Evaluation of two isoprene emission models for use in a long-range air pollution model

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Received: 29 February 2012 – Accepted: 22 March 2012 – Published: 10 April 2012

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

Knowledge about isoprene emissions and concentration distribution is important for chemistry transport models (CTMs), because isoprene acts as a precursor for tropospheric ozone and subsequently affects the atmospheric concentrations of many other atmospheric compounds. Isoprene has a short lifetime, and hence it is very difficult to evaluate its emission estimates against measurements. For this reason, we coupled two isoprene emission models with the Danish Eulerian Hemispheric Model (DEHM), and evaluated the simulated background ozone concentrations based on different models for isoprene emissions. In this research, results of using the two global biogenic emission models; GEIA (Global Emissions Inventory Activity) and MEGAN (the global Model of Emissions of Gases and Aerosols from Nature) are compared and evaluated. The total annual emissions of isoprene for the year 2006 estimated by using MEGAN is 732 Tg yr\(^{-1}\) for an extended area of the Northern Hemisphere, which is 50\% higher than that estimated by using GEIA. The overall feature of the emissions from the two models are quite similar, but significant differences are found mainly in Africa’s savannah and the rain forests of South America, and in some subtropical regions, such as the Middle East, India and the southern part of North America. Differences in spatial distribution of emission factors are found to be a key source of these discrepancies. In spite of the short life-time of isoprene, a direct evaluation of isoprene concentrations using the two biogenic emission models has been made against available measurements in Europe. Results show that the two models in general represent the measurements well and that the CTM is able to simulate isoprene concentrations. Additionally, investigation of ozone concentrations resulting from the two biogenic emission models show that isoprene simulated by MEGAN strongly affects the ozone production in the African savannah; the effect is up to 20\% more than that obtained using GEIA. In contrast, the impact of using GEIA is higher in the Amazon region with more than 15\% higher ozone concentrations compared to that of using MEGAN. Comparing the results for ozone concentrations for Europe obtained by using the two different models
with measurements, show that the MEGAN emission model improves the model performance significantly in the Mediterranean area.

1 Introduction

Volatile organic compounds (VOCs) are important air pollutants that play a central role in the atmospheric chemistry from urban to the global scale. On a global scale, natural emissions of non-methane VOCs (NMVOCs) equal or exceed anthropogenic emissions (Guenther et al., 2000). Guenther et al. (1995) estimated the annual global emissions of biogenic non-methane VOCs (BVOCs) to be 1150 TgC. This value represents about 90% of total NMVOC emissions (Poupkou et al., 2010). BVOCs react with oxides of nitrogen (NOx) in the presence of solar radiation to form various secondary air pollutants, such as ozone. Ozone is not only a pollutant, toxic for human beings and an inhabitant of agricultural products, but also a potent short-lived greenhouse gas in the troposphere. In addition, formation of secondary organic aerosols (SOA) is a process in which BVOCs play a key role (Tsigeridis and Kanakidou, 2003; Glasuis et al., 2000). Besides causing impacts on human health, SOA act as cloud condensation nuclei and influence the radiation balance of the Earth. Among BVOCs, isoprene is the most important species. It is one of the most reactive species with a short atmospheric lifetime of around minutes to hours (Ashworth et al., 2010). Moreover, it is the most abundant of BVOCs in the atmosphere (with total annual emissions equal to that of methane) (Guenther et al., 2006).

Three dimensional chemistry transport models (CTMs) are used to predict ozone concentrations based on emissions of VOCs and NOx. These models can also be used to study the impact of BVOC emissions on atmospheric chemistry. BVOC emissions have been incorporated as off-line static emission inventories into CTMs since the mid-1980s. However, coupling of biogenic emission models with CTMs is required in order to study the interactions between CTMs and surface fluxes of BVOCs. Because BVOC emissions are influenced by the surface conditions and weather, the coupled system
ensures that the BVOC models are forced by the same land-use type and weather as those used in the CTMs (Guenther et al., 2006).

Guenther et al. (1995) developed the global model GEIA on a 1 degree by 1 degree grid for use in global CTMs. On a regional scale, the Biogenic Emissions Inventory System (BEIS/BEIS2/BEIS3) was developed by Pierce et al. (1998). Among recent models, the new global Model of Emissions of Gases and Aerosols from Nature (MEGAN) was developed as the next generation emission model for biogenic emissions of gases and aerosols. It is suitable for regional modeling as well, due to the high spatial resolution (1 km² or 30 s latitude by 30 s longitude) database for emission factors (EF) and land cover distribution (Guenther et al., 2006).

