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FINAL TECHNICAL MEMORANDUM No. 9: BIOGENIC EMISSIONS

To: Tom Moore, Western Regional Air Partnership (WRAP)

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Subject: Biogenic Emissions for use in the WestJumpAQMS

INTRODUCTION

ENVIRON International Corporation (ENVIRON), Alpine Geophysics, LLC (Alpine) and the University of North Carolina (UNC) at Chapel Hill Institute for Environment are performing the West-wide Jump Start Air Quality Modeling Study (WestJumpAQMS) managed by the Western Governors' Association (WGA) and Western Regional Air Partnership (WRAP). WestJumpAQMS is setting up the CAMx and CMAQ photochemical grid models for the 2008 calendar year (plus spin up days for the end of December 2007) on a 36 km CONUS, 12 km WESTUS and several 4 km Inter-Mountain West domains. The WestJumpAQMS Team are currently compiling emissions to be used for the 2008 base case modeling, with the 2008 National Emissions Inventory (NEI) being a major data source. Seventeen Technical Memorandums discussing the sources of the 2008 emissions by major source sector are being prepared as part of the WestJumpAQMS:

1. Point Sources including Electrical Generating Units (EGUs) and Non-EGUs;
2. Area plus Non-Road Mobile Sources;
3. On-Road Mobile Sources that will be based on MOVES;
4. Oil and Gas Sources (5 separate memorandums for different Basins);
5. Fires Emissions including wildfire, prescribed burns and agricultural burning;
6. Fugitive Dust Sources;
7. Off-Shore Shipping Sources;
8. Ammonia Emissions;
9. Biogenic Emissions;

10. Eastern USA Emissions;

11. Mexico/Canada;

12. Sea Salt and Lightening Emissions; and

13. Emissions Modeling Parameters including spatial surrogates, temporal adjustment parameters and chemical (VOC and PM) speciation profiles.

This document is Technical Memorandum Number 9 that discusses the approach to be used for developing 2008 biogenic emission inputs for the CAMx and CMAQ models in the WestJumpAQMS. The discussion below is taken from the final report of the WRAP Biogenic Emissions Study (Sakulyanontvittaya, Yarwood and Guenther, 2012[1]).

INTRODUCTION TO BIOGENIC EMISSIONS

Emissions from vegetation, mostly from the leaves of plants, are the largest source of volatile organic compounds (VOC) in the global atmosphere, although VOC emissions from cars, factories and fires dominate in urban and industrial areas. In the atmosphere, the oxidation of VOC can influence aerosol particles, precipitation acidity, and regional ozone distributions. Accurate predictions of biogenic VOC emissions are important for developing regulatory ozone and aerosol control strategies for at least some rural and urban areas. One of the great challenges associated with characterizing biogenic VOC (BVOC) is the large variety of compounds involved. Isoprene is the single most important BVOC with an emission that is about half of the global BVOC emission and is highly reactive so can be an important component of ozone formation. Many monoterpenes have been observed in the atmosphere but only a few, such as α-pinene, make a significant contribution to the global total emissions. The dominant sesquiterpenes, such as β-caryophyllene, have lifetimes of only minutes in the atmosphere and so are present at very low levels, but their reaction products may be an important source of secondary organic aerosol (SOA). Oxygenated BVOC include a wide range of alcohols, aldehydes, ketones, acids, ethers, and esters but are dominated by relatively low molecular weight compounds such as methanol, acetaldehyde and acetone. Other BVOC include alkanes (e.g., heptane), alkenes (e.g., ethene), aromatic hydrocarbons (e.g., toluene), sulfur compounds (e.g., dimethyl sulfide), and nitrogen compounds (e.g., hydrogen cyanide). Observations of land–atmosphere interactions must include not only primary emissions but also the larger number of reaction products that impact atmospheric oxidants and particle formation and growth.

