Peak 8-hr Ozone Model Performance when using Biogenic VOC estimated by MEGAN and BIOME (BEIS)

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1. INTRODUCTION

Biogenic emissions are a large contributor of regional VOC in the central and eastern United States that participate in photochemical reactions which form ozone (Wiedinmyer et al, 2005). It is important to capture the magnitude and spatial scale of VOC emissions, especially isoprene, to appropriately model high ozone episodes in the Midwest United States. The Model of Emissions of Gases and Aerosols from Nature (MEGAN) was recently developed as the next generation emission model for biogenic emissions of gases and aerosols (Guenther and Wiedinmyer, 2006). MEGAN has been implemented into the CONsolidated Community Emissions Processing Tool (CONCEPT) emissions modeling framework (Wilkinson, 2006). The CONCEPT emissions framework (CONCEPT, 2007) also includes the biogenic emissions model BIOME, which is a combination of BEIS3 (Geron et al, 1994) and GloBEIS (Guenther et al 1999, 2000) methodologies. A slightly different version of BIOME was implemented in the EMS-2003 emissions model (Janssen and Hua, 2007; Wilkinson et al, 1994).

The biggest difference in BIOME implementations is in the canopy parameterization scheme. EMS/BIOME has a simple canopy formulation and CONCEPT/BIOME uses canopy and environmental adjustment factors from GloBEIS. MEGAN uses a canopy environmental correction factor based on photosynthetically activated radiation (PAR) and temperature for isoprene emissions, which is similar to the GloBEIS approach (Guenther and Wiedinmyer, 2006). The emissions estimation equation in MEGAN is augmented to include a factor to account for the natural cycle of the changing structure of leaves and a factor to account for plant stress due to the lack of soil moisture. Leaf area index and average temperature across the current and previous time period is used to estimate the factor that adjusts for leave structure. Soil moisture and wilting point data are used to estimate the factor that adjusts emissions based on moisture availability (Wilkinson, 2006).

MEGAN groups plants and area coverages by plant functional type (PFT) rather than treating plant species explicitly as in the BIOME (and BEIS) models. Total emissions are the sum of emissions estimated for each PFT in a given grid cell. PFTs include broadleaf trees, fine leaf evergreen trees, fine leaf deciduous trees, shrubs, grass, and crops. Plant functional type data has been gridded to a scale of 30 seconds by 30 seconds and made available with the MEGAN model (Guenther et al, 2006). Soil wilting point data and leaf area index are also gridded to the same scale and used as input to MEGAN.

MEGAN, CONCEPT/BIOME, and EMS/BIOME are used to generate emissions estimates for each day of the summer of 2002. Each of the 3 biogenic emissions estimates are modeled with a state of the science photochemical transport model, the Comprehensive Air Quality Model with Extensions (CAMx4), to determine how well model estimates of ozone compare with observations.

2. METHODS

The Comprehensive Air Quality Model with Extensions (CAMx) version 4.50 uses state of the science routines to model ozone formation and removal processes over regional and urban scales (Nobel et al, 2002; Chen et al, 2003; Morris et al, 2005). The model is applied with an updated carbon-bond 05 (CB05) gas phase chemistry module (ENVIRON, 2006). CAMx is applied using the PPM horizontal transport scheme and an implicit vertical transport scheme with the fast CMC chemistry solver (ENVIRON, 2006). The photochemical model is initiated at midnight Eastern Standard Time and run for 24 hours for each episode day. The summer simulations are initiated on June 2 and run through August 31. The first 11 days of the simulation are not used in any analysis to minimize the influence of initial concentrations (Baker, 2007).

The meteorological, emissions, and photochemical models are applied with a Lambert projection centered at (-97, 40) and true latitudes at 33 and 45. The 36 km photochemical modeling domain consists of 97 cells in the X direction and 90 cells in the Y direction covering the central and eastern United States (Figure 1). The 2-way nested 12 km domain covers most of the upper Midwest region with 131 cells in the X and Y directions. CAMx is applied with the vertical atmosphere resolved with 16 layers up to approximately 15 kilometers above ground level.

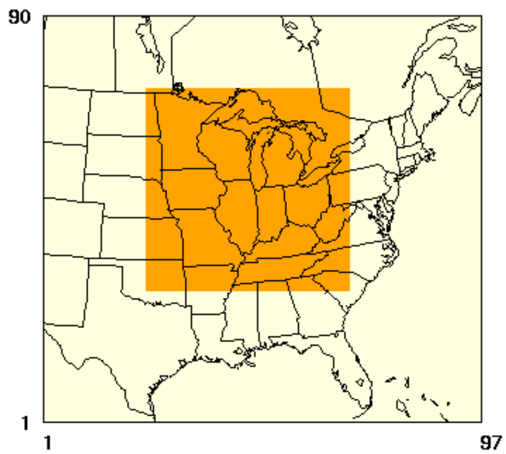

Fig. 1. 36 km (large box) and 12 km (small dark box) modeling domain.