During the last decade, several studies have been carried out to investigate the impact of isoprene on tropospheric ozone concentrations by incorporating BVOC models into CTMs (Steiner et al., 2008; Pfister et al., 2008; Bao et al., 2010; Souza et al., 2010). Im et al. (2011) simulated an enhancement of ozone concentration in the Greater Istanbul Area up to 25 ppb due to BNMVOC emissions. They also showed that the BNMVOC emissions are critical in the performance of the photochemical ozone modeling, and that the VOC/NOₓ ratio almost doubled due to the addition of BNMVOCs. The significant contribution of isoprene to atmospheric chemical budgets has also been confirmed in the recent modeling studies by using MEGAN as BVOC emission model on regional (Geng et al., 2011) and global scales (Pfister et al., 2008). Uncertainties in the isoprene emission inventories, modeling of chemical pathways and ambient NOₓ abundance accompany the modeling studies of isoprene impacts on atmospheric chemistry (Curci et al., 2009). For better prediction of the occurrence of atmospheric chemical compounds due to isoprene, particularly of ground-level ozone, it is necessary to implement more accurately calculated emissions from BVOC models in CTMs. Pouliot and Pierce (2009) summarized the differences in the isoprene algorithms of BEIS3 and MEGAN as a first step to use MEGAN in the CMAQ modelling system. They demonstrated substantial differences in all components of the algorithms, which resulted in 53% difference in the annual estimates of isoprene emissions over North
A number of studies have compared MEGAN with other BVOC models on regional scale; e.g. with BEIS in the US (Wiedinmyer et al., 2008; Poulolot, 2008; Lam et al., 2011) and e.g. with semi-empirical emission module (seBVOC) and Biogenic Emission Model (BEM) in Europe (Steinbrecher et al., 2009; Poupkou et al., 2010).

A number of studies have also been conducted to evaluate results of the integrated BVOC models e.g. MEGAN in air quality models with satellite, aircraft or ground-base observations (Geng et al., 2011; Steiner et al., 2008; Müller et al., 2008). Baker (2007), for example, evaluates the performance of two slightly different versions of BIOME, which is a combination of BEIS3 and GloBEIS (Guenther et al., 2000), and MEGAN using the CAMx4 model to capture high ozone episodes in the Midwest of the United States. Results show, compared to BIOME, MEGAN isoprene emissions improve CAMx4 simulation of high ozone. On the other hand, Warneke et al. (2010) demonstrate that MEGAN emissions are in most cases higher than those determined from the measurements (using isoprene airborne data of the Eastern United States). Such studies allow a detailed comparison and evaluation of MEGAN versus observations, but they are on regional scale and in the USA only. Over Europe, the isoprene emission estimated by MEGAN has been compared with that estimated by other biogenic emission models (e.g., Poupkou et al., 2010), but not evaluated with observations. On the other hand, an algorithm, developed based on the GEIA parameterization, was compared with a specific model described by Steinbrecher et al. (2009), and evaluated using the CHIMERE CTM model with ground-level ozone observations (Curci et al., 2009).

Up until now, none of the studies have addressed the comparison and evaluation of the MEGAN and GEIA global models with focus on sources of difference on the large (hemispheric) scale. On the other hand, because GEIA and MEGAN have been widely used in air quality models, the importance of evaluating these biogenic algorithms used in CTMs has been certainly recognised. In the present work, we focus our attention on the comparison and evaluation of these two global models with background ozone measurements using a long-range air pollution model covering the Northern America.
Hemisphere. Section 2 describes the biogenic models and the CTM used in this study. Results of simulations, comparisons and evaluations are showed and discussed in Sect. 3. Section 4 highlights the concluding remarks and an outlook for future studies.

2 Model descriptions

2.1 The DEHM chemistry-transport model

The model used in this study is the Danish Eulerian Hemispheric Model (DEHM), which is a 3-D large-scale Eulerian atmospheric chemistry transport model. The model has been applied in several long-range transport air pollution studies, covering most of the Northern Hemisphere (see e.g., Christensen, 1997; Hedegaard et al., 2011; Brandt et al., 2012), with a two-way nesting capability to obtain higher resolution over limited areas (Frohn et al., 2002). The model is defined on a polar stereographic projection true at 60° N and applied with two domains – a mother domain with a resolution of 150 × 150 km and a nested domain covering Europe with a resolution of 50 × 50 km. The model includes 29 irregular vertical layers extending to the 100 hPa pressure level in a sigma-coordinate system. It is designed to simulate both the gaseous and the aerosol phases, presently including 67 different species with 122 chemical reactions.

Most of emissions are derived from a combined dataset, which includes 1) EDGAR2000 Fast track and GEIA with a 1 × 1° resolution for the Northern Hemispheric domain; and 2) EMEP with a 50 × 50 km resolution for Europe. In DEHM, natural emissions from wildfires are included based on Schultz et al. (2008). Natural emissions of NOx from soil and lightning and Black Carbon, mainly from biomass burning, are based on the GEIA database. Biogenic emissions of isoprene are described in the following subsection.