Soil emissions of nitric oxide (NO) are also treated by biogenic emissions models. Investigations of NO emission from soils began in the 1960s with agronomists that were interested in the fate of fertilizer applied to soil, but the amount lost to the atmosphere was a relatively small part (a few percent) of the total fertilizer applied. NO emissions were later observed from unfertilized landscapes and it was recognized that this could be an important source of atmospheric NO in some regions. Early studies of the microbial and ecological processes and environmental controls over NO emissions led to what has been called the “hole-in-the-pipe” model (Firestone

1 http://www.wrapair2.org/pdf/WGA_BiogEmisInv_FinalReport_March20_2012.pdf

and Davidson 1989). This model conceptualizes NO emission regulation at two levels: (1) the rate of nitrogen cycling (the amount of nitrogen flowing through the pipe); and (2) factors influencing the ability of NO to escape from the soil into the atmosphere (the hole in the pipe). The nitrogen cycling includes two components: (1) nitrification (converting NH_4 to NO_3); and (2) denitrification (converting NO_3 to N_2). Nitrification is considered the main source of NO emission. Fertilizer, atmospheric nitrogen deposition, leaf litter, soil temperature and perhaps other factors can influence the rate of nitrogen cycling in the soil while soil properties and water content and perhaps other factors influence the amount that can leak into the atmosphere.

Although NO emissions have been observed from a wide range of landscapes under various conditions, the implementation in regional to global models has been relatively simple due to the lack of suitable databases for scaling observations to regional scales. The model of Williams et al. (1992), used for MEGAN v2.04, is a simple approach with emissions based on landcover type and soil temperature. Yienger and Levy (1995) improved on this approach by including the two factors (fertilizer rates and soil moisture) responsible for much of the observed variability. This is the approach used for MEGAN v2.10 and BEIS v3.14.

WRAP BIOGENIC EMISSIONS UPDATE STUDY

WRAP performed a biogenic emissions update study to develop improved methods for estimating biogenic VOC and NO emissions in the western states and to develop biogenic emissions to support the WestJumpAQMS modeling of the 2008 annual period. The major focus of the WRAP Biogenic Emissions Study was to improve data that drive biogenic emission inventories in the West to account for important factors such as inter-annual variability in vegetation due to drought, land cover change due to progressive urbanization, the biogenic VOC emission potential of Western plants and ecosystems, and the importance of correctly characterizing biogenic NO_X emissions in sparsely populated Western regions.

BIOGENIC EMISSIONS MODELS

The WRAP Biogenic Emissions Study presents several different biogenic emissions models with the main two being the Model of Emissions of Gases and Aerosols in Nature (MEGAN[2]) and the Biogenic Emissions Inventory System (BEIS[3]). The version of MEGAN that is publicly available on the MEGAN website is v2.04, whereas the latest version of BEIS is v3.14 that is implemented in the SMOKE-BEIS modeling system. There is also an updated version of MEGAN (v2.10) that includes several enhancements that was used as the basis for the WRAP Biogenic Emissions Study. There are considerable differences in biogenic emission models which often lead to emission estimates that differ by a factor of two or more. Much of these differences are due to the emission factors and landcover inputs used for the models so that by using similar inputs it is often possible to bring these models into agreement of better than 30%. Most of the observations available for evaluating the accuracy of these models are concentration measurements. Since ambient concentrations are dependent on emissions, chemical loss and

2 http://acd.ucar.edu/~guenther/MEGAN/MEGAN.htm
3 http://www.epa.gov/AMD/biogen.html

transport, they are reliable for evaluating emission estimates only if we have an accurate understanding of chemical loss rates and transport. Presently, our limited understanding of OH distributions, the dominant sink for most BVOC, means that ambient concentrations are only useful for constraining emissions to within about a factor of two, which is the same magnitude as the difference between model estimates. As a result, these observations are of limited value for identifying which model provides the better estimates. Recent advances in direct BVOC flux measurements, including airborne eddy covariance systems and a low cost tower-based relaxed eddy accumulation system, are beginning to provide a substantial database that can be used to constrain emission estimates to within ~30% which will improve our ability to evaluate BVOC emission models.

The major components of biogenic emissions models are as follows:

- Leaf Area Index (LAI).
- Plant Functional Type (PFT).
- Plant specific species composition data and averaging (speciation).
- Emissions factors, which includes the effects of:
    - Meteorological variables (e.g., temperature); and
    - Photosynthetically Active Radiation (PAR).

