly influenced by the soil moisture dependence of stomatal conductance which influences the leaf temperature estimated by the MEGAN canopy environment model. In addition, MEGAN includes an emission activity factor, dependent on soil moisture, estimated as

$$\gamma_{SM} = 1 \quad \text{for } \theta > \theta_1 \quad (14a)$$

$$\gamma_{SM} = (\theta - \theta_w) / \Delta\theta_1 \quad \text{for } \theta_w < \theta < \theta_1 \quad (14b)$$

$$\gamma_{SM} = 0 \quad \text{for } \theta < \theta_w \quad (14c)$$

where  $\theta$  is soil moisture (volumetric water content,  $\text{m}^3 \text{m}^{-3}$ ),  $\theta_w$  ( $\text{m}^3 \text{m}^{-3}$ ) is wilting point (the soil moisture level below which plants cannot extract water from soil) and  $\Delta\theta_1$

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(=0.06) is an empirical parameter based on the observations of Pegoraro et al. (2004), and  $\theta_1 = \theta_w + \Delta\theta_1$ . MEGAN uses the high resolution ( $\sim 1 \text{ km}^2$ ) database developed by Chen and Dudhia (2001) which assigns  $\theta_w$  values that range from 0.01 for sand to 0.138 for clay soils. Soil moisture varies significantly with depth and the ability of a plant to extract water is dependent on root depth. We follow the PFT dependent approach described by Zeng (2001) to determine the fraction of roots within each soil layer and use the weighted average  $\gamma_{SM}$  for each soil layer.

### 3.2.4. Other factors that influence isoprene emission activity

Isoprene emission activity can also be influenced by other environmental conditions including ozone (Velikova et al., 2005) and carbon dioxide (Buckley, 2001; Rosenstiel et al., 2003) concentrations, nitrogen availability (Harley et al., 1994), and physical stress (e.g., Alessio et al., 2004). In addition, there may be significant diurnal variations that are not entirely explained by variations in environmental conditions (Funk et al., 2003). Emission activity factors accounting for these processes will be included in MEGAN as more reliable algorithms are developed. Existing observations have been used to qualitatively assess the importance of these factors and are discussed in Sect. 7.

### 3.3. Canopy loss and production, $\rho$

Chemicals emitted into the canopy airspace do not always escape to the above-canopy atmosphere. Some molecules are consumed by biological, chemical and physical processes on soil and vegetation surfaces while others react within the canopy atmosphere. Some emissions escape to the above-canopy atmosphere in a different chemical and/or physical (i.e. gas to particle conversion) form. The  $\varepsilon$  defined by MEGAN is a net canopy emission factor but is not the net flux. This is because the MEGAN isoprene  $\varepsilon$  accounts for isoprene losses on the way out of the canopy but does not account for isoprene deposition from the above-canopy atmosphere. The net ecosystem-atmosphere isoprene flux can be determined from the MEGAN isoprene emission rate

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estimate and an isoprene deposition rate based on the above canopy concentration and a deposition velocity.

Inverse modeling of within-canopy gradients of isoprene suggests that at least 90% of the isoprene emitted by tropical and temperate forests escapes to the above-canopy atmosphere (Karl et al., 2004; Stroud et al., 2005). The remainder is removed through a combination of chemical losses and dry deposition. While ambient mixing ratios within the canopy and roughness layer can change on the order of 10–30% due to chemistry (Makar et al., 1999), the bias of canopy scale isoprene flux measurements is small (i.e., on the order of 5–10%). This can be attributed to (1) near field effects within the canopy and (2) limited processing time between the location of isoprene emission (occurring mostly within the upper canopy) and the top of the canopy. Comparisons between canopy-scale emissions based on leaf-level emission measurements extrapolated with a canopy environment model and above-canopy flux measurements tend to show that any loss of isoprene is less than the uncertainty associated with these two approaches (Guenther et al., 2000).

MEGAN includes a canopy loss and production factor,  $\rho$ , that is equal to unity for standard conditions and varies with changes in canopy residence time and isoprene lifetime which is determined by canopy oxidative capacity. Variations in isoprene canopy production and loss are estimated as

$$\rho = \rho_o - H / [\lambda \cdot u^* \cdot \tau + H] \quad (15)$$

where  $H$  is canopy height (m),  $u^*$  is friction velocity ( $\text{m s}^{-1}$ ),  $\tau$  is the above canopy isoprene lifetime (s),  $\lambda$  ( $=1.5 \pm 0.1$ ) and  $\rho_o$  ( $=1.01$ ) are empirically determined parameters. Equation (15) was parameterized with the above-canopy isoprene lifetime, rather than the within-canopy lifetime, because this is the value more readily available for regional and global modeling. Standard conditions ( $\rho=1$ ) are defined as  $u^*=0.5 \text{ m s}^{-1}$ ,  $\tau=3600 \text{ s}$  and  $H=30 \text{ m}$ . Since variations in  $\rho$  for isoprene are typically less than 5%,  $\rho$  can be assigned a constant value of unity for many isoprene emission estimation efforts. Equation (15) is based on measured isoprene emission profiles and turbulence

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profiles obtained during recent tropical and temperate forest field studies (Karl et al., 2004, Stroud et al., 2005). The variation of the isoprene lifetime inside the canopy was scaled to the above-canopy lifetime and based on measured  $O_3$  profiles and modeled OH and  $NO_3$  levels reported by Stroud et al. (2005). A random walk model similar to the one described by Baldocchi (1997) and Strong et al. (2004) was used to estimate the first order decay of isoprene. Trajectories for 5000 particles were released at 4 levels (25%, 50%, 75% and 100% of canopy height) and computed for typical daytime conditions. The chemical loss by the ensemble mean was used to assess  $\rho$  integrated over the whole canopy. A sensitivity analysis indicated that canopy height, friction velocity and lifetime were the most important variables controlling  $\rho$ . Model simulations were performed for a range of canopy heights (13.5 m, 27 m and 54 m), isoprene lifetimes (1370 to 6870 s) and friction velocities (0.1 to 2 m s<sup>-1</sup>).

Model simulations of the impact of isoprene on atmospheric chemistry depend on estimates of net isoprene emission as well as estimates of the regional uptake of isoprene and its oxidation products, e.g. methylvinylketone, methacrolein and peroxyacetyl nitrate (PAN), from the above-canopy atmosphere. Karl et al. (2004) conclude that current model procedures can underestimate the uptake of these oxidation products which would cause an overestimate of the impact of isoprene on oxidants and other atmospheric constituents. They also report that isoprene oxidation products deposit more rapidly during night than predicted by standard dry deposition schemes. During daytime, the net effect of deposition and in-canopy production of these compounds can be on the same order. These observations raise the possibility that various products of isoprene chemistry are taken up by the forest canopy more efficiently than previously assumed. This could lead to an incorrect characterization of the impact of isoprene by chemistry and transport models that have correctly simulated isoprene emission rates and oxidation schemes, and could explain why some chemistry and transport models are forced to use isoprene emission rates that are lower than observed.

## 4. Driving variables

The MEGAN algorithms described in Sect. 3 require estimates of landcover (LAI and PFT distributions) and weather (solar transmission, air temperature, humidity, wind speed, and soil moisture). The driving variables used for MEGAN are described in this section and are compared with alternative databases.

### 4.1. Leaf area

MEGAN requires leaf area estimates with a time step of  $\sim 4$  to 40 days in order to simulate seasonal variations in leaf biomass and age distribution. MEGAN does not assume that LAI is uniformly spread over a grid cell but assumes that foliage covers only that part of the grid cell containing vegetation. The average LAI for vegetated areas is estimated by dividing the grid average LAI by the fraction of the grid that is covered by vegetation. We refer to this as LAI<sub>v</sub> (the LAI of vegetation covered surfaces) and we set an upper limit of LAI<sub>v</sub>=8 to eliminate the very high values that can be estimated for grids with very little vegetation. The standard MEGAN LAI<sub>v</sub> database (MEGAN-L) was estimated by this approach using the LAI estimates of Zhang et al. (2004) and estimates of vegetation cover fraction from Hansen et al. (2003).

Figure 4 illustrates how LAI<sub>v</sub> variations with time and location result in isoprene emission variations of more than an order of magnitude, independent of variation in other driving variables which are held constant in these simulations. These emission variations are driven by changes in only leaf age and quantity. Isoprene is reduced by more than 80% at higher latitudes in winter but varies only  $\sim 15\%$  for croplands, forests and grasslands during the growing season. Most of the extra-tropical regions of the southern hemisphere do not exceed a level of  $\sim 30\%$  of the maximum emission while tropical forests regions rarely fall below a level of 70%.

Table 2 includes descriptions of six LAI databases that have been used to estimate global isoprene emissions with MEGAN. Satellite-derived LAI estimates provide high resolution variability but are not available for all years. Dynamic vegetation models

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allow predictions of past and future emissions. The MEGAN-L database contains monthly estimates for years 2000 to 2004 at 30 s ( $\sim 1 \text{ km}^2$ ) resolution. Table 2 includes a comparison of annual global isoprene emissions estimated with alternative LAIv databases. The estimates range from 11% lower to 29% higher than the MEGAN-L values. Some of the differences are due to interannual variations, which can be seen in Fig. 5 by the comparison of July average isoprene emissions estimated with the AVHRR3 databases for years 1990 and 2000. The emission estimates using MODIS based estimates of LAI, including the MEGAN-L database, are generally  $\sim 20\%$  lower than emission estimates using the other LAI databases. All of the databases shown in Fig. 5 have regions of more than a factor of 3 lower emissions and regions with more than a factor of 3 higher emissions. However, the regions with the greatest percent differences tend to be areas with relatively low emissions.