The chemical scheme used in DEHM is based on the explicit approach of Strand and Hov (1994). The scheme has been extended by updating several original photolysis as well as the inorganic and organic chemistry rates. Furthermore, several reactions
concerning particulate sulphate and a detailed description of the ammonia chemistry have been included to improve the origin chemical scheme in the model. The chemical scheme of isoprene oxidation with OH and NO$_3$ in DEHM is described by Frohn (2004).

The required meteorological inputs are provided by the mesoscale meteorological model MM5v3.7 (Grell et al., 1994) and defined on the same domains and resolutions as in DEHM. The National Centers for Environmental Prediction (NCEP) Final Analyses (FNL) data ($1 \times 1^\circ$ spatial and 6 h temporal resolution) have been used to provide the initial and boundary conditions required by the MM5 (http://dss.ucar.edu/datasets/ds083.2/).

2.2 Isoprene emission models

In this section, a brief description of the two BVOC models used in this study is presented and the differences between these isoprene algorithms are summarized.

In the last version of DEHM, isoprene emissions are calculated online based on the GEIA biogenic emission model as described by Guenther et al. (1995). The algorithm simulates the light and temperature dependency of isoprene emissions and estimates the flux of isoprene from vegetation given by

$$F = E D \gamma$$

where $E$ is an ecosystem dependent emission factor ($\mu$g C g$^{-1}$ dry mass h$^{-1}$), which represents the rate of isoprene emission at standard conditions; $D$ is the foliar density (g dry mass m$^{-2}$ ground); $\gamma$ is a non-dimensional activity factor that takes into account the effects of temperature and photo-synthetically active radiation (PAR) (Guenther et al., 1995). For each grid cell within the model domain, the total flux of isoprene is calculated as the sum of emissions from each ecosystem within that cell. Each area of the Earth’s land surface is assigned by one of 59 different ecosystem types with a resolution of $0.5 \times 0.5^\circ$ that are compiled by Olson (1992).

Alternatively, isoprene emissions have been calculated with MEGAN v2.04 that implements the empirical algorithm PCEEA presented by Guenther et al. (2006). The
algorithm for modeling isoprene emission in MEGAN is based on empirical relationships between key drivers and emission as in GEIA, while the model is extended to include more processes that control emissions. The standard conditions for the emission factors in MEGAN include not only air temperature and radiation (as in GEIA), but also leaf area index (LAI), foliage age, solar angle, relative humidity, wind speed, soil moisture, and past weather conditions (Guenther et al., 2006; Arneth et al., 2008). MEGAN includes, for instance, short- to long-term weather history to account for the seasonal cycle of the emissions. It has also several significant improvements to account for the influences of leaf age, CO$_2$ concentration, soil moisture, and within-canopy variation in light and temperature. Moreover, the model estimates the net emission to the atmosphere and includes a term to account for variations in canopy production and loss of isoprene. This study neglects the impact of soil moisture and any loss of isoprene in the canopy. One of the differences between MEGAN and GEIA model is in the treatment of plant species area coverage. In GEIA, plant species are mostly treated explicitly and grouped into 59 different ecosystems, whereas MEGAN uses a suite of six plant functional types (PFTs): broadleaf tree, needle leaf evergreen tree, needle leaf deciduous tree, shrub, crop and grass. In this study, we use the MEGAN v2.04 dataset, which comprises the geographical distribution of both the fractional cover and the standard emission factor of the six PFTs. These parameters as well as the leaf area index were all supplied by the National Center for Atmospheric Research (http://cdp.ucar.edu/). These monthly LAI datasets are used as the driving land cover variables for MEGAN to estimate the response of emissions to temporal variations in leaf age and LAI. Monthly LAI data, averaged over the fraction of land area covered by vegetation, is needed for the months of the model simulation and the preceding month.

We have applied the MEGAN and GEIA models with temperature and cloud cover variables generated by MM5v3.7 on the same domain and grid configuration, i.e. the projection and grid size as in DEHM. In order to compare the results of these two BVOC models, the isoprene emissions have been calculated for the last decade (1999–2009). Here, we focus on 2006 as an example thus allowing comparison to be made
between the results of this study and emission estimates previously reported by Guen-
ther et al. (2006).

2.3 EMEP measuring network

In order to evaluate the DEHM model performance with different isoprene emission
inventories, comparisons have been made using observations of isoprene and ozone
concentrations. The observations used for this evaluation originates from the EMEP
measuring network, which includes a large number of chemical components. Details
about the measurement period and the location of the measuring sites are presented
in Hedegaard et al. (2008).