Meteorological input data for the photochemical modeling runs are processed using the National Center for Atmospheric Research (NCAR) 5th generation Mesoscale Model (MM5) version 3.6.1 (Dudhia, 1993; Grell et al, 1994). Important MM5 parameterizations and physics options include mixed phase (Reisner 1) microphysics, Kain-Fritsch 2 cumulus scheme, Rapid Radiative Transfer Model, Pleim-Chang planetary boundary layer (PBL), and the Pleim-Xiu land surface module. Analysis nudging for temperature and moisture is only applied above the boundary layer. Analysis nudging of the wind field is applied above and below the boundary layer. These parameters and options are selected as an optimal configuration for the central United States based on multiple MM5 simulations using a variety of physics and configuration options (Johnson, 2003; Baker, 2004).

Anthropogenic emission estimates are made for a weekday, Saturday, and Sunday for each month. The biogenic emissions are day-specific. Daily emissions estimates for June through August 2002 from each biogenic model are merged with the same 2002 anthropogenic emissions. Volatile organic compounds are speciated to the Carbon Bond 05 chemical speciation profile. The BELD3 land use dataset is input to the BIOME biogenic models for fractional land-use and vegetative speciation information (US EPA, 2006; Kinnee et al, 1997). Inputs to all 3 biogenic models include hourly satellite photosynthetically activated radiation (PAR) and 15 m (above ground level) temperature data output from MM5 (Pinker and Laszlo, 1992).

Other inputs to MEGAN include plant functional type emission factors, PFT area coverage, soil wilting point data, leaf area index, and additional meteorological variables including soil moisture. Soil moisture estimated by MM5 for the 1 m soil depth is used as input to MEGAN because it represents the plant root layer.

3. RESULTS & DISCUSSION

3.1 Biogenic Emissions Modeling

MEGAN estimated VOC is compared to estimates from alternative biogenic emissions models including the CONCEPT and EMS-2003 implementations of the BIOME model. Total isoprene emissions over the entire summer for the entire modeling domain are 3.6 Mt from MEGAN, 3.1 Mt from EMS/BIOME, and 2.9 Mt from CONCEPT/BIOME. Daily total isoprene emissions estimated by MEGAN, EMS/BIOME, and CONCEPT/BIOME over the entire modeling domain are shown in Figure 2.

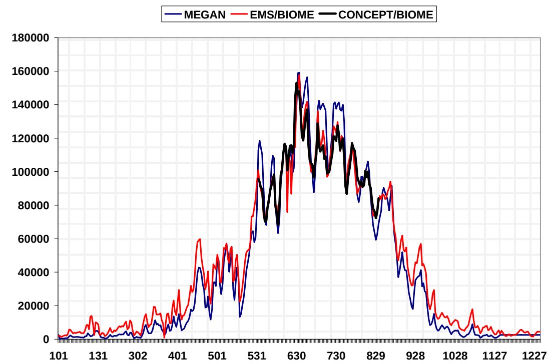

Fig. 2. Daily total isoprene emissions (tpd) for 2002.

Emissions estimates for each of the BIOME implementations are very similar, which is expected given the similarities in formulation. The CONCEPT implementation estimates slightly less isoprene on high emission days than the EMS version. Typically in the summer MEGAN estimates more total isoprene than BIOME. MEGAN tends to estimate less daily isoprene emissions in the early fall and late spring than BIOME. Total daily emissions for all species are shown in Table 1 for July 1, 2002.

Table 1. Total daily emissions (tpd) by model.

	Model		
Species	megan	concept/biome	ems/biome
ALD2	8,633	14,294	16,149
ALDX	1,732		
CO	25,343		
ETH	4,956		
ETHA	770		
ETOH	6,233		
FORM	1,442		
IOLE	2,549		
ISOP	158,793	146,376	149,575
MEOH	46,651		
NO	4,970	4,684	3,921
NR	22,591	2,561	2,424
OLE	4,683	9,887	10,230
PAR	14,333	72,129	73,498
SQT	8,918		
TERP	37,210	40,499	22,877
TOL	322		
XYL	170		

MEGAN outputs more explicit species than BIOME: carbon monoxide, ethane (ETHA), ethene (ETH), ethanol (ETOH), methanol (MEOH), formaldehyde, toluene, xylene, and sesquiterpenes. BIOME estimates much more mass in the more reactive VOC groupings of paraffins, olefins, and aldehydes as opposed to MEGAN which estimates much more mass as non-reactive (NR) VOC. This decrease in reactive VOC groups may offset some of the increases in ozone formation expected from the higher isoprene emissions estimated by MEGAN.

The spatial pattern of isoprene emissions varies between models. Figure 3 shows daily total emissions of isoprene in each grid cell for July 1, 2002.

