BIOME3

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Introduction

The third generation Biogenic Model for Emissions (BIOME3) has been developed and sensitivity analyses conducted to determine the impacts to biogenic emissions predictions over the Midwest United States. BIOME3 includes a revised canopy model as well as a revised algorithm to estimate isoprene emissions; however, the monoterpene, oxygenated VOCs, and biogenic nitric oxide formulations remain unchanged. Further, BIOME3 has been designed to utilize version three of EPA's Biogenic Emissions Landuse Data (BELD3). Finally, along with the new BELD3 data, EPA has also updated the biogenic emissions factors most notably the oxygenated VOCs. As will be shown, BIOME3 coupled with the BELD3 and new biogenic emissions factors, predicts somewhat lower isoprene emissions than does BEIS2 though the oxygenated VOCs show dramatic changes depending on the choice of biogenic emissions factors.

The first generation model, BIOME which is a component of the GEMAP emissions modeling system, was built in 1993. BIOME was designed to emulate version two of EPA's Biogenic Emissions Inventory System (BEIS2). LADCO used BIOME coupled with land use and biomass data derived specifically for the Chicago/Milwaukee/Gary/Muskegon area. When the BEIS2 model was introduced, LADCO turned to it but did not take the steps necessary to update the BEIS2 data with the land use and biomass data, which as previously noted were used in BIOME, that had been specifically developed for the Lake Michigan area. This resulted in different biogenic emissions predictions BIOME and BEIS2. Though, at that time, the BEIS2 predictions were chosen for use and the use of BIOME languished.

However, there were several shortcomings of the BEIS2 model. Because BEIS2 was written in FORTRAN, it was difficult to prepare adequate emissions summaries or visualize the emissions estimates. Also, the FORTRAN code was difficult to read and inadequately documented, leading to difficulty in interpreting the code. This resulted in an extended period where LADCO did not seriously question the results of the BEIS2 model.

After LADCO embarked on the study of biogenic emissions from oak trees in the Ozarks (i.e. Missouri), it became clear that LADCO needed a biogenics model which gave the user the freedom to modify the data and model code easily and to better understand how the calculations were done. LADCO approached Alpine Geophysics with the idea of re-invigorating the BIOME model by updating the datasets to include many of the datasets and methods likely to be included in future releases of the BEIS3 model. This version emulates BEIS3, but more importantly, it allows users the flexibility of EMS-2001. The system uses many of the old BIOME processors with updated methodologies. In addition, the new processors read the newer datasets available in BEIS3. This new model and associated data are called BIOME3.

Model Improvements

BIOME3 has three major improvements over BIOME. The first improvement is inclusion of the BEIS3 canopy model as derived from GLOBEIS (Environ, 2001; Yarwood et al., 1999). Unlike the BEIS2 formulation which had only a five layer, fixed canopy model based on forest type (e.g. pine, coniferous, deciduous), the new canopy model is more general and more rigorous in its treatment of energy transfer through a leaf canopy. Leaf-level estimates of temperature and photosynthetically active radiation (PAR) are required in the biogenic isoprene emissions algorithms. Numerous approaches have been used to account for energy transfer through the leaf canopy. Lamb et al. (1993) introduced a simple scaling model, which was incorporated into BEIS (Pierce and Waldruff, 1991), to adjust above canopy observations of temperature, PAR, wind speed, and humidity as a function of height in the canopy. In BEIS3 and in BIOME3, a revised version of the BEIS leaf energy balance is used to adjust PAR levels for sun and shaded leaves as a function of height in the canopy (Guenther et al., 2000).

The second improvement is the inclusion of an option to define the isoprene ratio. "Isoprene ratio" is used to scale the isoprene emission factors. In GLOBEIS, this value is set to 1.43 which is close to the ratio of isoprene rates determined from cuvette measurements versus leaf enclosure measurements though this has not been confirmed. However, after discussions with Mr. Tom Pierce (2001), this value should be set to 1.0.