3 Results

3.1 Evaluation of isoprene emissions and driving factors

The MEGAN and GEIA platforms have been used to estimate grid-based emissions
on an hourly time scale for an extended area of the Northern Hemispheric for the year
2006. The total annual isoprene emission in the study area estimated using MEGAN
is 732 Tgyr\(^{-1}\), which is higher than the 488 Tgyr\(^{-1}\) isoprene emission estimated by
GEIA. Our estimated emissions are within the range of about 460–770 Tgyr\(^{-1}\) reported
in previous studies (Guenther et al., 2006; Arneth et al., 2008; Ashworth et al., 2010).
Ashworth et al. (2010) have pointed out that the MEGAN estimates of total annual
isoprene emissions increase with the temporal resolution of the input weather data
and recommended using the highest possible temporal resolution. As the temperature
and radiation data from MM5 used for running MEGAN is based on hourly data in the
present study, the estimated isoprene emission is close to the higher end of previously
reported values.

The spatial distribution of total annual isoprene emissions calculated with MEGAN
and GEIA are shown in Fig. 1, together with their absolute differences. Both models
estimate the largest isoprene emissions in the tropics. These are obtained from a combination of warm temperatures, high levels of radiation and higher foliar density (Arnhet al., 2011). Temperate regions in South-Eastern United States have high fluxes throughout the summertime. As shown in the figure, largest differences emerge clearly over African savannah and subtropical regions, such as the Middle East and India.

In Fig. 2, daily isoprene emissions are displayed for 2006. Peak emission rates occur in the summer months when the two driving forces, i.e. temperature and solar radiation, are highest. The MEGAN estimation shows a stronger seasonality compared to GEIA. The discrepancies between GEIA and MEGAN estimates of monthly isoprene emissions vary from 25% in wintertime up to 40% in summer season. The stronger seasonality in MEGAN emissions can be attributed to the influence of the past weather conditions in the MEGAN algorithm (Guenther et al., 2006; Arnhet al., 2008). Different parameterizations, different land cover data, and/or different emission factors might have contributed to the differences observed between the MEGAN and GEIA estimations. For instance, Fig. 3 shows the GEIA and MEGAN emission factors; emission rates at standard conditions of 303 K and 1500 µmol m$^{-2}$ s$^{-1}$ at the top of the canopy. In GEIA, All ecosystem types were assigned with one of the five values of emission factors given in Guenther et al. (1995) and summed to estimate the total emission for a location, while MEGAN uses an approach that accounts for geographic variations in the emission factors attributed to each PFT. Comparison of these maps with corresponding emission rates in Fig. 1 indicates that the differences between GEIA and MEGAN are primarily from the use of different base emission factors. To confirm this hypothesis, we carried out MEGAN simulations with an alternative emission factor scheme. This alternative includes a single isoprene EF for each PFT based on the approach used in GEIA (Fig. 4). This scheme introduces different distributions for both emission factors (Fig. 4a) and emission rates (Fig. 4b) compared to Figs. 3 (top right) and 1 (top right), respectively. It is apparent that even in the same model (MEGAN), the differences between emission rate distributions are mainly due to different corresponding emission factor maps. As Guenther et al. (2006) pointed out the estimated
emissions using a constant emission factor for each PFT (like the approach used in Fig. 4) lead to significant errors; we have used the standard MEGAN emission factor scheme in the following.

Figure 5 shows the distribution of isoprene emission rates calculated by the models for summer (JJA) and winter (DJF) in 2006. The discrepancy of the emission rate distributions in tropical Savannah is more apparent in winter than in summer. As already noted by Guenther et al. (2006), accounting for the soil moisture stress factor significantly reduces the emissions in regions having dry season with little rainfall but high annual precipitations (e.g. the African savannah). In this study, the effect of soil moisture is not included, which can reduce the emission up to one order of magnitude (Müller et al., 2008). Hence, MEGAN estimates higher emissions in the dry season in the subtropical Africa and tropical savannah. In addition, Fig. 6 shows the temperature pattern, used as a driving variable in the emission models, for 2006. The highest temperatures are found over the subtropics (e.g., Middle East and north of India) and African savannah in the summer. On the other hand, MEGAN has a larger sensitivity of isoprene emission to the climate inputs compared with GEIA (not shown). This is why MEGAN estimates considerable emissions in these regions in the summer. Moreover, the global distribution of each PFT in the MEGAN database, given by Guenther et al. (2006), shows that these regions are covered mostly by shrubs, which are associated with relatively higher emission factors.

3.2 Evaluation of isoprene concentrations

In this subsection, we present results of implementing MEGAN and GEIA into DEHM for online calculation of the isoprene emissions and evaluation the DEHM simulations with measurements.

Figure 7 shows the spatial distributions of the annual isoprene concentrations in the lowest model layer using MEGAN and GEIA for the year 2006. Due to the short atmospheric lifetime (around 0.5–2 h), isoprene cannot be transported far from its sources. Therefore, it is reasonable to assume that the spatial distribution of isoprene
concentrations is similar to that of the corresponding emissions. The highest concentrations, with values up to 4 ppbV, occur similarly in the tropics, where the largest isoprene emissions have been obtained by both models. However, the additional isoprene emissions (2–3 times higher) in MEGAN strongly affect the concentrations in the African savannah and the south-eastern part of the United States. It is apparent that the discrepancies of the emission distributions result in differences between the isoprene concentration simulations of the two models.