#### 4.2. PFT distributions

The PFT databases described in Table 2 use a variety of inputs including satellite observations, vegetation inventories, ecosystem maps, and ecosystem model output. The satellite data provide the highest spatial and temporal resolution while models can be used to simulate future scenarios. Vegetation inventories based on field observations are expected to provide the most accurate estimates of PFT distributions but they have limited coverage.

Landcover data were processed to generate the MEGAN PFT categories from each data source shown in Table 2. Landcover data that included PFT estimates (AVHRR1-P, MODIS1-P), were converted into the MEGAN PFT scheme with a straightforward collapsing of the fifteen PFTs into the six MEGAN PFTs. The ecosystem scheme databases (HYDE, GED, IBIS, IMAGE, MODIS2, SPOT) contain a discrete landcover type for each location that are based on either observed vegetation distribution maps, vegetation model output or satellite observations. A PFT distribution was assumed for each ecosystem type in each database. For example, the temperate mixed forest ecosystem in the GED database was assumed to be composed of 40% broadleaf trees,

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40% fineleaf evergreen trees, 1% fineleaf deciduous trees, 1% shrubs, 1% crops, 2% herbaceous and 15% bare ground or water. The PFT assignments were based on qualitative descriptions of the ecosystems and are somewhat subjective. The IMAGE database includes estimates for years 2000 and 2100 and the HYDE database has estimates for 50 year intervals between 1700 and 1950 and 20 year intervals between 1950 and 1990. The AVHRR2 and MODIS3 databases use satellite derived tree cover data that include total cover, deciduous and broadleaf fractions and provide the most direct estimates for the MEGAN tree PFTs and constrain the total fraction assigned to the other three MEGAN PFTs. The standard MEGAN PFT database (MEGAN-P) combines the MODIS3 database with available quantitative tree inventories based on ground observations (e.g., Kinnee et al., 1997). The global distribution of each PFT in the MEGAN database is shown in Fig. 6. The regions dominated by broadleaf trees are the major global isoprene sources. Shrubs dominate at high latitudes, where, despite relatively high emission factors, cool weather generally results in low isoprene emissions. However, shrubs have a fairly wide global distribution and so contribute to isoprene emissions in many regions.

Global vegetation cover area estimated with the eleven databases range from about 90 to  $120 \times 10^6 \text{ km}^2$ , which represents  $\sim 60$  to  $80\%$  of the global land surface (Table 1). Most of the PFT database estimates are within  $\sim 10\%$  of the mean value of  $104 \times 10^6 \text{ km}^2$ . While there is considerable variation in estimates of crops, grass/other and fineleaf deciduous tree areas, these PFTs make only a small contribution to the global total isoprene emission. Shrub and fineleaf evergreen tree area estimates from the different PFT databases agree relatively well. Area estimates of broadleaf trees, which contribute over half of the total global isoprene emission, are more variable and thus are a significant component of the overall uncertainty in global annual emissions. However, the sum of broadleaf tree area plus shrub area is less variable and all but one database is within  $20\%$  of the  $40 \times 10^6 \text{ km}^2$  estimated by the MEGAN-P database. Figure 7 shows that large differences in regional isoprene emission estimates ( $>$  factor of 4) are obtained using the different PFT databases. All of the databases have areas of



both lower and higher emission so that the global total difference (Table 2) ranges only from 13% lower to 24% higher than the value estimated with the MEGAN-P database.

Ecosystem databases can be used to generate reasonable estimates of annual global isoprene emissions but may not produce accurate regional distributions. For example, the 72 ecosystem types in the GED database used for the Guenther et al. (1995) emission inventory were assigned PFT distributions that resulted in a global annual emission within a few percent of the MEGAN-P database, but Fig. 7 shows that there are large regional differences.

Global total emissions from all of the databases derived directly from 1 km resolution data agree reasonably well. However, large global total differences in PFT area estimates occur among databases that are based on MODIS observations but use different procedures to assign PFT areas. This indicates that the method for assigning PFT cover has a greater effect than the satellite sensor that is used. Approaches (e.g. DeFries et al., 2000) that use continuous vegetation fields (e.g. percent tree cover, percent broadleaf vegetation, percent herbaceous cover) could result in more accurate PFT distributions.

### 4.3. Weather

MEGAN weather input variables include ambient temperature, PPFD transmission, humidity, wind speed and soil moisture. Figure 8 shows that both seasonal and spatial weather variations can result in monthly average isoprene emission estimates that vary by more than an order of magnitude. In particular, the cool weather conditions at high latitudes result in much lower isoprene emissions. Previous estimates of seasonal variations in tropical rainforests indicate fairly constant monthly emission rates (Guenther et al., 1995) but MEGAN estimates much larger (factor of 3) variations. These large seasonal variations are a result of the MEGAN algorithms that account for the influence of the weather of the past 24 to 240 h. Substantial seasonal variations in isoprene emissions have been reported for tropical rainforest sites (e.g., Guenther et al., 1999a; Andreae et al., 2002; Trostorf et al., 2004) but additional observations are

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needed for a rigorous evaluation.

The sensitivity of MEGAN hourly isoprene emission estimates to different global weather data was examined using the databases listed in Table 2. These include estimates based on interpolated observations (IIASA and CRU), estimates from global weather models with assimilated observations (NCEP-DOE reanalysis and MM5), and two global climate models (HadCM2 and CSM1). The NCEP-DOE reanalysis, which is the only one that included soil moisture, was used as the standard database (MEGAN-W). The NCEP-DOE soil moisture was used to estimate  $\gamma_{SM}$  for all emission estimates. Hourly estimates were generated from 4 times daily values for MEGAN-W, MM5 and CSM1 data and from monthly mean values for IIASA, CRU and HadCM2. Hourly temperature and PPFD variations were estimated for an average day for each month for the latter databases. Annual global emission estimates for the five alternative databases are all within  $-11\%$  to  $+15\%$  of the MEGAN-W estimate. The alternative weather databases result in annual global emission estimates are within  $\sim 15\%$  of the MEGAN-W estimate. However, regional estimates differ by as much as a factor of two to three for specific locations and months. The difference in isoprene emission estimated for alternatives of the same database type (e.g., observations) is similar to the level of difference between database types (e.g., observations compared to climate models).

The Guenther et al. (1995) isoprene emission estimates used the IIASA database without including diurnal temperature variations (which underestimated emissions) but also used a method for estimating PPFD from cloud cover (based on Pierce and Waldruff, 1991) that overestimated emissions. The two compensating errors resulted in an annual global emission estimate that is within  $\sim 3\%$  of the annual global emission that is estimated when using a diurnal temperature range and more accurate estimates of surface solar radiation.

The soil moisture algorithm (Eq. 14) reduces annual global isoprene emissions by only  $\sim 7\%$  but can reduce regional emissions to zero for days to months. As expected, the soil moisture emission activity factor has the greatest impact on isoprene emissions estimated for arid regions. However, significant reductions in estimated emissions also

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occurred in regions that have moderate to high total annual precipitation but also have dry seasons with little rainfall.

## 5. MEGAN-EZ model description

Application of the MEGAN algorithms (Sect. 3) and the associated driving variables (Sect. 4) may require more effort than is desirable for some modeling studies. We have developed a simplified approach, referred to as MEGAN-EZ, with relatively simple methods for estimating the three factors used to estimate emissions with Eq. (1). The factor,  $\rho$ , is simply assigned a constant value of unity. Instead of calculating landscape average  $\varepsilon$  from the PFT specific emission factors described in Sect. 3.1 and the MEGAN-P PFT distribution database described in Sect. 4.2, a global gridded average  $\varepsilon$  can be downloaded from the MEGAN data portal. The global distribution of  $\varepsilon$  is shown in Fig. 9 with a base resolution of 30 s ( $\sim 1$  km). Global hotspots include the southeastern U.S. and southeastern Australia. Figure 9 illustrates the considerable variation in  $\varepsilon$  that occurs on both global and regional (10–100 km) scales. The small scale variability estimated by MEGAN is important for regional modeling simulations due to the short lifetime of isoprene and the non-linear chemistry that determines the impact of isoprene on the chemistry of the atmosphere.

The MEGAN-EZ approach for estimating the isoprene emission activity factor is as follows,

$$Y = Y_{LAI} \cdot Y_P \cdot Y_T \quad (16)$$

where  $Y_{LAI}$ ,  $Y_P$  and  $Y_T$  account for variations associated with LAI, PPFD and temperature. The relationships between these factors and canopy scale isoprene emissions are based on MEGAN canopy environment model simulations for the canopies and environmental conditions that dominate global isoprene emissions (i.e., warm broadleaf forests). The MEGAN-EZ canopy-scale isoprene emission response to PPFD varia-

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tions is simulated as

$$\gamma_P = \text{Sin}(a)[1 + 0.0005 \cdot (PPFDm - 400)][2.46\phi - (0.9\phi^2)] \quad (17)$$

where  $PPFDm$  is monthly average PPFD ( $\mu\text{mol m}^{-2} \text{s}^{-1}$ ),  $a$  is solar angle (degrees) and  $\phi$  is PPFD transmission (non-dimensional) which can be estimated from solar angle and PPFD or cloud cover. The MEGAN-EZ temperature response factor,  $\gamma_T$ , is estimated as

$$\gamma_T = E_{\text{opt}} \cdot \exp(0.08(T_{\text{mon}} - 297))[C_{T_2} \cdot \exp(C_{T_1} \cdot x)/(C_{T_2} - C_{T_1} \cdot (1 - \exp(C_{T_2} \cdot x)))] \quad (18)$$

where  $x = [(1/T_{\text{opt}}) - (1/T_{\text{hr}})]/0.00831$ ,  $T_{\text{hr}}$  is hourly average air temperature (K),  $T_{\text{mon}}$  is monthly average air temperature (K),  $E_{\text{opt}}$  (=1.75),  $C_{T_1}$  (=80),  $C_{T_2}$  (=200), are empirical coefficients and  $T_{\text{opt}}$  is estimated using Eq. (8). Emission responses to LAI variations are estimated as

$$\gamma_{\text{LAI}} = 0.49\text{LAI}/[(1 + 0.2\text{LAI}^2)^{0.5}]. \quad (19)$$

When the standard MEGAN driving variables are used, the annual global isoprene emission estimated by MEGAN-EZ is within ~5% of the value estimated by MEGAN. However, differences can exceed 25% for estimates at specific times and locations.