The third improvement is a revised isoprene emissions estimates algorithm based on the work of Guenther et al. (2000). However, these revisions are only small modifications to the original work of Guenther et al. (1991, 1993). Of note, the work of Guenther et al. (2000) introduces the concept of "leaf aging." Early in the growing season (i.e. at and shortly after budbreak), isoprene emissions appear to be very low or nonexistent. Whereas late in the growing season, isoprene emissions decline as leaves rapidly age. Results from Monson et al. (1994), Geron et al. (1997), and Goldstein et al. (1998) suggest that isoprene emission onset is initiated after 650 heating degree days, defined as number of days with mean temperature above 65° F, which occurs several weeks after budbreak. Peak isoprene emissions occur after 1050

heating degree days. At the time BIOME3 was constructed, it was unclear whether BEIS3 would account for leaf aging; therefore, leaf aging was not accounted for in BIOME3. However, it is now apparent that the leaf aging concept will be included in BEIS3, and it will be necessary to revise BIOME3 to accommodate this as well.

Data Improvements

By far the greatest change in BIOME3 is the incorporation of updated land use and biogenic emissions factors datasets. The BELD3 (EPA, 2001) is a major revision to the BELD2 data (Kinnee et al., 1997). The BELD3 covers 230 land use characteristics and is based on the blending of the United States Geological Survey (USGS) North America Land Cover Characteristics (LCC) (USGS, 2000), the United States Forest Service's Forest Inventory Analysis (FIA) data base (Pierce et al., 1998), and the United States Department of Agriculture county-level crop acreage statistics for 1992 (USDA, 2001) data. The BELD3 covers most of North America including much of Canada and all of Mexico. Further, unlike BELD2 which is resolved to the county level, BELD3 is resolved on a one kilometer by one kilometer grid cell basis.

Though the biogenic emissions factors have been revised, the isoprene, monoterpenes, and nitric oxide emissions factors remain basically unchanged since their development for use in BEIS2. However, two new developments have occurred with the biogenic emissions factors: the biogenic species are now available in species-specific form as well as the lumped monoterpenes and oxygenated VOCs (OVOCs) forms; and methanol (MEOH) and 2-methyl-3-butenol (MBO) are now included as oxygenated VOCs (OVOCs).

Until now, the OVOCs and monoterpenes were treated as lumped species emissions factors from which emissions were estimated. After the OVOCs and monoterpenes were estimated, it was necessary to speciate the estimates per the chemical mechanism that the air quality model used. The process of speciating the emissions for use by the air quality model introduced yet one more level of uncertainty. Now, with the introduction of individual species emissions factors, the speciation process is mitigated to some degree though it is now necessary to map the individual species biogenic emissions estimates into the lumped chemical mechanism species which is a somewhat easier process.

Also MEOH and MBO have been included as OVOCs. Of note, MBO is predominantly emitted from western pines and should not impact biogenic emissions elsewhere in the United States. However, with the inclusion of MEOH into the OVOCs, the OVOCs emissions rate, as a lumped species, jumps dramatically for some plant species. Though, because MEOH is somewhat unreactive, it is not clear what impact this OVOC increase will have on air quality model predictions.

**********END JGW COMMENTS**********

Running BIOME3.

Biome3 is written is SAS and is integrated with the EMS-2001 model. It can be run outside of the EMS-2001 framework because many of it's components are modular. There are 4 actions

required to complete a model run.

The first step in running the model is to read the emission factor data base, This is done by running the load_efact.sas processor. This processor will load 1 of the 3 currently available sets of emissions factors. The command line for this processor would read:

sas -sysparm “V2" load_efact.sas

This example would read version 2 of the available emissions factors. Later in this document there is a brief discussion of the differences between the different emission factors which are included with the model.

Next the modeler would need to subset the BELD3 database for the local modeling grid. This is done with the subset_beld3.sas processor. This processor needs to be told the definition of the modeling grid as it relates to the BELD3 projection system. An example of this for the 12km Eastern Unified grid is:

Sas -sysparm “5524;3012;2808;2412;12" subset_beld3.sas

Where 5524= the X origin of the photochemical modeling cell within the BELD grid
3012= the Y origin of the photochemical modeling cell within the BELD grid
2808= the number of BELD3 X cells to include
2412= the number of BELD3 Y cells to include
12= Number of BELD cells to use to create one Photochemical modeling cell.

The output of this processor is a set of emission estimates based on the emission factors and the BELD data for standard meteorological conditions. These estimates are then run through the btap.sas processor to adjust the emission for the specific temperature and solar radiation by cell and hour in the photochemical modeling grid. The model has a number of options to shape the output values. Here is an example of how to run the model:

sas -sysparm “BEIS3;7;1.43" btap.sas

where: BEIS3 = is the algorithm set the model should use(beis2 or beis3)
7 = the number of layers in the canopy model
1.43 = the Isoprene adjustment factor.