Hourly isoprene concentrations simulated using DEHM are compared with isoprene measurements from the EMEP network (http://www.nilu.no/projects/ccc/emepdata.html). The available observed data for year 2006 are obtained from 9 stations in Europe located in Germany, France, Czech Republic and Switzerland. The number of stations with available isoprene measurements is quite small and cannot constitute the basis for a full scale evaluation; however, the results can give an indication of whether the model simulations are in the right order of magnitude. Also, for one of the stations (Rigi, Switzerland), the time variation can be evaluated. Table 1 shows the comparison between mean observed and mean simulated isoprene concentrations using GEIA and MEGAN. Taking into account the very short lifetime of isoprene, the results based on both models are in an acceptable agreement with observations; the agreement is within a factor of two for several stations. The mean isoprene concentrations based on MEGAN simulations tend to be more consistent with in situ measurements than those based on GEIA. The numbers of valid measurements for each station, during the period of study are also shown in the table. The data are infrequent, making an accurate analysis and comparison of measurements from the different sites very difficult. The Rigi station in Switzerland is the only station for which continuous measurements (3 h) are available. In other stations, samples were acquired twice a week. The measured 3-hourly and daily isoprene concentrations for the Rigi station are compared with those calculated using MEGAN and GEIA, in Fig. 8. Simulations of both models agree well with the measurements. As shown in Table 1, MEGAN results have a very small difference from observed mean values. The results are in agreement with
Poupkou et al. (2010) concluding an average level of uncertainty within a factor of 4 for isoprene estimations in Europe. This indicates that the emission models may be used to produce representative isoprene emission in the European region. It should also be emphasized that the relatively coarse spatial resolution applied in DEHM in these simulations (50 × 50 km for Europe) is not able to represent the high spatio-temporal variation in the isoprene concentrations. Due to the coarse resolution, the model cannot take into account effects from local sources. The isoprene concentrations can easily vary by a factor of 4 or more within the individual grid cells. However, the purpose of the evaluation of isoprene concentrations in the present study is to examine whether the model results are in the right order of magnitude.

3.3 Evaluation of ozone concentrations

Due to the scarcity of isoprene measurements and its short lifetime, we have also evaluated the DEHM simulations of ozone concentrations, in order to check possible benefits in using the newly developed MEGAN compared to GEIA. We first study the simulated impact of isoprene on ozone concentrations in the lowest model layer, and then evaluate background ozone values against the measurements in Europe.

Biogenic isoprene is one of the key ozone precursors due to the oxidation by hydroxyl radical and nitrate proxy radical in the areas of high anthropogenic emissions. The gas phase chemistry of isoprene and its by-products in the DEHM model are presented by Frohn (2004). Hedegaard et al. (2011) discussed the main photochemical processes involved in the formation of tropospheric ozone.

Figure 9 shows the contributions of isoprene to the ozone concentrations based on the two different models for biogenic emissions. These results are also compared with the case of running the model without the biogenic emissions to qualify the contributions from BVOC to the ozone levels in general. The model results show that the highest ozone concentrations occur over industrial or high NOx emission regions where they coincide with biogenic emission or biomass burning regions with high isoprene emissions. This can explain the higher ozone concentrations in South-Eastern USA, African
savannah, and large parts of Asia (e.g., tropical regions) with a maximum annual value of more than 60 ppbV over the densely populated areas.

The comparison of the results based on the two BVOC models with the model results where the biogenic isoprene emissions are set to zero (non-isoprene) demonstrates that isoprene has a significant impact on the ozone concentrations over land. The BVOC contribution to ozone formation is more than 40% in the tropics. Adding biogenic isoprene with MEGAN also leads to an enhancement of ozone production at several locations in the subtropics with up to 35% and 20% in the South-Eastern USA and in the Mediterranean region, respectively. The differences in impacts on ozone between MEGAN and GEIA are largely consistent with the differences in their isoprene emissions (see Fig. 1).

As mentioned earlier, compared to GEIA, MEGAN estimates higher isoprene emission by a factor of 2 in the African savannah, where the additional isoprene increases the ozone production by up to 20%. In contrast, the isoprene emission by GEIA is higher than that of MEGAN in the Amazon region. This results in a higher ozone concentration of around 15% by GEIA compared to MEGAN in the Amazon. At higher latitudes, the ozone concentrations simulated using the two biogenic models are quite similar (in the range of 25–30 ppbV). Generally, isoprene has less impact on ozone at higher latitudes. In Europe, the simulated effect of isoprene on ozone by MEGAN is up to 20% more than that by GEIA in the Mediterranean region, where some of the most effective isoprene emitters exist. The difference between the two models decreases toward higher latitudes and declines to 5% in the Scandinavian countries.