## 6. Isoprene emission estimates

Guenther et al. (1995) estimated a global annual emission of ~570 Tg of isoprene (503 Tg of carbon), which was somewhat higher than prior estimates which had ranged from ~200–500 Tg of isoprene. The higher emission estimate of Guenther et al. (1995) is primarily due to increased emission factors, although there were also substantial differences in other model components. Earlier isoprene emission factor measurements tended to underestimate the canopy average emissions because they were biased towards leaves and branches from the lower part of the canopy or were otherwise not representative. Wang et al. (1998) used methods similar to Guenther et al. (1995) and

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5 estimated a global annual isoprene emission that was  $\sim 20\%$  higher. This difference was attributed to the use of a diurnal temperature cycle, rather than monthly average temperatures, which results in higher emission estimates because of the exponential increase in emissions with temperature and because emissions occur only during the daylight hours when temperatures are highest. Other investigators (e.g., Adams et al., 2001; Potter et al., 2001; Levis et al., 2003; Sanderson et al., 2003) based their emission factors and algorithms on the Guenther et al. (1995) values but used considerably different landcover and climate data. The reported global annual totals calculated by these six studies are all within  $\sim 10\%$  of Guenther et al. (1995) which is a small range  
10 considering the large uncertainties associated with these estimates.

### 6.1. MEGAN isoprene emission estimates

The annual global isoprene emission estimated by MEGAN using the standard MEGAN input databases for year 2003 is  $\sim 600$  Tg isoprene. This estimate is similar to the annual global emission (570 Tg isoprene) reported by Guenther et al. (1995). Monthly average isoprene emissions estimated using MEGAN with the standard driving variables are shown in Fig. 10. Emissions range from  $>150$  mg isoprene  $\text{m}^{-2} \text{day}^{-1}$  (e.g., some locations in Australia, eastern U.S., Amazon) to  $<2$  mg isoprene  $\text{m}^{-2} \text{day}^{-1}$  (e.g., higher latitudes in winter). Figures 4 and 8 show that monthly variation in isoprene distributions are controlled by weather and, to a lesser degree, by LAI variations.

15 Isoprene emission estimates based on the 20 year AVHRR3 LAIv database indicates that interannual LAI variations result in  $\sim 4\%$  variation in global annual isoprene emissions. However, isoprene emission estimates for specific regions and months, especially arid landscapes and boreal forests, vary by more than 30% due to interannual LAI variations. NCEP-DOE database interannual weather variations for years 1996 to  
20 2004 result in  $\sim 8\%$  variation in global annual isoprene emissions but differences for specific months and locations exceed 50%.

The annual global isoprene emission estimated by MEGAN using alternative driving variable databases (see Table 2) range from  $\sim 15\%$  lower to  $\sim 30\%$  higher. Weather,

PFT and LAI databases can all contribute to these differences in estimated emissions. Emission estimates for specific regions and months can differ by more than a factor of 3 but are typically within ~30% for the regions that dominate global emissions.

## 6.2. Top-down emission estimates using satellite observations

Recent studies have demonstrated that formaldehyde (HCHO) column data from the Global Ozone Monitoring Experiment (Palmer et al., 2001) provide important constraints to regional and global isoprene emission estimates (e.g., Abbot et al., 2003; Palmer et al., 2003; Shim et al., 2005). Formaldehyde is a high yield oxidation product of VOCs. Palmer et al. (2003) developed a methodology to relate HCHO columns to emissions of its parent VOC, taking into account the lifetimes of HCHO and the VOC.

Over North America during the growing season, isoprene is the dominant contributor to measured HCHO columns (Palmer et al., 2003). The spatial distribution and magnitude of GOME HCHO columns is consistent with in situ surface data (Palmer et al., 2003); and the seasonal and interannual variability of HCHO columns is broadly consistent with MEGAN-EZ isoprene emission estimates (Abbot et al., 2003). Typical monthly mean values for GOME HCHO columns over North America during summer months are  $1-2.5 \times 10^{16}$  molec  $\text{cm}^{-2}$ , with the largest values over the Southeast United States (Fig. 11); the fitting uncertainty of the columns is  $\sim 4 \times 10^{15}$  molec  $\text{cm}^{-2}$ . Isoprene emissions, estimated from these data using a regression between modeled isoprene fluxes and modeled HCHO columns, have an estimated uncertainty of ~30% (Palmer et al., 2006). Past work has shown that GOME isoprene emission estimates are spatially correlated with BEIS2 isoprene emission estimates but have a significant positive bias, and have a negative bias relative to the Guenther et al. (1995) isoprene emission estimates (Palmer et al., 2003). There remain a number of differences between GOME and MEGAN-EZ isoprene emission estimates in both the magnitude and the distribution of isoprene emissions, particularly over the Southeast United States (Fig. 11). These discrepancies could be due to a number of unresolved issues with both the model chemistry and MEGAN estimates.

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The HCHO yield from isoprene oxidation has been the subject of only a few studies (e.g., Atkinson and Arey, 2003, and references therein) but the intermediate chemical kinetics are generally thought to be fairly well known at NO<sub>x</sub> levels >1 ppbv, as often experienced over North America. Terpenes, sesquiterpenes, and other highly reactive VOCs emitted by vegetation, also lead to the production of HCHO but current model calculations suggest that they make a relatively small contribution to observed HCHO columns (Palmer et al., 2006). Better quantitative understanding of the HCHO yields from these reactive VOCs is required. Work has begun to assess the role of anthropogenic hydrocarbons on the observed HCHO column signal. Aircraft observations during the Texas Air Quality Study in August–September 2000 (Wert et al., 2003) saw HCHO plumes of 100 km length originating from a number of smoke stacks close to Houston; the primary source of this HCHO was saturated alkenes (Wert et al., 2003). Analysis of GOME data does not show an enhancement over these regions (Martin et al., 2004), possibly due its crude horizontal resolution (320×40 km<sup>2</sup>). However, Martin et al. (2004) found that anthropogenic VOCs play a role in determining HCHO columns over eastern Texas although biogenic VOCs appear to dominate on a regional scale. The role of anthropogenic VOCs in determining HCHO columns is a subject of ongoing work, but taking into account these possible contaminations to the analysis of the observed HCHO columns will not explain the model discrepancy in the observed seasonal variability shown by Fig. 11. It is possible that the GOME data is describing a large-scale stress factor that affects isoprene emissions (e.g., ozone) but is not accounted for by MEGAN-EZ.

Initial studies of GOME HCHO data have focused on North America because there is a relative abundance of in situ observations with which to evaluate the HCHO column data and the methodology used to estimate isoprene emissions (Palmer et al., 2003). Extending this analysis to the rest of the world is clearly desirable but requires careful separation of the biomass burning and anthropogenic contributions to HCHO from the biogenic signal (as discussed above). Taking this difficulty into consideration, Shim et al. conducted Bayesian inversions for 10 biogenic, biomass burning, and industrial

sources over 8 separate continental regions based on GOME HCHO measurements. GEOS-CHEM was used as the forward model. Over the selected inversion regions, isoprene is the major contributor to the observed variability of HCHO columns. They showed that the posteriori isoprene emissions are generally higher at northern mid latitudes but lower in the tropics compared to the Guenther et al. (1995) estimates. The posteriori annual global isoprene emissions are 641 Tg isoprene, slightly higher than MEGAN or Guenther et al. (1995) estimates. The posteriori biomass burning HCHO sources are higher by a factor of 2–4 over the regions with significant biomass burning except for India. The industrial HCHO sources are higher by about 20% except for northern East Asia and India (about 60%). The posteriori uncertainties of isoprene emissions are greatly reduced but are still high at about 90%, reflecting the relatively large uncertainties in GOME retrievals.

## 7. Isoprene emission response to earth system changes

Isoprene emissions are a dynamic part of the earth system and respond to changes in the physical, chemical and biological components of this system. Our current limited understanding of the likely response of isoprene emissions to these changes is based primarily on studies using greenhouse grown plants. Additional studies are needed under realistic growth conditions that include potential synergistic variables. Predictions of future isoprene emissions are very challenging due to the uncertainties in characterizing future physical, chemical and biological variables and the isoprene emission response to each. Potential interactions add additional complications. It is difficult to predict even the sign of the response of isoprene emission to the multiple effects of some driving variables. For example, increasing CO<sub>2</sub> levels may reduce isoprene emission activity (a direct effect) but increase LAI and the abundance of isoprene emitters (indirect effects).

Figure 12 illustrates MEGAN predictions of the response of July average isoprene emissions to past and future changes in PFT distributions, LAI and weather (using the

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databases described in Table 2). Estimates of PFT changes generally indicate that isoprene emissions have increased in the past 50 to 300 years and will decrease over the next 50 to 100 years. This is primarily due to simulated changes in agricultural land use. Future increases in isoprene are predicted for some regions due to climate driven PFT and LAI changes. Future temperature simulations result in a substantial increase in isoprene emissions in most regions. Predicted changes in PPFD result in increased emissions in some regions and decreases in other regions. The MEGAN estimates clearly show that isoprene emissions are sensitive to earth system changes but there are large uncertainties associated with these estimates and it is currently not possible to make robust predictions of future changes in isoprene emissions. The potential importance of the known driving variables is discussed below.