Table 1 compares the main biogenic emissions model components for the MEGAN V2.10 and BEIS 3.14. While improved landcover and emission factors could be incorporated into any BVOC emission model, the WRAP Biogenic Emissions Study has adopted the MEGAN model primarily because (1) it is easier to incorporate new landcover and emission factors, and (2) it is the only available model that already includes recent (i.e., past 5 years) advances in BVOC emission process understanding. The WRAP Biogenic Emissions Study focused on developing improved inputs for MEGAN modeling of the 2008 period and started with the latest version of MEGAN (v2.10). MEGAN v2.10 has the following improvements over the publicly available MEGAN v2.04 that was released October 29, 2007:

- Implementation of an explicit canopy environment and leaf energy balance models that calculate solar radiation and leaf temperature of sun and shade leaf components for 5 canopy depths.
- Modification of the 20 emission categories to emphasize and add some categories (e.g., compounds with bi-directional exchange, compounds that are sensitive to stress levels) and de-emphasize others (e.g., methane no longer has its own category but is included in the other category).
- Revised parameterization for the temperature dependence of light-dependent emissions.
- Revised emission factors and emission algorithm coefficients.
- Introduction of a deposition term to account for bi-directional exchange.

- The code was made more modular, to simplify future changes, and more parameters were included as input files to facilitate future changes.

The WRAP Biogenic Emissions Study made the following improvements to MEGAN v2.10 (Sakulyanontvittaya, Yarwood and Guenther, 2012):

- Code modification to allow input of improved landcover data including 8-day LAI and 17 of PFT categories.
- Update NO emissions scheme to the soil NO_X model of Yienger and Levy (1995) that will result in improved soil NO_X emissions that account for fertilizer application rates and soil moisture variations from precipitation.

Table 1. Comparison of MEGAN v2.10 and SMOKE-BEIS v3.14 landcover and emission factors.

Model	Approach	Advantages
	LAI	
MEGANv2.10	MODIS observations	This is the best available option because it provides a means to represent 1) interannual variations due to climate, insects and other factors, 2) seasonal variations of deciduous vegetation, and 3) spatial variations in canopy density.
BEISv3.14	Constant maximum LAI for individual species	Minimal effort is required to use this approach.
	PFT	
MEGANv2.10	30-m LANDSAT-TM NLCD and 56-m AWiFS CDL satellite data.	This is the best available option because the high resolution data can characterize the heterogeneous landscapes found in much of the western U.S. The approach is also arguably easier to apply.
BEISv3.14	1000-m MODIS based landcover data for western U.S.	None
	Species Composition Data and Averaging	
MEGANv2.10	Average over ecoregions. FIA tree data and NRCS grass and shrub data. CDL for crops.	This is the best available option because ecoregions provide an area with more consistent species composition in comparison to a county-based approach. The addition of NRCS shrub and grass species composition and CDL crop distributions provides a substantial improvement for these plant functional types.
BEISv3.14	Average over counties. FIA tree data. USDA crop data. No shrub and grass data.	None
	Emission factors	
MEGANv2.10	Emission factor database updated in 2011	This is the best available option because it includes recent measurements including field campaigns in the western U.S.
BEISv3.14	Emission factor database has not been updated recently	None

DEVELOPMENT OF 2008 BIOGENIC EMISSIONS USING UPDATED MEGAN V2.10

Below we summarize the application of the updated v2.10 of MEGAN to generate 2008 biogenic emissions for the WestJumpAQMS. WestJumpAQMS is developing emissions inputs for three modeling domains, which are depicted in Figure 1, a 36 km continental U.S. (CONUS) domain, a 12 km western U.S. (WESTUS) domain and a 4 km Inter-Mountain West Processing Domain (IMWPD). More details on WRAP Biogenic Emissions Study are available on the WRAP website[4].

Development of MEGAN v2.10 Model Inputs

Biogenic emissions were generated using the updated MEGAN v2.10 for the WestJumpAQMS 2008 annual period and the 36/12/4 km domains as shown in Figure 1. Vegetation inputs used were as follows:

> Leaf Area Index (LAI): A set of 46 8-day LAI files for North America were generated for the 2008 year at 1 km resolution. This allowed the representation of the seasonal variation in LAI in the biogenic emissions modeling.
>
> Plant Functional Type (PFT): A set of 9 PFTs were developed at both a 1 km and 56 m resolution across the domains. Although MEGAN can address 17 PFTs, only 9 were contained in the North America modeling domains. Various databases were used to define the spatial variations in the PFTs.
>
> Emission Factor (EF): EF data were updated using data from the latest literature that included 6 western U.S. (Arizona, California, Colorado, Nevada, New Mexico, and Oregon) specific plant type measurements. For example, the pinyon pine and juniper emissions parameterization were updated using data collected by the University of New Mexico[5]. A set of 10 EF files at 56 m and 1 km spatial resolution were developed for NO and 9 VOC species (isoprene, methyl butenol, alpha-pinene and 6 other monoterpenes).