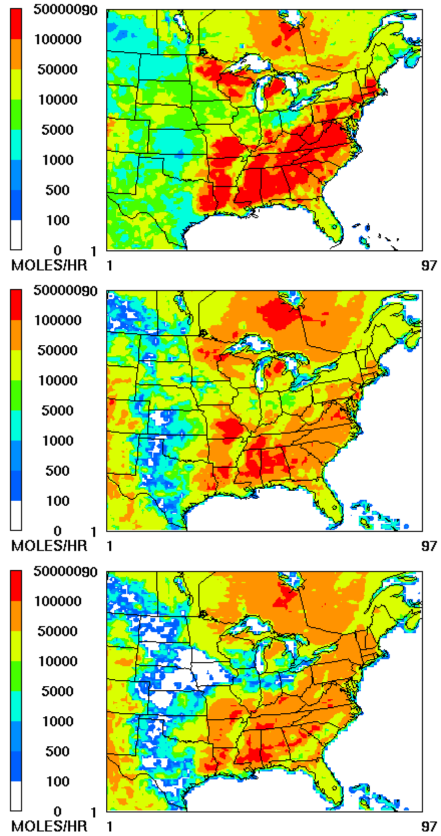

Fig. 3. Total emissions for July 1, 2002 estimated by MEGAN (top), EMS/BIOME (middle) and CONCEPT/BIOME (bottom).

The spatial plots in Figure 3 show higher regional isoprene emissions in the southeast United States, mid-Appalachian region, and mid-Great Lakes region estimated by MEGAN. There are less isoprene emissions estimated with MEGAN in Canada and Mexico. The implications about the change in spatial pattern of isoprene emissions are that more regional isoprene is available for ozone formation in the central and eastern United States when using MEGAN estimates.

3.2 Photochemical Modeling

When modeled with a photochemical transport model, each set of biogenic emissions result in a similar spatial pattern of peak ozone formation. The MEGAN emissions have the highest ozone peaks of the 3 sets of biogenic emissions. The 99th percentile daily maximum 8-hourly average ozone observation for each monitor is paired with model estimates. The mean bias of 99th percentile 8-hourly average maximum ozone over all stations (N=303) in the 12 km domain is -16.5 ppb with MEGAN biogenics, -18.0 with CONCEPT/BIOME biogenics, and -19.4 with EMS/BIOME biogenics. The isoprene estimated by MEGAN resulted in ozone estimates closest to peak observations over the entire 12 km modeling domain.

Figure 4 shows daily average mean gross error over all stations in the 12km modeling domain estimated for 8-hr ozone greater than 80 ppb. This high minimum threshold is selected to assess model performance for high ozone that is used as part of ozone attainment model demonstrations (US EPA, 2007). The ozone predictions using MEGAN biogenic emissions tend to be closest to high observed ozone values in the upper Midwest United States, but all three are fairly close on most days.

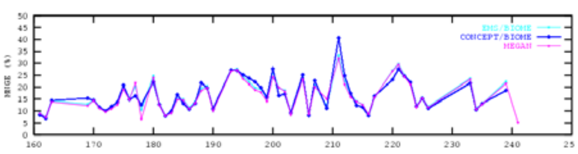

Fig. 4. Daily average mean gross error for all 3 simulations for 8-hr ozone > 80 ppb.

The day to day model performance features in daily average mean gross error change little when using different biogenic emissions. This suggests the day to day performance for ozone is more closely related to anthropogenic emissions and meteorology. The difference in mean normalized gross error for 8-hr ozone greater than 80 ppb between MEGAN and EMS/BIOME simulations is shown for each monitor in Figure 5. The blue shades (cool colors) represent monitor locations where the error is lower using MEGAN biogenics and red shades (hot colors) represent monitor locations where the error is lower using EMS/BIOME biogenics.

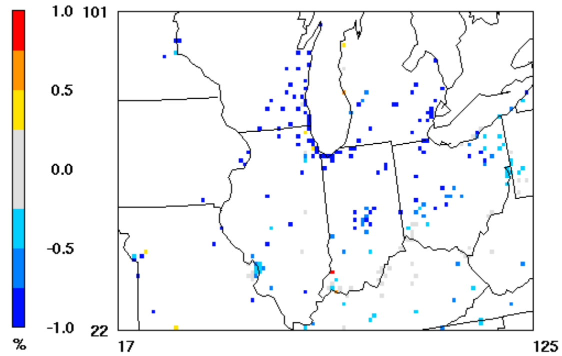

Fig. 5. MNGE (%) difference between simulations (megan – ems/biome).

Most stations in the region have better performance when the MEGAN biogenic emissions are used. This is seen in particular in urban areas like Indianapolis, St. Louis, Chicago, Milwaukee, Detroit, Columbus, and Cleveland.

4. CONCLUSIONS

The MEGAN isoprene emissions improve model estimates of high ozone in the upper Midwest compared to 2 implementations of the BIOME model. In general, each of the 3 biogenic emissions estimates resulted in similar spatial patterns of ozone formation in the region which suggests that ozone performance is more closely related to anthropogenic emissions and meteorology. Future work will include a comparison of photochemical model estimated secondary organic aerosol using emissions from MEGAN and BIOME.

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