### 7.1. Physical climate: temperature, light, and soil moisture

Physical climate influences isoprene emissions through physiological and ecological processes that operate on different time scales. The relationship between isoprene emission and these driving variables is non-linear and the response depends on canopy structure, climate (e.g., a temperature increase in a warm climate may have a different effect than in a cool climate), and the temporal and spatial pattern of these changes. Isoprene emission can increase non-linearly with increasing PPFD transmission because increasing transmission is accompanied by a decrease in diffuse light which is more effective at penetrating plant canopies. MEGAN isoprene emission estimates increase with increasing leaf temperature which is primarily driven by air temperature but is also influenced by solar radiation, humidity, wind speed and soil moisture. MEGAN isoprene emission estimates are less sensitive to air temperature changes than they would be if the model assumed that leaf temperature is equal to air temperature. This behavior reflects the ability of broadleaf canopies to minimize leaf temperature increases by transpiring. However, this ability is diminished during drought conditions. MEGAN predicts a greater response to long term changes in temperature and PPFD than other models that use only the Guenther et al. (1993) algorithms. Thus

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MEGAN isoprene emission estimates are more sensitive to long-term changes in temperature and PPFD. Model simulations of isoprene emission response to long-term climate variations are difficult to evaluate due to a lack of observational studies that are needed to characterize this behavior. In addition to the direct effects of climate, estimates of long-term changes in isoprene emissions must also consider the indirect effects of climate-driven changes in vegetation. Our ability to predict the response of isoprene to these vegetation changes is limited both by uncertainties in model predictions of these changes and uncertainties in assigning emission factors to the landcover types used in these models.

Previous studies have described the potential sensitivity of isoprene emissions to long-term (centuries) changes in physical climate. Adams et al. (2001) estimate that global isoprene emissions are presently more than a factor of 2 higher than they were during the last glacial maximum. The estimated increase was associated with the direct effect of higher leaf temperature, resulting in a 60% increase in isoprene emissions, and the indirect effect of climate-induced changes in vegetation distributions, resulting in a 40% increase in isoprene emissions. They note that lower BVOC emissions during the last glacial maximum would significantly increase OH which could contribute to the low methane concentrations observed in ice core samples. Several studies have examined the response of global isoprene emission to potential future climate (Turner et al., 1991; Sanderson et al., 2003; Wiedinmyer et al., 2006). Turner et al. predict that climate-induced landcover changes will result in a 25% increase in isoprene emissions while Sanderson et al. and Wiedinmyer et al. predict slight (~5%) decreases in isoprene emission. All three studies predict a much larger (35% to 70%) increase associated with increased temperature. They all assumed a similar isoprene emission response to temperature change so it is likely that the differences in estimated emissions are primarily due to differences in the climate model predictions.

MEGAN simulations using the IMAGE and MAPSS-P PFT databases predict isoprene emission responses to future (year~2100) PFT distributions that range from a 30% decrease with IMAGE to a 6% increase with MAPSS. The difference is proba-

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bly because IMAGE accounts for changes in cropland area while MAPSS does not. MEGAN isoprene emission distributions shown in Fig. 12 demonstrate that these changes vary considerably for different regions. These MEGAN simulations, and the results of previous studies described above, demonstrate that future PFT changes could result in significant isoprene emission variations, especially at regional scales, but it is difficult to even predict whether these PFT changes will result in an increase or decrease in emissions.

Global climate model predictions of future PPFD result in small (~5%) changes in annual global isoprene emissions that range from a small increase (HadCM2) to a small decrease (CSM1). CSM1 estimates of future PPFD resulted in regional isoprene emission changes ranging from about -50% to +50%. The isoprene emission changes associated with HadCM2 PPFD estimates are shown in Fig. 12 and range from -16% to +58%. Solar radiation trends observed at sites in the U.S., China and other locations (e.g., Liepert, 2002; Che et al., 2005) indicate that substantial reductions (>10%) in solar transmission have occurred in many regions in the past four decades. The response of isoprene emission is sensitive to the pattern of solar radiation decrease, i.e. whether there is an increase in the number of overcast days or a change in the transmission on clear days, but Fig. 3 shows that isoprene emission is expected to decrease nearly linearly with solar transmission.

The response of isoprene to future temperature increases is highly dependent on the model and scenario used to predict future temperatures. For a given prediction of future temperature increases, the associated isoprene emission increase predicted by MEGAN is about a factor of 2 higher than what would be predicted by previous studies (e.g. Turner et al., 1991; Sanderson et al., 2003; Wiedinmyer et al., 2006). This is because MEGAN includes algorithms (Eqs. 8 and 9) that account for changes in the temperature of the past 24 to 240 h. As a result, MEGAN predicts that annual global isoprene emissions in the year 2100 could be more than a factor of 2 higher than present day emissions. Isoprene emission increases of more than a factor of 3 are estimated for some regions. PPFD and temperature variations tend to be correlated

which can result in larger increases in isoprene emissions. For example, the HadCM2 simulation predicts a 4% increase in annual global emission due to PPFD alone and a 72% increase due to temperature alone. An increase of 81% is estimated when both PPFD and temperature are considered.

## 5 7.2. Chemical climate: CO<sub>2</sub>, ozone, nitrogen and aerosols

Laboratory and field enclosure measurements have shown that the chemical composition of the atmosphere can influence isoprene emission rates (e.g., Rosenstiel et al., 2003; Velikova et al., 2005). Aerosols in the atmosphere or deposited on leaf surfaces can indirectly influence isoprene emissions by modifying light levels. Atmospheric nitrogen, ozone, and CO<sub>2</sub> concentrations can have both direct and indirect impacts on isoprene emissions. The indirect effects are associated with their ability to influence climate and plant species distributions. The direct effects are related to biochemical and physiological responses.

Isoprene emission from plants can be significantly suppressed by high CO<sub>2</sub> concentrations (Rosenstiel et al., 2003) but minimal decreases have been observed in some field studies (Buckley, 2001; Rapparini et al., 2004). Pegoraro et al. (2004) found that isoprene emission correlates with internal CO<sub>2</sub> concentration which is a function of ambient CO<sub>2</sub> levels and stomatal conductance. A lower stomatal conductance, which occurs with higher vapor pressure deficits and water stress, reduces the internal CO<sub>2</sub> concentration and so can minimize the impact of elevated CO<sub>2</sub> levels on isoprene. This suggests that the elevated CO<sub>2</sub> concentrations that can substantially decrease isoprene emission from well-watered plants will have less of an impact under most field conditions. Elevated CO<sub>2</sub> tends to increase foliar density which can result in an increase in isoprene emission. Centritto et al. (2004) found that the decrease in isoprene per unit leaf area was balanced by an increased leaf area associated with elevated CO<sub>2</sub> levels. However, isoprene emission from most plant canopies is limited by light and not leaf area, so increased foliage will have the greatest impact on isoprene emission from open canopies. Elevated CO<sub>2</sub> concentrations may result in changes in species dis-

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tributions, which can also have a significant impact on landscape average isoprene emission factors. This has the potential to significantly impact isoprene emissions but it is not known how this will affect regional to global scale isoprene emission.

Harley et al. (1994) observed a strong correlation between nitrogen fertilization and isoprene emission from potted plants. This indicates that increased nitrogen availability from fertilizer application or atmospheric deposition could lead to elevated isoprene emissions. Field studies of this phenomenon are needed in order to assess the potential impact on regional or global isoprene emissions.

Large increases in the emission of isoprene have been observed from leaves exposed to short-term elevated ozone levels (Velikova et al., 2005). The response occurs rapidly and persists for hours after ozone levels are reduced. In contrast, Ennis et al. (1990) found that isoprene emission did not respond to long term exposure to elevated ozone. This may indicate that isoprene emissions are not influenced by the long-term average ozone but respond only when plants are exposed to shorter-term ozone concentration fluctuations. The response of isoprene emissions to ozone, and other stresses, is likely complex and a reliable description of this behavior will require a better understanding of the biochemical and physiological processes that control emissions.

### 7.3. Land management: grazing, crops, urbanization, tree plantations and fire suppression

Landscape-scale isoprene emissions are very sensitive to the changes in foliar density and species composition that are a direct or indirect result of land management practices. Examples of practices that have had major impacts on regional isoprene emissions include overgrazing, cropland abandonment and urbanization. Guenther et al. (1999a) examined the response of a subtropical rangeland to overgrazing. They estimate that a shrub invasion associated with overgrazing resulted in a factor of 3 increase in isoprene emissions. Schaab et al. (2000) simulated the response of regional isoprene emissions to cropland-to-woodland conversion in southern France over a 35-

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year period and estimated that regional isoprene emissions increased by a factor of four (~50% increase per decade). The impact of urbanization on isoprene emission is dependent on the landscape that is being converted and by urban tree planting practices. Cities in drier regions tend to have more vegetation than the natural landscape while cities in wetter regions typically have less vegetation than the potential natural state. The recognition that some vegetation has very high VOC emission rates could lead municipal governments to recommend or mandate the planting of vegetation with low isoprene emissions.

Tree plantations represent a small fraction (~5%) of total forest land but they dominate in some regions and the global total is rapidly increasing. The total land area covered by tree plantations has increased by about a factor of 10 in the past century, with much of the increase in the tropics. Landcover inventories (e.g., FAO, Global Forest Resource Assessment 2000, National Forestry Action Plans (NFAP)/Forest Resources Assessment (FRA), FAO <http://www.fao.org/forestry/fo/fra/index.jsp>, 2001) indicate that at least half of this land area is covered by bamboo or trees (e.g., *Eucalyptus*, *Cocos*, *Elaeis*, *Casuarina*, *Picea*, *Populus*, *Salix* and *Platanus*) with high isoprene emissions that are likely to cause a large regional increase (greater than a factor of 10) in isoprene emission. While the impact of this land management activity on global scale emissions is currently minimal, the regional perturbations can be significant.