The DEHM model has been run for the Northern Hemisphere with a two-way nested domain covering Europe (with a resolution of 50 × 50 km). This enables a thorough evaluation of the ozone concentrations based on the two BVOC emission models against measurements over Europe. In Fig. 10, the annual mean concentrations for Europe are displayed. At higher latitudes, the ozone production is less influenced by the isoprene emission, and hence the ozone concentrations simulated by both models are within the range of 30–35 ppbV, e.g., in Central Europe, Great Britain and the Scandinavian
countries. At lower latitudes, especially over the Mediterranean countries (Portugal, Cyprus, Spain, Italy, Southern France and Greece), where the land is covered by high isoprene emitting trees such Oak, Eucalyptus and Macchia (Steinbrecher et al., 2009), the ozone concentration increases to 35–45 ppbV. Compared to GEIA, MEGAN results in up to 10 ppbV higher ozone concentrations throughout the Mediterranean Sea and the Mediterranean countries. Higher emission of precursors, higher solar radiation, higher temperatures, and a longer growing season of vegetation may all contribute in the higher ozone concentrations in Southern Europe. Furthermore, the much lower rate of dry deposition to water surfaces may be the reason for higher ozone concentrations over the sea. Maximum efficiency near populated and industrialized areas with large NOx emissions may also be responsible for the enhanced build-up of ozone in the Mediterranean region.

In order to evaluate the indirect effect of using the two different BVOC models, the model simulations of annual mean values of daily maximum ozone concentration for the year 2006 are plotted against measurements obtained from 117 European rural background monitoring sites in Fig. 11. The performance of DEHM is evaluated using the Pearson correlation coefficient and the fractional bias (FB) (see Fig. 11). Results show that DEHM in general performs better using with MEGAN (correlation = 0.70; FB = −0.03) than with GEIA (correlation = 0.67; FB = −0.10). The standard deviation of the simulated ozone using DEHM/MEGAN is also closer to that of observations. We can conclude from the results that both emission models produce good isoprene estimates on the European scale.

Figure 10 showed that in the Mediterranean region the simulated mean ozone concentration by DEHM was higher using the MEGAN model than that using the GEIA model. We now compare the daily maxima of ozone concentration in the year 2006 simulated using the two BVOC models with observations at all sites in the region in order to assess the isoprene emission by the two models. Table 2 summarizes the comparison statistics for 13 stations in Italy, France, Spain, Portugal and Cyprus. As seen in the table, the DEHM model based on MEGAN outperforms (much higher correlation
coefficients and smaller FBs) that based on GEIA at all stations in the Mediterranean, implying that MEGAN estimation of isoprene emission is closer to reality.

As an example of the improved performance of DEHM using MEGAN compared to GEIA, time series of modelled and measured ozone concentrations at two background monitoring sites in Spain (Viznar; 37.23° N, −3.53° E) and Southern France (Iraty; 43.03° N, −1.08° E) are shown in Fig. 12. The results are given for daily means, hourly values and daily maxima of ozone concentrations for the year 2006. The GEIA-based simulations of daily mean \( O_3 \) and daily maxima \( O_3 \) show relatively high correlation with the measurements in both Viznar (0.72 and 0.75, respectively) and Iraty (0.59 and 0.73, respectively). However, the model highly underestimates the mean ozone concentration by around 33% in Viznar and 34% in Iraty, and is unable to capture the large daily maximum values observed. The corresponding correlation coefficients using the MEGAN model are increased to, respectively, 0.86 and 0.88 in Viznar and 0.66 and 0.79 in Iraty. DEHM still underestimates the mean ozone concentration, but using MEGAN decreases the fractional bias to 18% in Viznar and only 27% in Iraty. The better performance using MEGAN can be attributed to a better parameterisation of environmental activity factors or more accurate emission factors in MEGAN.

4 Conclusions and outlook

In this paper, a comparison and evaluation of isoprene emissions estimated by the MEGAN and GEIA models has been carried out. The overall goal of the work is to address the issue of better algorithms for biogenic emissions for integrating and application into CTMs on a large scale. In general, the differences in the algorithms result in a 50% difference in the annual estimate of isoprene emissions in the study area covering the Northern Hemisphere. Differences between the two models are present in both the description of model processes and the environmental factors. We found that the single most important parameter is the PFT emission factors, since emission rates depend linearly on these values.
Isoprene measurements for the year 2006 in Europe were used to perform a direct evaluation of the two biogenic emission models coupled in DEHM. Overall, a good agreement with the available measurement was found for both modelled results. However, we found that the model results for isoprene using the MEGAN model performed better and had an agreement in the mean observed values better than GEIA. Due to the scarcity of observed isoprene data and the short lifetime of isoprene (making it difficult to compare with a large scale model), an indirect evaluation was made based on measurements of ozone concentration in Europe. Large differences were found between the two models results where the results based on isoprene emissions from MEGAN gave up to 20% higher concentrations of ozone in the Mediterranean area. Two DEHM simulations based on the two different isoprene emission models were evaluated against measurements at 117 rural background monitoring sites in Europe. We found that the performance of the DEHM model based on the MEGAN model improved significantly with respect to ozone in Europe, particularly in the Mediterranean area.