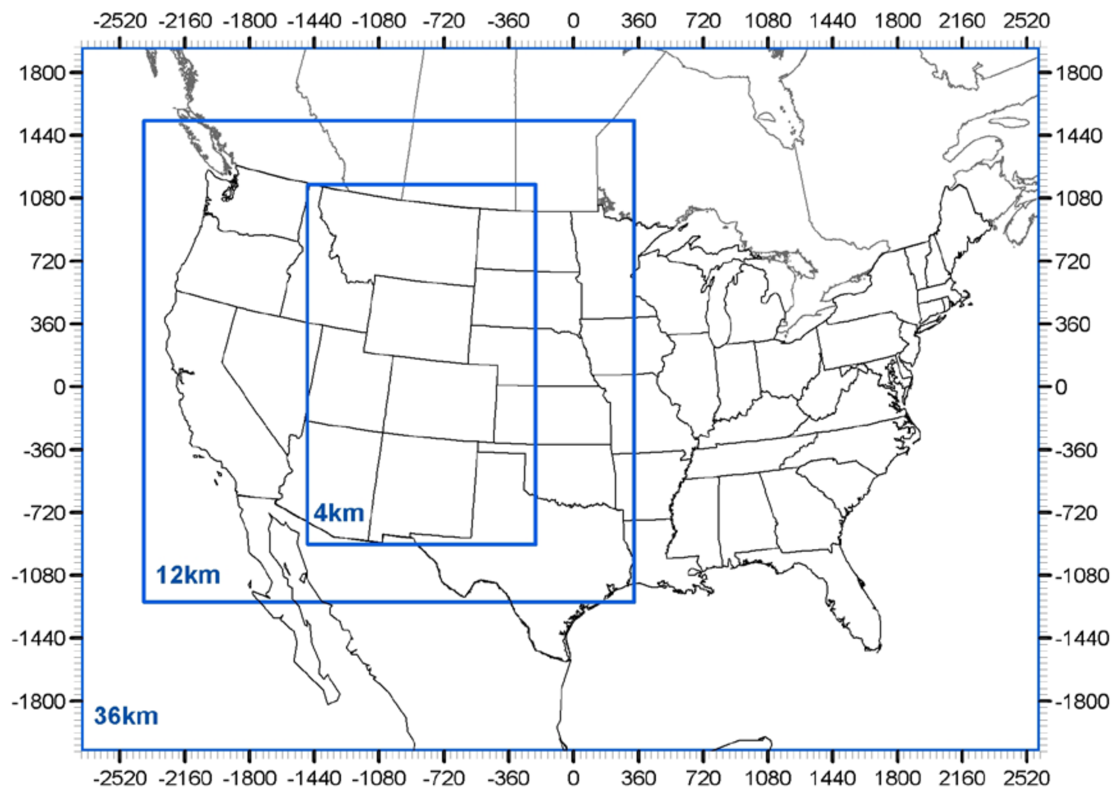
Meteorological Data for MEGAN v2.10 Model

The MEGAN model requires meteorological data, e.g. temperature, solar radiation, soil temperature and moisture, and wind speed, to drive algorithms for light, temperature, canopy, and soil-NO_X. Hourly gridded meteorological data for 2008 and the 36/12/4 km domains were mainly obtained from the WestJumpAQMS WRF meteorological model modeling[6] and were processed through MCIP version 3.6

Photosynthetically Active Radiation (PAR) is the solar radiation in the 400-700 nm spectral region and is an important variable in MEGAN for generating biogenic VOC emissions. MEGAN has two options for providing PAR inputs to MEGAN: (1) PAR obtained as a ratio off of the total

4 http://www.wrapair2.org/emissions.aspx
5 http://biology.unm.edu/litvak/Pinyon%20Juniper/Pinyon%20Juniper.html
6 http://www.wrapair2.org/pdf/WestJumpAQMS_2008_Annual_WRF_Final_Report_February29_2012.pdf

solar radiation (SRAD) from a meteorological model (i.e., WRF in this case) where PAR = CF x SRAD with a CF default value of 0.5; or (2) PAR data from satellite. The first option is always available, whereas satellite PAR data can be spotty. The WRAP Biogenic Emissions Study did an extension comparison and evaluation of the two PAR approaches and found that use of the WRF scaled SRAD approach resulted in higher isoprene values than use of satellite PAR. Under clear sky comparisons they found that the 0.5 ratio for PAR to SRAD is too high. They also found that WRF sometimes failed to capture clouds that were present, which was due in part to thin layers of clouds that WRF's vertical resolution could not resolve. In the end, the satellite PAR data was used with data gaps filled with the WRF SRAD ratio approach using an updated and lower CF PAR to SRAD scaling factor of 0.45.