Fire suppression during the past century has led to large increases in tree foliar density distributions in many regions (e.g., the western United States). Increased foliar density would be expected to increase isoprene emissions but the change in species composition may be equally important. Brown and Smith (2000) summarize the response of various ecosystems to fire and note that large changes in species composition occur with varying fire frequency. Fire resistant species include trees that emit isoprene (e.g., oaks) and those that do not (e.g., pines). The impact of fire suppression on isoprene emission appears to be ecosystem dependent but is likely to result in large changes in most ecosystems.

## 8. Conclusions

Global geographically-referenced estimates of isoprene emission are necessary for characterizing global carbon cycling, distributions of trace gases and aerosols and their radiative forcing, and investigations of regional air quality (Guenther 2002; Geron et al., 1994; Sanderson et al., 2003). The isoprene emission rates recommended in the mid to late 1990s (e.g., Guenther et al., 1995; Pierce et al., 1998) were more than a factor of two greater than those previously used in regional air quality models and global chemistry and transport models (e.g., Zimmerman et al., 1979; Pierce and Waldruff, 1991; Muller, 1992). The higher isoprene emission rates resulted in unrealistically high predictions of boundary layer isoprene and ozone concentrations when they were introduced in some chemistry and transport models (e.g., Houweling et al., 1998). This led to the development of global isoprene emission inventories that were based on the Guenther et al. (1995) geographical and seasonal emission distributions but included a scaling factor to uniformly reduce emissions by 20% or more (e.g., Houweling et al., 1998; Poisson et al., 2000) or reduce isoprene emissions by as much as a factor of three in selected landscapes (Bey et al., 2001). The Intergovernmental Panel on Climate Change (IPCC) Working Group on Atmospheric Chemistry and Greenhouse Gases (Ehhalt and Prather 2001) recommended using a global isoprene emission rate that is 56% lower than the Guenther et al. (1995) estimates. This emission reduction was used to produce chemistry and transport model simulations of CO and isoprene concentrations that were similar to observations. However, the poor model performance could have been due to factors other than isoprene emission rates. For example, deposition rates, chemical oxidation schemes, or boundary layer dynamics could have been responsible. The ability of other models (e.g., Granier et al., 2000; Sanderson et al., 2003) to simulate reasonable distributions of chemical constituents when using annual global isoprene emissions of ~500 Tg carbon (~570 Tg isoprene), indicates that the rates estimated by Guenther et al. (1995) and by MEGAN are not unrealistic. Future improvements in simulations of the relevant chemical, phys-

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ical, and biological processes in global chemistry and transport models may provide stronger constraints on isoprene emissions. At present, these models neither confirm nor disprove the validity of the emission rates estimated by MEGAN. However, top-down emission estimates based on satellite measurements of formaldehyde distributions (see Sect. 6.2) generally agree with the emission rates estimated by MEGAN.

While considerable progress has been made to improve our understanding of the processes controlling isoprene emission rates for some regions and seasons, substantial uncertainties remain. Robust algorithms that accurately predict the response of isoprene emission to long term changes in the physical (e.g., temperature and light) and chemical (e.g., carbon dioxide and ozone) environments are needed and require additional observations. Advances in aircraft regional flux measurement capabilities and top-down remote sensing approaches are improving our ability to constrain regional to global scale isoprene emissions. The isoprene emission calculation methods developed for MEGAN require significant refinement but are suitable for chemistry and transport modeling on regional and global scales.

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**Table 1.** Global average emission factors,  $\varepsilon$  (mg isoprene  $\text{m}^{-2} \text{h}^{-1}$ ), land area ( $10^6 \text{ km}^2$ ) and percent contribution to the annual global isoprene emission associated with each of the six MEGAN plant functional types. The range of land area estimates is based on the PFT databases described in Table 2.

		Broadleaf Trees	Fineleaf Evergreen Trees	Fineleaf Deciduous Trees	Shrubs	Crops	Grass and other
$\varepsilon$ :	Average	12.6	2.0	0.7	10.7	0.09	0.5
	Range	0.1 to 32	0.01–13	0.01–2	0.1 to 30	0.01 to 1	0.004 to 1.2
Land Area:	Average	22.9	14.8	2.7	19.8	17	24.3
	Range	13.4 to 38.5	8.6 to 20.0	1.3 to 3.9	15.6 to 24.4	8 to 36.5	17.2 to 38.6
Annual global emission		54%	4%	0.5%	40%	0.2%	1.1%

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**Table 2.** MEGAN global input databases. Annual global isoprene emissions estimated for alternative (present day) databases are compared (% difference) to the emission estimated with the standard (MEGAN-P, MEGAN-L and MEGAN-W) databases.

Data Type	Name	Spatial Scale	Time Period	Description	Base Data	Global Emission (% difference)	Base Data Reference
PFT	AVHRR1-P	~50 km	~2000	PFT	AVHRR	-7%	Bonan et al. (2002)
PFT	MODIS1-P	~50 km	~2000	PFT	MODIS	+15%	Tian et al. (2004)
PFT	MODIS2	~50 km	~2000	ecosystem	MODIS	+18%	Friedl et al. (2002)
PFT	G95-P	~50 km	~2000	ecosystem	Inventory	+2%	Olson (1992)
PFT	HYDE	~50 km	1700–1990	ecosystem	Model, inventory	-13%	Klein Goldewijk et al. (2001)
PFT	IMAGE	~50 km	2000–2100	ecosystem	Model	-11%	Alcamo et al. (1998)
PFT	MAPPS-P	~50 km	2000, 2100	ecosystem	Model	+24%	Neilson (1995)
PFT	IBIS	~8 km	1992	ecosystem	Model, inventory	+3%	Ramankutty and Foley (1999)
PFT	SPOT	~1 km	~2000	ecosystem	SPOT	-7%	<a href="http://www-gvm.jrc.it/glc2000">http://www-gvm.jrc.it/glc2000</a>
PFT	AVHRR2	~1 km	~2000	land char.	AVHRR	+2%	DeFries (2000); Hansen (2000)
PFT	MODIS3	~1 km	~2000	land char.	AVHRR/MODIS	-0.3%	DeFries (2000); Hansen (2003)
PFT	MEGAN-P	~1 km	2001	land char.	MODIS, inventory	standard case	Kinnee et al. (1997)
LAI	AVHRR1-L	~50 km	~2000	Monthly	AVHRR	-11%	Bonan et al. (2002)
LAI	MODIS1-L	~50 km	~2000	Monthly	MODIS	+12%	Tian et al. (2004)
LAI	AVHRR3	~50 km	1981–2000	Monthly	AVHRR	+25%	Myneni et al. (1997)
LAI	G95-L	~50 km	~2000	Monthly	model, AVHRR	+24%	Guenther et al. (1995)
LAI	MAPSS-L	~50 km	~2000, 2100	Monthly	model	+29%	Neilson (1995)
LAI	MEGAN-L	~1 km	2000–2004	Monthly	MODIS	standard case	Zhang et al. (2004)
Weather	IIASA	~50 km	1960–1990 mean	Hourly	observations	+13%	Leemans and Cramer (1992)
Weather	CRU	~50 km	1900s–1980s	Hourly	observations	-11%	a
Weather	HadCM2	~300 km	1980s, 2080s	Hourly	A1 scenario	+15	b
Weather	CSM1	~300 km	1990s, 2090s	Hourly	A1 scenario	-11%	c
Weather	MEGAN-W	~200 km	1979–2004	Hourly	NCEP obs/model	standard case	d
Weather	MM5	~100 km	2001–2004	Hourly	MM5 obs/model	-14%	Dudhia and Bresch (2002)

<sup>a</sup> [http://ipcc-ddc.cru.uea.ac.uk/obs/get\\_30yr\\_means.html](http://ipcc-ddc.cru.uea.ac.uk/obs/get_30yr_means.html)

<sup>b</sup> [http://ipcc-ddc.cru.uea.ac.uk/sres/hadcm2\\_download/is92/gcm\\_data.html](http://ipcc-ddc.cru.uea.ac.uk/sres/hadcm2_download/is92/gcm_data.html)

<sup>c</sup> <http://www.cesm.ucar.edu/experiments/ccsm1.0/b030.A1/>

<sup>d</sup> NCEP/DOE Reanalysis II. ([http://nomad3.ncep.noaa.gov/ncep\\_data/index.html](http://nomad3.ncep.noaa.gov/ncep_data/index.html))