The output of this processor is a dataset called ems_run.bioemis. Dataset contains estimates by icell, jcell, hour, plant species and pollutant. It is a day specific emissions estimate.
These emission estimates can then be speciated into the photochemical/aerosol model format using the fastspec_bio.sas processor to create UAMV/CAMX style output files. Additional processor can then be used to convert those files into IOAPI files for use in CMAQ and Models3.

Finally, The user can run a small set of reports which help the user see potential problems with the data. These reports are run with the web/biorep.sas processor and will create 5 reports.

The first is a report by state and pollutant, this report shows tons per day. The second report shows the state and County total emissions. The third and final report shows the emissions by state and plant species. This will give the user a rough idea of the impact of certain plant species by state. Finally the processor automatically draws a tile plot by pollutant of emissions for the photochemical modeling grid. Examples of these reports can be found on the LADCO web site at www.ladco.org/emis/biome3/reports.htm . In the past, the number of reports has increased over time as the modelers needed new reports to diagnose newly identified problems. Because BIOME3 is written in SAS the inclusion of new reports is easy.

LADCO BIOME3 Sensitivity runs.

This portion of the document is intended to show the results of changes to the inputs or calculation methods of the BIOME3 model. The intent of this analysis is to show the potential impact of changes to the inputs of the model. It is not intended to suggest the changes that LADCO or any other organization should make to the model without further analysis. It only suggest the impact of those changes on the emissions estimates

Table 1. Shows the results and describes each run. For relative purposes we are using run B0 as a baseline run. Initially, we believed that this should be the de-facto methodology for modeling biogenics. We now know that there are better schemes within the model but this is the starting point. We attempted to change only one variable for each sensitivity test.

Run1. Version 1 Emissions Factors.

There were three sets of emissions factors included with the model. These factors are best described by portions of Jim Wilkinson's BIOME3 Code:

1) beis3_efact_version_1.dat

The newest version of the biogenic emissions factors for use with the BELD3 data base with updated isoprene, monoterpene, nitric oxide, and especially the OVOC category which now contains methanol and 2-methyl-3-butenol (MBO). By including methanol and MBO, the OVOC go up substantially.

2) beis3_efact_version_2.dat

The newest version of the biogenic emissions factors for use with the BELD3 data base with updated isoprene, monoterpene, nitric oxide, and especially the OVOC category, but unlike the file described in Item (1) the OVOC does not contain methanol and MBO; hence the resulting OVOC estimates are much closer to those estimated by BEIS2.

3) beis3_efact_version_3.dat

The third version is identical to Version 1 except that it explicitly identifies the individual chemical species instead of the summed groups.

The version 1 and 3 emissions factors include Methanol(and to a lesser extent MBO) in OVOC.

The emission factors increase dramatically. This sensitivity analysis shows a 230% increase in OVOC emissions with the new emissions factors. Further discussion of this issue should include the agreements on what level of reporting methanol is included in the modeling and how to modify speciation methods to include this increase in methanol. It should be pointed out that the number of pollutants resulting from the version 3 of the emissions factors for a domain as large as the eastern unified results large files. In the future we will need to re-think the entire Biogenics to chemical mechanism(CB-IV, SAPRC) method within all emissions models. It will use more direct calculation of individual species instead of the 4 main groups(ISOP, NOX, OVOC, TERP) for a larger number of directly calculated emissions estimates for as many as 30 individual chemical species. This will be especially important for particulate and haze modeling because monoterpene species have such important roles in particulate formation.

Run 2 Meteorological Inputs Change.

This run was an attempt to look at the change due to modifying the meteorological inputs from the Meteorological model MM5. This review was to look at the effect of changing the temperature from the 15 meter height to the Surface temperature as defined by MM5. In the past modelers have used the Surface temperature in biogenic emissions processing. The term 15M height is somewhat deceptive, In fact it is really the average temperature of the first layer in the meteorological model which for our modeling is 30 meters thick. Not all meteorological modelers will use this configuration. We believe that the best future value for Temperature in the biogenics models is the 15 meter height, This run will give us a good comparison to what change can be attributed to this recent change in modeling techniques.