Modeling Domain

36km: 148 x 112 (-2736, -2088) to (2592, 1944)
12km*: 227 x 230 (-2388, -1236) to (336, 1542)
04km*: 317 x 515 (-1480, -904) to (-212, 1156)

* includes buffer cells

Figure 1. WestJumpAQMS 36-km CONUS, 12-km WESTUS and 4-km IMWPD domains that will be used to develop meteorological and emission PGM inputs.

2008 BIOGENIC EMISSIONS MODELING RESULTS

The WRAP Biogenic Emissions Study compared biogenic emission estimates for a two-week period in January and July 2008 using the MEGAN v2.04 (Mv2.04) and v2.10 (Mv2.10) and SMOKE-BEIS v3.14 (SBEIS) biogenic emissions models. MEGAN v2.10 was also run for the full 2008 calendar year on the 36/12/4 km modeling domains (Figure 1). Table 2 compares the domain wide isoprene (ISOP), monoterpene (TERP), nitric oxide (NO) and carbon monoxide (CO) emissions for the 2 two-week periods and the 36 km CONUS, 12 km WESTUS and 4 km IMWPD modeling domains. The units of the emissions are as two-week averages in mass per time per area ($kg/hr\text{-}km^2$), which allows an intercomparison of the emission rates across the three domains.

Mv2.04 vs. Mv2.10: The main differences between Mv2.04 and Mv.2.10 are the inclusion of a canopy model, updates to the NO emissions algorithm and updates to the landcover data. These updates result in lower ISOP emissions of -14%, -17% and -38% for the summer period and the 36 km CONUS, 12 km WESTUS and 4 km IMWPD domains, respectively. The ISOP reductions between Mv2.04 and Mv2.10 are even greater (-40% to -67%) for the winter period. The TERP emissions estimates for Mv2.04 and Mv2.10 are more similar with differences ranging from -16% to +21%. The new NO algorithm in Mv2.10 produces substantially more NO emissions than Mv2.04 for the summer period (+26% for 36 km, +31% for 12 km and +58% for 4 km domains), but less (-16% to -40%) NO emissions for the winter period.

SBEIS vs. Mv2.10: The summer period ISOP emission estimates are comparable for SBEIS and Mv2.10 with Mv2.10 having from +12% (36 km) and +5% (12 km) more, to -12% (4 km) less than SBEIS. For the winter period, Mv2.10 has comparable ISOP emissions for the 36 km CONUS domain (+4%) to less (-30%) and much less (-61%) for the 12 km and 4 km domains, respectively. Mv2.10 has less TERP emissions than SBEIS ranging from -31% to -47% less for the summer period and -45% to -71% less for the winter period. Mv.2.10 NO emissions are approximately half of those from SBEIS for the summer period and a small fraction of the SBEIS NO emissions for the winter period.

Figures 2 and 3 compare the spatial distribution of the three biogenic emission models isoprene emissions for the 4 km IMWPD for, respectively, for July 3-18 and January 3-18 periods. The Mv2.10 spatial distribution of the ISOP emissions for the summer period is more similar to SBEIS than Mv2.04. Whereas for the winter period, all three models estimate that most of the biogenic ISOP comes from the southern states where there are higher temperatures and PAR and less snow on the ground. The isoprene emission distribution from SMOKE-BEIS follows the state boundaries, which is especially noticeable for Idaho and Wyoming. This is because SMOKE-BEIS uses county-level tree species distribution. MEGAN does not have this issue.

In general, MEGAN v2.04 and 2.10 estimate lower monoterpene, NO_X, and CO emissions than SMOKE-BEIS. MEGAN v2.04 isoprene emission estimates are about 30% higher than SMOKE-BEIS while MEGAN v2.10 is about the same as SMOKE-BEIS. MEGAN v2.10 estimates lower isoprene and lower CO emissions than MEGAN v2.04 for all domains in both January and July. Monoterpene emissions from MEGAN v2.10 are lower than MEGAN v2.04 except for the 12 km and 4 km domains in July. NO_X emissions from MEGAN v2.10 are higher than MEGAN v2.04 in July but lower in January.