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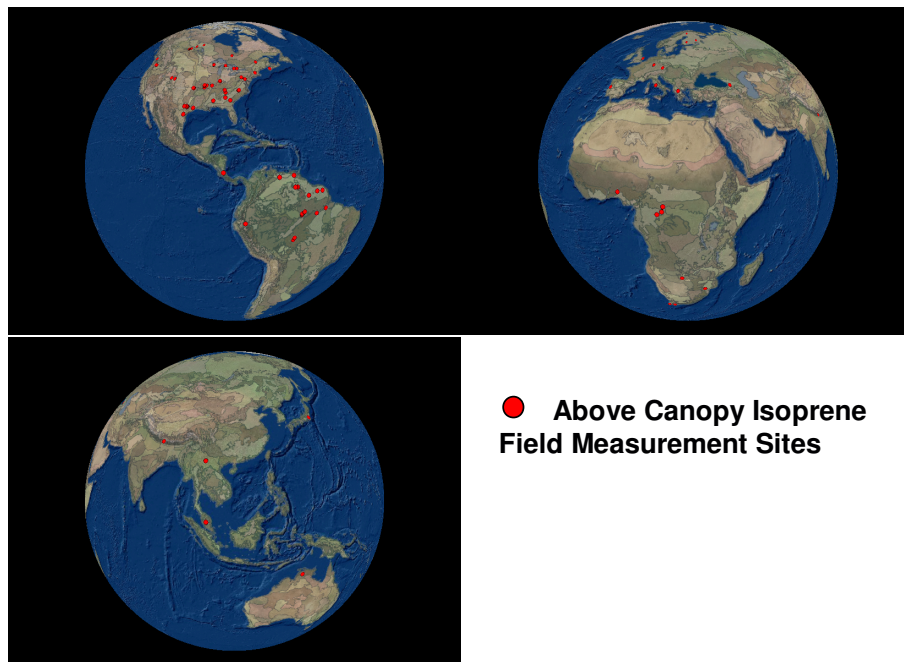
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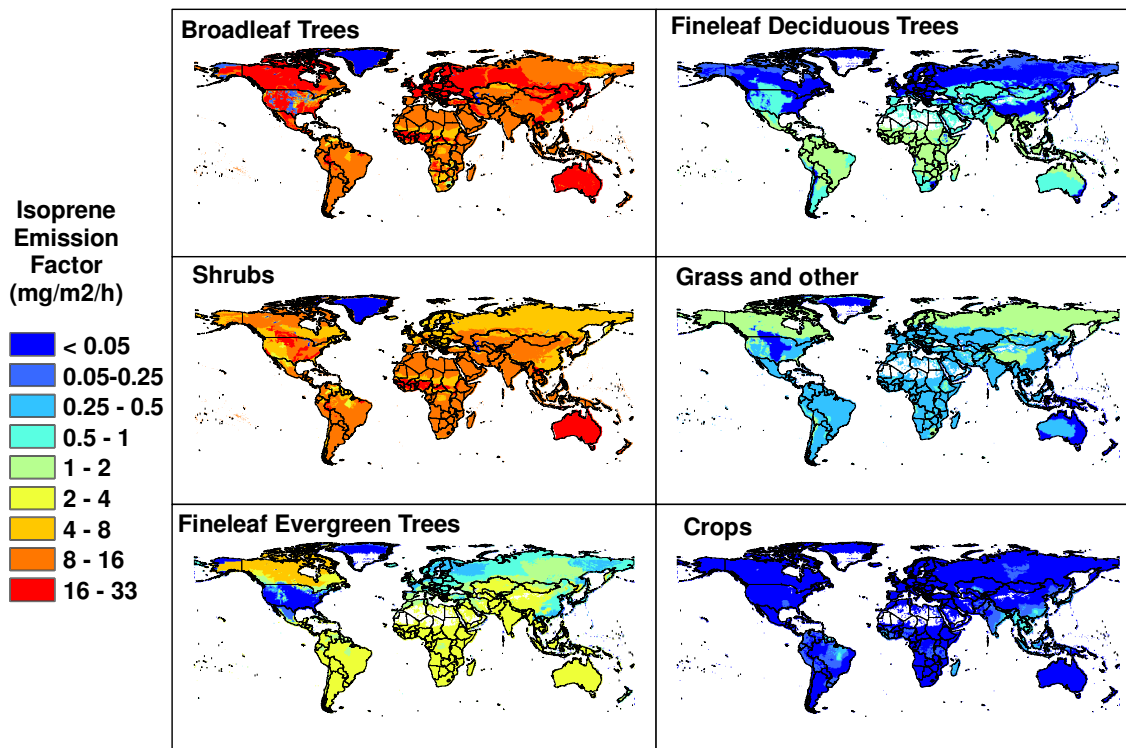
**Fig. 1.** Geographic distribution of Olson et al. (2001) ecoregions and the locations of isoprene field measurement studies used to develop isoprene emission factors.

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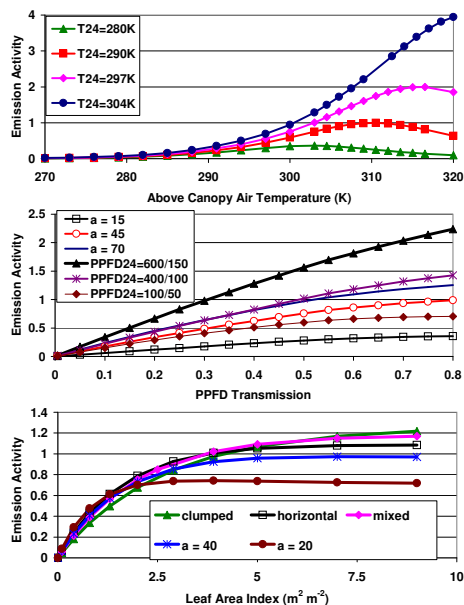
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**Fig. 2.** Global distribution of isoprene emission factors for the six MEGAN PFTs.[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[◀](#)[▶](#)[◀](#)[▶](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Print Version](#)[Interactive Discussion](#)

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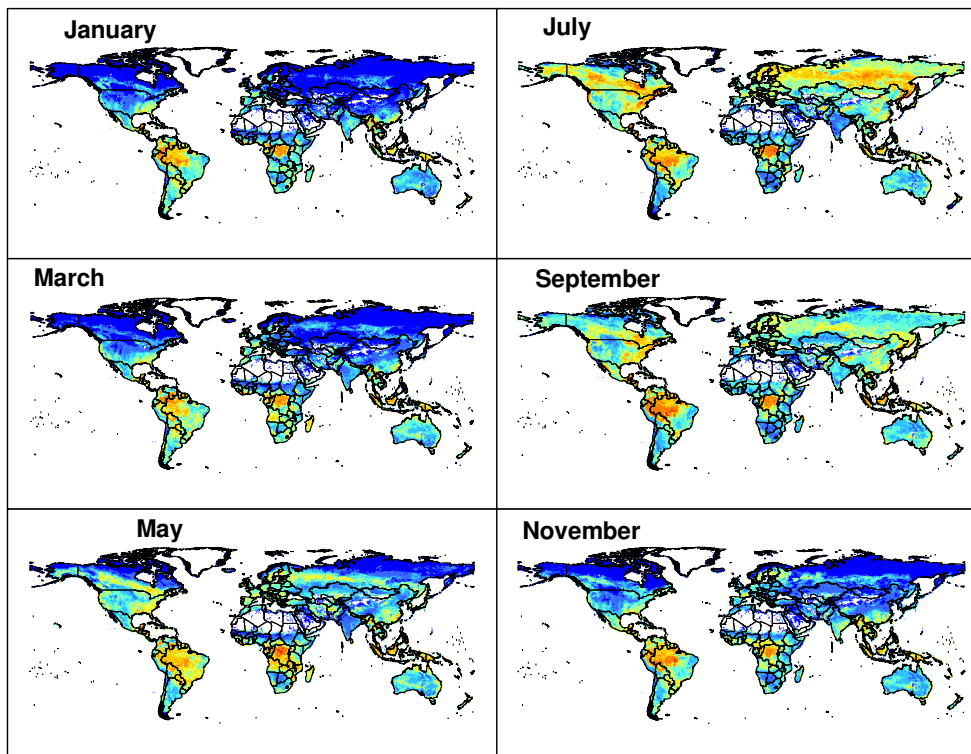
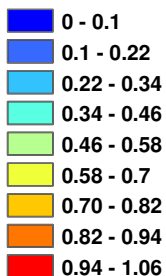
**Fig. 3.** MEGAN estimates of isoprene emission response to current temperature (top), PPFD transmission (middle) and LAI (bottom). The response to current temperature is estimated for leaves exposed to different average temperatures (280 K, 290 K, 297 K and 305 K) during the past 24 to 240 h ( $T_{24}=T_{240}$  in each case). The response to current PPFD transmission is estimated for leaves exposed to different solar angles (15, 45 and 70 degrees) and for average PPFD levels for the past 24 to 240 h ( $PPFD_{24}=PPFD_{240}$  in each case) that include 600 and 150  $\mu\text{mol m}^{-2} \text{s}^{-1}$ , respectively, for sun leaves and shade leaves, 400 and 100  $\mu\text{mol m}^{-2} \text{s}^{-1}$  for sun and shade leaves, and 100 and 50  $\mu\text{mol m}^{-2} \text{s}^{-1}$  for sun and shade leaves. The response to LAI (for a constant PPFD transmission of 60%) is estimated for different canopy leaf orientations (clumped, horizontal and mixed leaves with a solar angle of 60 degrees) and solar angles (20 and 40 degrees with a mixed leaf orientation).

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LAI and  
leaf age  
normalized  
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**Fig. 4.** Monthly normalized isoprene emission rates estimated with MEGAN for 2003. Rates are normalized by the emission estimated for standard LAI ( $=5\text{ m}^2\text{ m}^{-2}$ ) and leaf age (92% mature leaves). These normalized rates illustrate the variations associated with changes in only LAI and leaf age; i.e. all other model drivers are held constant.