In general, the results of our study, point out the potentially high impact of isoprene on the atmospheric composition and the need for further measurements of isoprene for better evaluations of the emissions and the modelled concentrations of isoprene, especially in the sub-tropical and tropical regions. Future work will be devoted to evaluate the DEHM model performance for ozone with different biogenic emission models in other areas of the model domain. Moreover, further work will be devoted to improve DEHM with emissions and chemistry of other biogenic NMVOCs (e.g. mono-terpenes), which also contribute to the air quality (ozone and particulate matter).

Acknowledgement. The authors would like to thank Kirsti Ashworth (Lancaster University) for communication of her results and Associate Professor Marianne Glasius (Aarhus University) for fruitful discussions.
References


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Table 1. Comparison of the mean (M) isoprene concentrations between observed and calculated data by DEHM using both biogenic models in 2006. H is the height of the station above sea-level.

<table>
<thead>
<tr>
<th>Country/Station</th>
<th>Lat/Lon</th>
<th>M_{obs} (ppbv)</th>
<th>M_{MEGAN} (ppbv)</th>
<th>M_{GEIA} (ppbv)</th>
<th>Ratio Obs./ MEGAN</th>
<th>Ratio Obs./ GEIA</th>
<th>No. data</th>
<th>H (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Switzerland/Rigi</td>
<td>47.04° N/8.28° E</td>
<td>0.073</td>
<td>0.073</td>
<td>0.054</td>
<td>0.99</td>
<td>1.35</td>
<td>1991</td>
<td>1030</td>
</tr>
<tr>
<td>Germany/Langenbrugge</td>
<td>52.48° N/10.45° E</td>
<td>0.040</td>
<td>0.040</td>
<td>0.026</td>
<td>0.99</td>
<td>1.53</td>
<td>76</td>
<td>74</td>
</tr>
<tr>
<td>Germany/Schauinsland</td>
<td>47.54° N/7.54° E</td>
<td>0.065</td>
<td>0.10</td>
<td>0.05</td>
<td>0.65</td>
<td>1.3</td>
<td>73</td>
<td>1205</td>
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<tr>
<td>Germany/Neuglobsow</td>
<td>53.10° N/13.02° E</td>
<td>0.010</td>
<td>0.039</td>
<td>0.028</td>
<td>0.26</td>
<td>0.36</td>
<td>77</td>
<td>65</td>
</tr>
<tr>
<td>Germany/Schmuecke</td>
<td>50.39° N/10.46° E</td>
<td>0.024</td>
<td>0.093</td>
<td>0.051</td>
<td>0.25</td>
<td>0.46</td>
<td>79</td>
<td>937</td>
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<tr>
<td>Germany/Zingst</td>
<td>54.26° N/12.44° E</td>
<td>0.125</td>
<td>0.063</td>
<td>0.016</td>
<td>1.98</td>
<td>7.53</td>
<td>78</td>
<td>1</td>
</tr>
<tr>
<td>France/Donon</td>
<td>48.30° N/7.0° E</td>
<td>0.468</td>
<td>0.110</td>
<td>0.050</td>
<td>4.25</td>
<td>9.36</td>
<td>85</td>
<td>775</td>
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<tr>
<td>France/Peyrusse Vieille</td>
<td>47.37° N/0.10° E</td>
<td>0.690</td>
<td>0.029</td>
<td>0.030</td>
<td>23.54</td>
<td>22.84</td>
<td>59</td>
<td>236</td>
</tr>
<tr>
<td>Czech Rep./Kosetice</td>
<td>49.35° N/15.05° E</td>
<td>0.051</td>
<td>0.078</td>
<td>0.057</td>
<td>0.64</td>
<td>0.88</td>
<td>70</td>
<td>633</td>
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</table>
**Table 2.** Statistical parameters of maximum daily ozone simulated with DEHM-MEGAN and DEHM-GEIA against observations from 12 EMEP stations in the Mediterranean area together with the statistics of the maximum daily values taken as a mean over all the 12 stations as well as statistics the mean value of 117 monitoring stations in Europe for 2006.