For a monoterpene comparison between SMOKE-BEIS and MEGAN models, SMOKE-BEIS estimates higher emissions in desert regions of western Arizona and Southern Nevada. The lower monoterpene emissions estimated by MEGAN are more reasonable for these regions with sparse vegetation cover.

Conclusions

The WRAP Biogenic Emissions Study updated the MEGAN V2.10 model and delivered CAMx-ready and CMAQ-ready biogenic emissions for the WestJumpAQMS 36/12/4 km modeling domains and the 2008 annual period. Although it is difficult to determine which biogenic emissions estimates are more correct, the MEGAN v2.10 biogenic emission estimates have technical improvements over past inventories, particularly for the western states. In summary, advantages of MEGAN v2.10 are the most up-to-date scientific algorithms for emission estimates, year specific 2008 land cover/vegetation inputs with high temporal resolution (8 day LAI), and the most up-to-date emission factors. In addition, the emission distributions from MEGAN v2.10 are more reasonable than SMOKE-BEIS in that SMOKE-BEIS estimates unreasonably high emissions in some desert regions with sparse vegetation, and county boundaries are noticeable in the SMOKE-BEIS isoprene emissions. The WestJumpAQMS proposes to use the MEGAN v2.10 biogenic emission inventories for their photochemical modeling analysis. More details are available on the WRAP website: http://www.wrapair2.org/emissions.aspx.

Future Topics

Additional improvements in the treatment of biogenic emissions can be made in the future. Although the WRAP biogenic emissions study updated the plant types in certain areas in the western U.S. where the ground truth of plant species was performed, these were very limited areas involving urban areas and their surroundings (e.g., Phoenix and the desert shrubland around Phoenix). There are vast expanses of the western U.S. where further refinement of specific plant species can be made. The sensitivity of the MEGAN biogenic emissions to site-specific plant species updates should be investigated.

Although the updates to the MEGAN model have brought the MEGAN and BEIS biogenic isoprene emission estimates closer together, there are still large differences in the other species. The biogenic NO_X emissions, in particular, are quite different between the two models. The sensitivity of western U.S. ozone formation to the biogenic NO_X emissions is a topic that should be analyzed in the future.

Table 2. Domain total summary table of period average biogenic emissions from SMOKE-BEIS V3.14 (SBEIS), MEGAN v2.04 (Mv2.04), and MEGAN v2.10 (Mv2.10). ISOP is isoprene, TERP is monoterpene, NO_X is mono-nitrogen oxides, and CO is carbon monoxide.

Period	Domain	Pollutant	Emission (kg/hr-km^2)			Percent Difference		
			SBEIS	Mv2.04	Mv2.10	(Mv2.04 - SBEIS)	(Mv2.10 - SBEIS)	(Mv2.10 - Mv2.04)
3-18 July, 2008	36 km	ISOP	4,212.4	5,474.2	4,735.0	30.0	12.4	-13.5
		TERP	2,019.2	1,537.1	1,388.8	-23.9	-31.2	-9.6
		NOx	298.5	140.6	176.4	-52.9	-40.9	25.5
		CO	1,610.1	1,377.9	817.4	-14.4	-49.2	-40.7
	12 km	ISOP	12,289.0	15,585.8	12,921.8	26.8	5.1	-17.1
		TERP	7,426.1	4,243.4	4,388.9	-42.9	-40.9	3.4
		NOx	1,594.7	637.8	833.6	-60.0	-47.7	30.7
		CO	7,862.2	5,293.9	3,112.6	-32.7	-60.4	-41.2
	4 km	ISOP	22,395.1	31,603.5	19,641.9	41.1	-12.3	-37.8
		TERP	23,244.7	10,143.2	12,293.1	-56.4	-47.1	21.2
		NOx	5,698.6	1,649.2	2,597.7	-71.1	-54.4	57.5
		CO	26,749.3	14,513.8	7,636.0	-45.7	-71.5	-47.4
3-18 January, 2008	36 km	ISOP	87.2	152.7	91.1	75.1	4.4	-40.4
		TERP	283.2	173.6	155.8	-38.7	-45.0	-10.3
		NOx	86.1	11.6	9.8	-86.5	-88.7	-16.0
		CO	163.6	125.9	22.5	-23.1	-86.2	-82.1
	12 km	ISOP	145.5	200.0	101.8	37.5	-30.0	-49.1
		TERP	860.0	404.5	340.3	-53.0	-60.4	-15.9
		NOx	398.6	29.8	18.0	-92.5	-95.5	-39.7
		CO	663.3	333.1	30.8	-49.8	-95.4	-90.8
	4 km	ISOP	203.8	241.6	80.1	18.5	-60.7	-66.8
		TERP	2,219.4	662.3	645.8	-70.2	-70.9	-2.5
		NOx	1,379.8	61.0	38.3	-95.6	-97.2	-37.2
		CO	1,982.2	683.4	50.8	-65.5	-97.4	-92.6