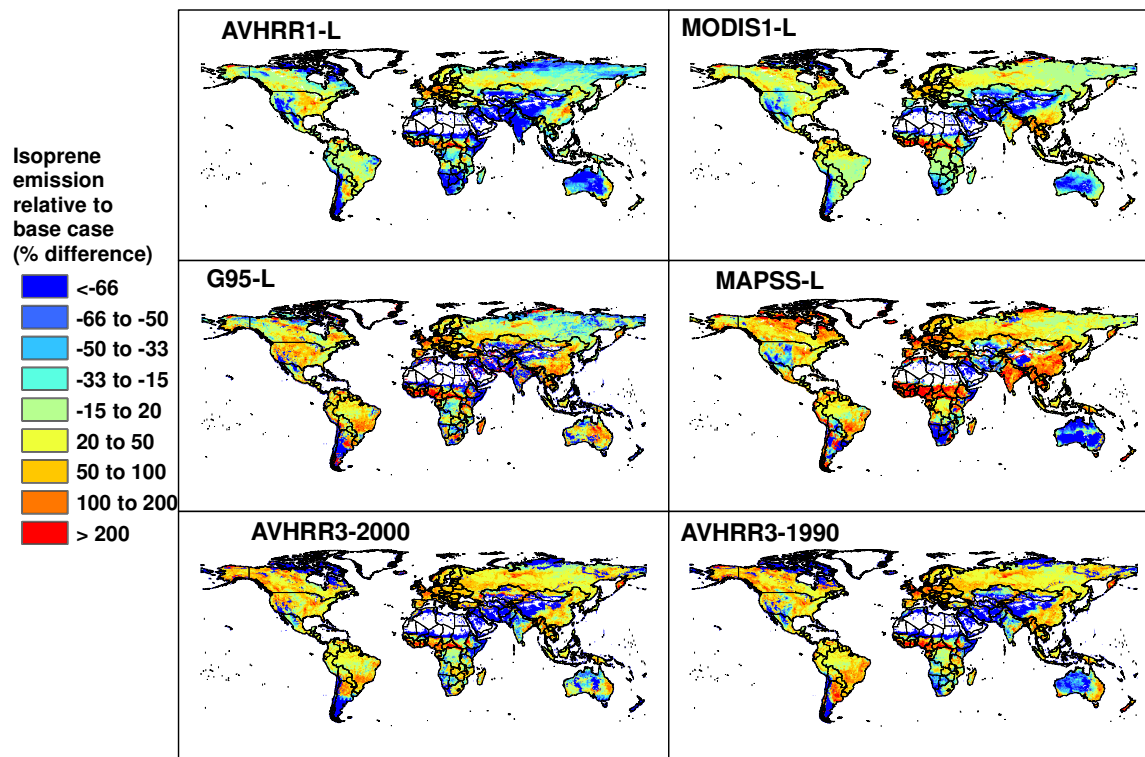
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**Fig. 5.** Percent difference in July 2003 average isoprene emission estimated by MEGAN with the LAI databases described in Table 2 in comparison with the standard MEGAN-L database.

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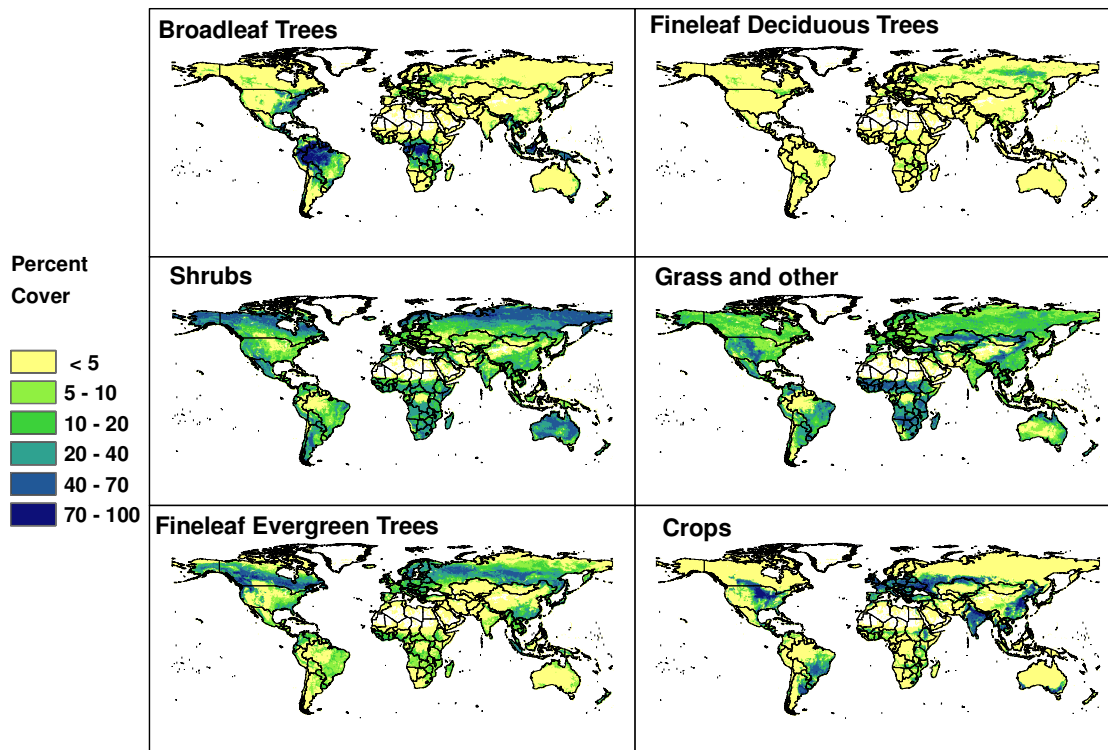
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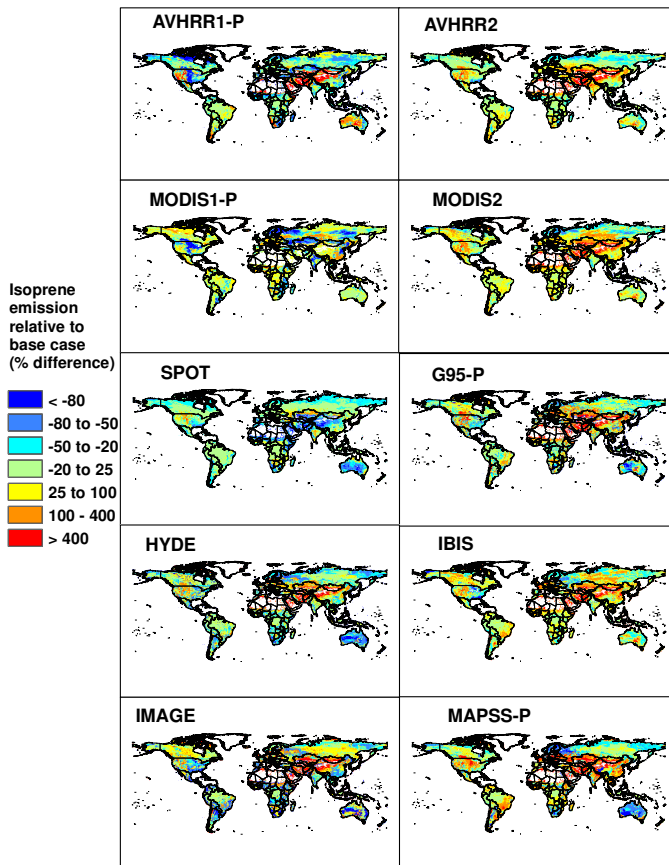
**Fig. 6.** Global distributions of ground cover percentage of each of the six MEGAN PFTs.[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[◀](#)[▶](#)[◀](#)[▶](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Print Version](#)[Interactive Discussion](#)

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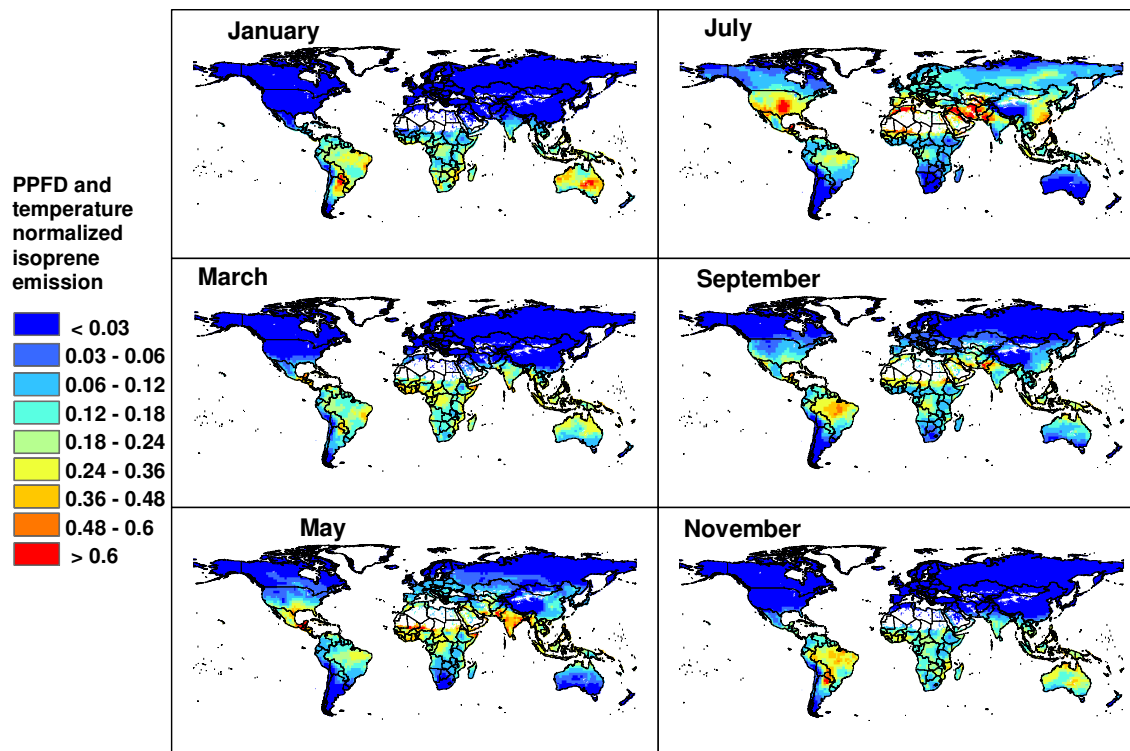
**Fig. 7.** Percent difference in July 2003 average isoprene emission estimated by MEGAN with the PFT databases described in Table 2 in comparison with the standard MEGAN-P database.