<table>
<thead>
<tr>
<th>Country/Station</th>
<th>Lon/Lat</th>
<th>Fractional bias MEGAN</th>
<th>Fractional bias GEIA</th>
<th>Correlation MEGAN</th>
<th>Correlation GEIA</th>
</tr>
</thead>
<tbody>
<tr>
<td>Portugal/Monte Velho</td>
<td>8.80° W/38.08° N</td>
<td>0.03</td>
<td>-0.07</td>
<td>0.70</td>
<td>0.63</td>
</tr>
<tr>
<td>Cyprus/Ayia Marina</td>
<td>33.05° E/33.03° N</td>
<td>0.04</td>
<td>-0.08</td>
<td>0.54</td>
<td>0.32</td>
</tr>
<tr>
<td>Spain/Viznar</td>
<td>3.53° W/37.23° N</td>
<td>-0.11</td>
<td>-0.25</td>
<td>0.88</td>
<td>0.75</td>
</tr>
<tr>
<td>Spain/Campisabalos</td>
<td>3.13° W/41.27° N</td>
<td>-0.04</td>
<td>-0.14</td>
<td>0.83</td>
<td>0.77</td>
</tr>
<tr>
<td>Spain/Barcarrola</td>
<td>6.92° W/38.47° N</td>
<td>0.00</td>
<td>-0.11</td>
<td>0.86</td>
<td>0.74</td>
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<tr>
<td>Spain/Penasusende</td>
<td>5.87° W/41.28° N</td>
<td>-0.02</td>
<td>-0.10</td>
<td>0.77</td>
<td>0.73</td>
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<tr>
<td>Spain/Risco</td>
<td>4.35° W/39.52° N</td>
<td>-0.04</td>
<td>-0.16</td>
<td>0.80</td>
<td>0.62</td>
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<tr>
<td>Spain/Els Torms</td>
<td>0.72° E/41.40° N</td>
<td>0.01</td>
<td>-0.14</td>
<td>0.87</td>
<td>0.84</td>
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<tr>
<td>Spain/O Savinao</td>
<td>7.68° W/43.22° N</td>
<td>-0.04</td>
<td>-0.11</td>
<td>0.62</td>
<td>0.57</td>
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<tr>
<td>France/Iraty</td>
<td>1.08° W/43.03° N</td>
<td>-0.17</td>
<td>-0.24</td>
<td>0.79</td>
<td>0.73</td>
</tr>
<tr>
<td>France/Le Montfrance</td>
<td>2.07° E/45.80° N</td>
<td>-0.04</td>
<td>-0.12</td>
<td>0.76</td>
<td>0.75</td>
</tr>
<tr>
<td>Italy/Montelibretti</td>
<td>12.63° E/42.10° N</td>
<td>0.00</td>
<td>-0.10</td>
<td>0.85</td>
<td>0.82</td>
</tr>
<tr>
<td>Mediterranean St. (No: 12)</td>
<td>-0.02</td>
<td>-0.12</td>
<td>0.71</td>
<td>0.63</td>
<td></td>
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<tr>
<td>All European St. (No: 117)</td>
<td>-0.04</td>
<td>-0.10</td>
<td>0.92</td>
<td>0.93</td>
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</tr>
</tbody>
</table>
Fig. 1. Spatial distribution of the annual isoprene emission rates calculated with GEIA and MEGAN, together with their difference for 2006.
Fig. 2. Daily total isoprene emissions calculated by both GEIA and MEGAN in the study area for 2006.
Fig. 3. Spatial variability of isoprene emission factors (mg isoprene m$^{-2}$ h$^{-1}$) used in the simulations with the MEGAN and GEIA models, together with their difference.
Fig. 4. Distributions of emission rate and its corresponding emission factor as a standard alternative method in MEGAN simulation. The total emission of each location is calculated from sum of a single isoprene EF for each PFT.
Fig. 5. Seasonal isoprene emission rates estimated by MEGAN and GEIA, together with their differences for summer (JJA) and winter (DJF), 2006.
Fig. 6. Mean temperature pattern of the lowest model layer provided by MM5v3.7 in 2006; the entire year, summer (JJA) and winter (DJF).
Fig. 7. Annual isoprene concentrations simulated by DEHM in the lowest model layer using the MEGAN and GEIA biogenic emission models.
Fig. 8. Validation of the DEHM model results of isoprene concentrations using the MEGAN and GEIA biogenic models in 2006 against measurements for the background station Rigi in Switzerland.
Fig. 9. Upper panel: ozone concentration simulated by DEHM with the MEGAN and GEIA isoprene models against the platform without isoprene emission. Lower panel: ozone changes due to isoprene estimated by both biogenic models and the differences of MEGAN and GEIA runs in simulations of ozone for 2006.
Fig. 10. Annual concentrations of ozone for the year 2006 calculated by the DEHM model using GEIA and MEGAN in the nested domain covering Europe with a 50 × 50 km resolution.
Fig. 11. Comparison of measured and predicted mean values of the daily maximum ozone concentrations with DEHM-GEIA and DEHM-MEGAN at 117 rural background stations of EMEP for the year 2006.
Fig. 12. Validation of the DEHM model results for ozone of daily mean concentrations, daily maximum ozone concentrations and hourly concentrations using both the GEIA and MEGAN isoprene emission models for the year 2006 against measurements from two typical background stations (Viznar, Spain and Iraty, France) in south of Europe.