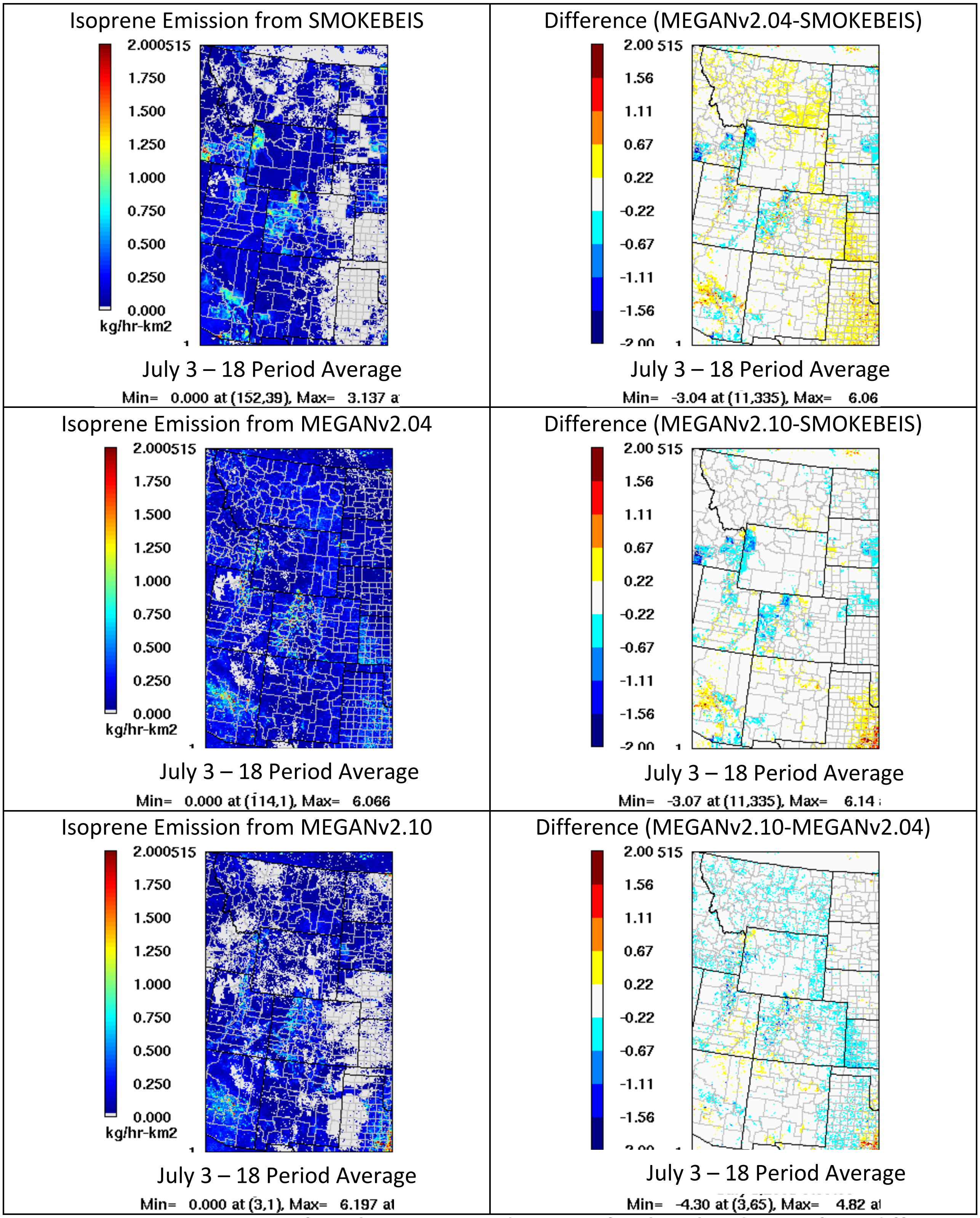


Figure 2. Isoprene emission for July 3 – 18 period average for the 4 km domain from different models, and the emission difference.