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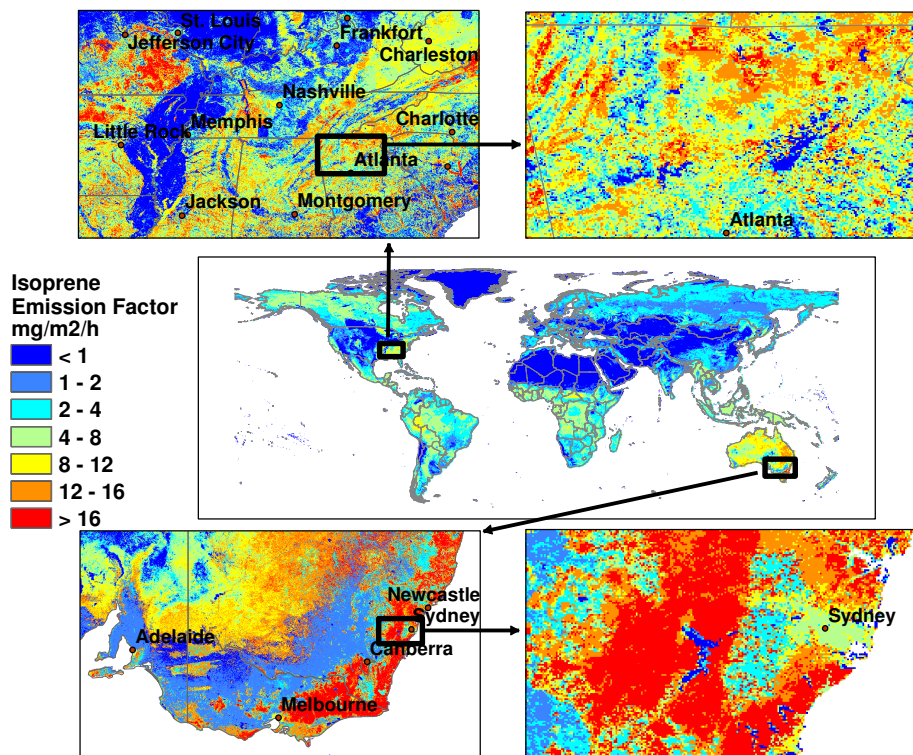
**Fig. 8.** Monthly normalized isoprene emission rates estimated with MEGAN for 2003. Rates are normalized by the emission estimated for standard temperature ( $=303\text{ K}$ ) and PPFD transmission (60%). These normalized rates illustrate the variations associated with changes only in temperature and PPFD transmission; i.e. all other model drivers are held constant.

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**Fig. 9.** Global distribution of landscape-average isoprene emission factors ( $\text{mg}$  isoprene  $\text{m}^{-2} \text{h}^{-1}$ ). Spatial variability at the base resolution ( $\sim 1$  km) is shown by regional images of the southeastern U.S. and southeastern Australia.

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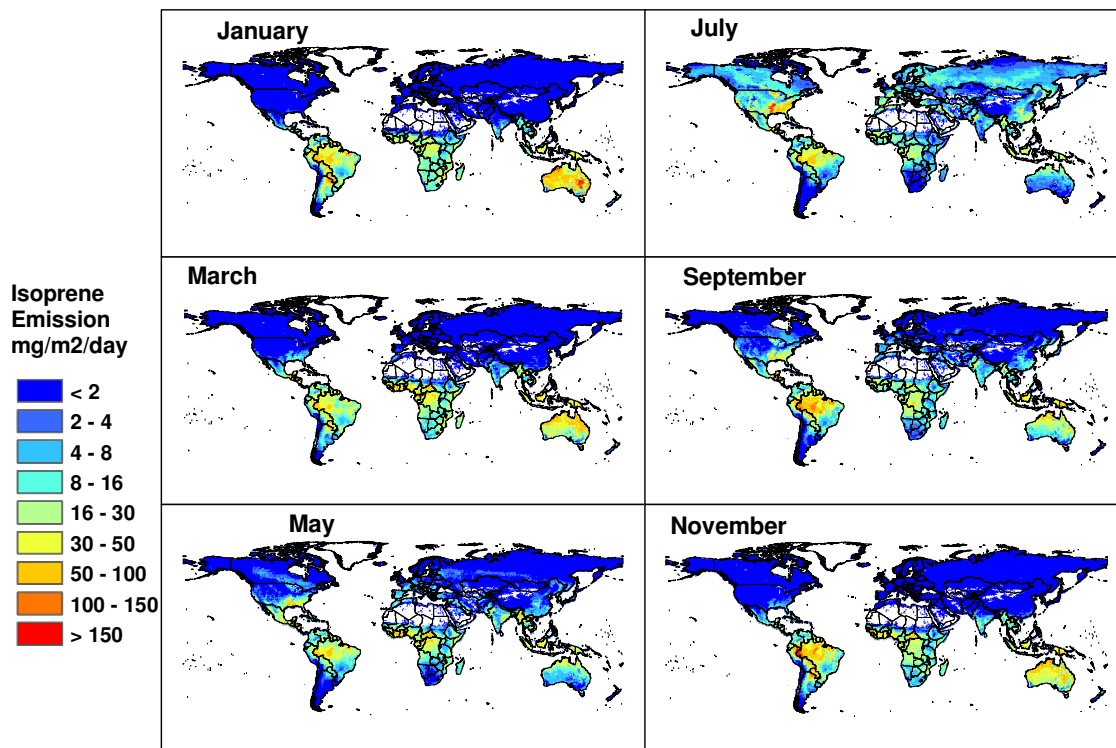
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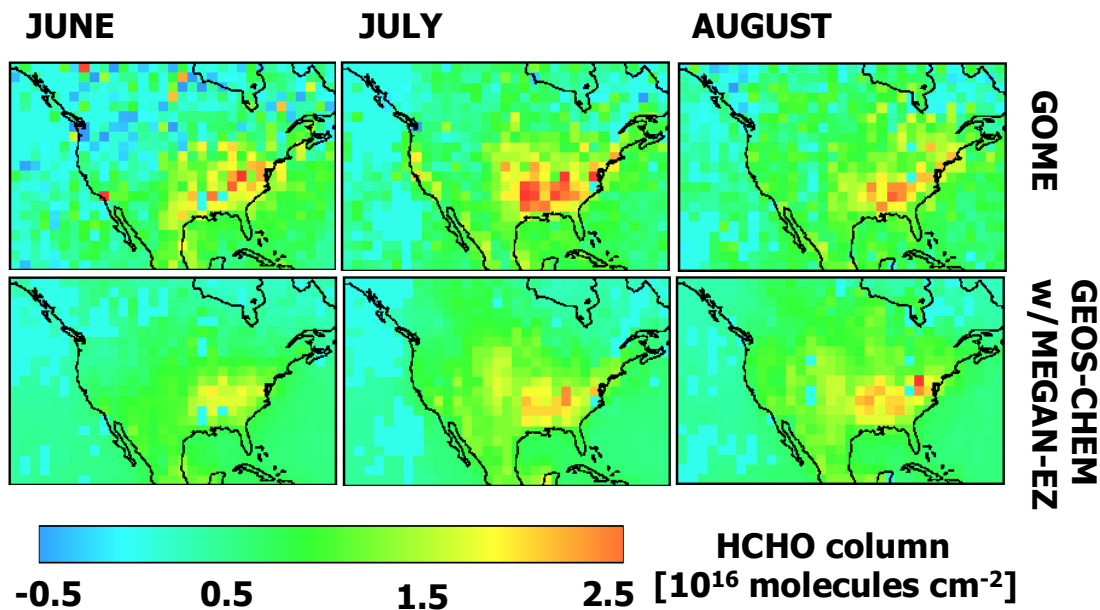
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**Fig. 10.** Monthly average isoprene emission rates estimated with MEGAN for 2003.[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[◀](#)[▶](#)[◀](#)[▶](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Print Version](#)[Interactive Discussion](#)

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**Fig. 11.** Monthly mean HCHO columns over North America for June–August 2001. GOME observed (top panels) and GEOS-CHEM modeled using MEGAN-EZ (bottom panels) vertical columns are shown on a  $2 \times 2.5$  degree grid for 10:00–12:00 LT and for cloud cover  $< 40\%$ .

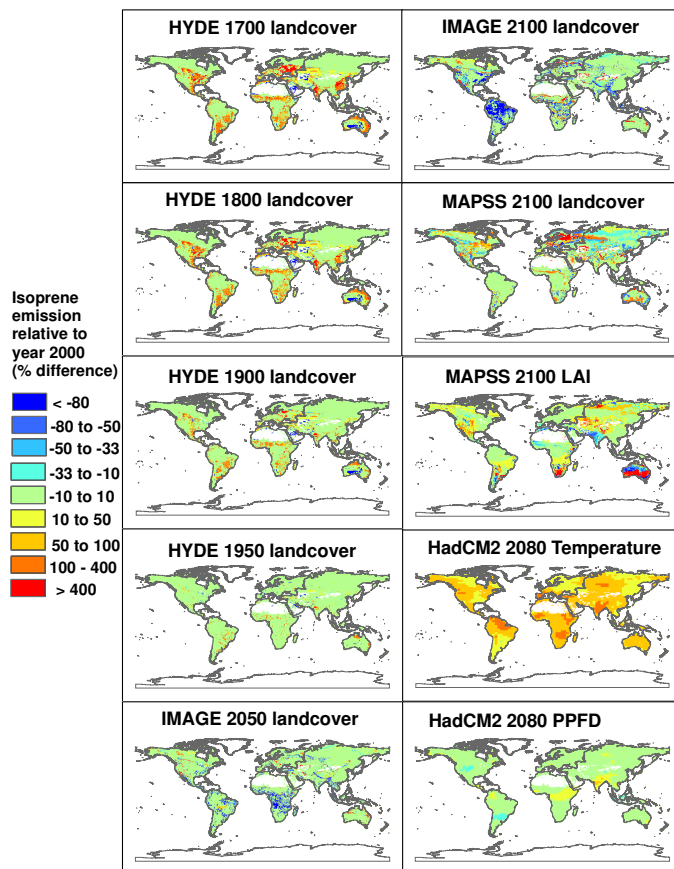
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**Fig. 12.** Percent difference (future/past – present) in July average isoprene emission estimated by MEGAN with past/future databases (Table 2) in comparison with MEGAN present day estimates.

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