Run3. Number of Canopy Layers

This run was an attempt to use the canopy layer within BIOM3 to calculate emissions. The result of this run showed a very small change in isoprene emissions. In future runs we will further stress the model by using 20 and 2 layers to see if there is a significant difference between these widely varying values.

Run 4 and Run 5. Oak Isoprene Reduction.

These runs test the potential reduction in isoprene emissions if the oak emissions factor were divided by 2 and 5(50% and 80% reductions). As we see, for the eastern unified domain, changing the oak emissions has a large effect on isoprene emissions, Nearly cutting total biogenic isoprene in half for the domain. It is not the intent of this run to suggest that users should adjust emissions factors for oak. This run was intended to look at the impact of oak and any possible over-prediction in the Oak estimates. We believe that problems with oak could be in any or all of biomass, landuse, emissions factors, or photochemical model chemistry. This run is not intended to answer where the problems are, Only how potential problems are likely to effect modeling.

Run 6. BEIS2 Methodology

This run examined the impact on the total inventory of using the BEIS2 calculation methodology

instead of the BEIS3 methodology. The results show an increase of 25% when using the BEIS2 methodologies. This result is based only on calculation differences and uses all of the same inputs including biomass emissions factors, and Solar radiation.

Future Directions.

Like most sensitivity runs, These runs have raised new questions as they have answered. Based on these results, The following sensitivity run would be suggested.

1.Run with 20 and 2 canopy layers.

Future Directions for BIOME3

Biome3 is a dynamic model over the next several months we will continue to update and improve the model to include new methods and greater Quality Assurance and reporting capabilities. These capabilities will improve where the users need them. Most likely improvements will include.

1. Further speed improvements to the BTAP.SAS processor.
2. Reporting improvements for input data.
3. BELD3 updates for local areas(Oak in Chicago)

Table 1. BIOME 3 Results for Selective sensitivities(Estimates for July 19th 1998).

Run#	Biogenics Algorithm	EF Version	Canopy Layers	Isoprene Divisor	PAR Source	Temp. Height	Isoprene tons/day	NOX Tons/Day	OVOC Tons/Day	TERP Tons/Day
B0	B3	V2	7	1	Pierce	15M	139,773	5,206	38,747	34198
B1	B3	**V1**	7	1	Pierce	15M	139,773	5,206	129,148	34198
B2	B3	V2	7	1	Pierce	**surf**	142,328	5217	38,865	43,297
B3	B3	V2	**5**	1	Pierce	15M	139,322	5,206	38,747	34,198
B4	B3	V2	7	**2**	Pierce	15M	102,521	5,206	38,747	34,198
B5	B3	V2	7	**5**	Pierce	15M	80,171	5,206	38,747	34,198
B6	**B2**	V2	7	1	Pierce	15M	131444	5,206	38,747	34,198
B7	B3	V2	7	1	Wilkinson	15M	119,983	5,206	38,747	34,198
B8	B3	V2	20	1	Pierce	15M	139,981	5,206	38,747	34,198
B9	B3	V2	3	1	Pierce	15M	134,043	5,206	38,747	34,198

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Attachment A. Photosynthesis Activated Radiation

Calculation algorithms:

1. Tom Pierce/EPA/CMAQ method:

RGRND * PF * CF = PAR

- RGRND = ground level radiation (watts/m2) calculated by CMAQ's MCIP processor based on MM5 output fields
- PF = percent of the radiation that is in the PAR spectrum based on observed data = .45
- CF = conversion factor to convert radiation in watts/m2 to micro-moles/m2-sec, which is what the BEIS model in SMOKE needs PAR units to be = 4.6

RGRND * .45 * 4.6 = PAR

-or-

RGRND * 2.07 = PAR

5. Jim Wilkinson method:

SWDWN * PF = PAR

- SWDWN = shortwave downward radiation variable as output by MM5 model (watts/m2)
- PF = percent of the radiation that is in the PAR spectrum = .5 based on literature
- CF = conversion factor to convert radiation in watts/m2 to micro-moles/m2-sec, which is not needed since the BIOME3 model needs PAR units to be watts/m2

SWDWN * .5 = PAR

Issues/Questions:

1. How different are RGRND and SWDWN?
2. How do PAR values calculated by these methods compare to GOES satellite data?

This table was produced by Kirk Baker at LADCO