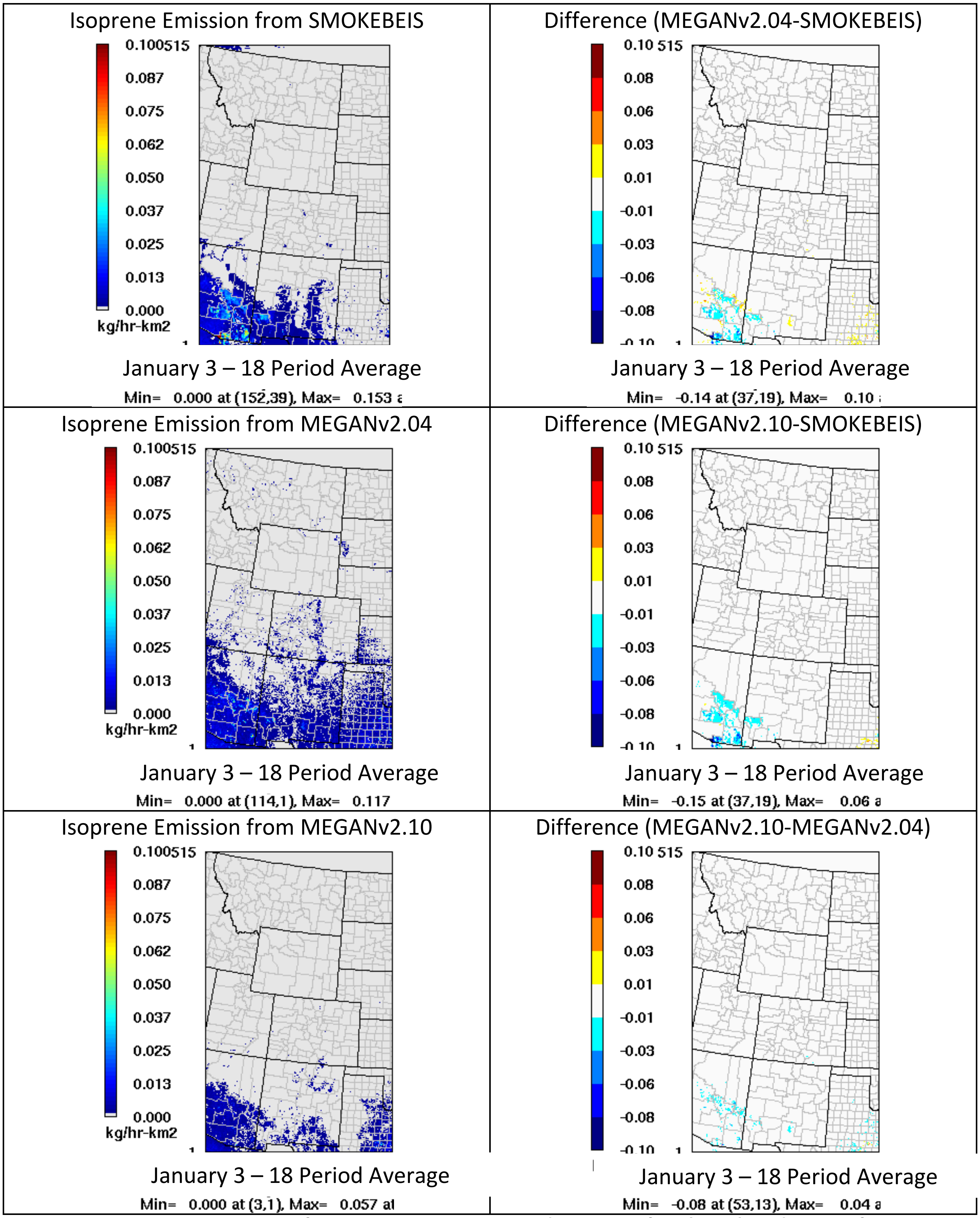


Figure 3. Isoprene emission for January 3 – 18 period average for the 4 km domain from different models, and the emission difference.