MODELING EMISSIONS INVENTORY PREPARATION FOR THE CALGRID PHOTOCHEMICAL AIR QUALITY MODEL

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Abstract

The CALGRID photochemical air quality model was originally developed as part of a project to upgrade and modernize the Urban Airshed Model (UAM). More recent versions of the CALGRID model were developed for the Ozone Transport Commission (OTC) for use in screening and evaluating the effectiveness of emissions control strategies. The earlier versions of the OTC CALGRID modeling platform were designed to take UAM-style emissions files as input. However, the goal of the current OTC CALGRID modeling effort is to supplement the SIP-quality modeling being done with the Community Multiscale Air Quality Model (CMAQ). To best achieve this goal, it was decided that the CALGRID model would be run on a common set of inputs as the CMAQ model, including boundary conditions, meteorology, and emissions. This presented a special challenge in processing and formatting the modeling emissions inventory for use with the CALGRID air quality model.

1. Introduction

As many states are in the process of preparing their State Implementation Plans (SIPs) for ozone attainment, they have relied on the air quality modeling being done on the Community Multiscale Air Quality Model (CMAQ) platform. This modeling is very resource intensive and requires the use of a Unix-based system. Therefore, the SIP-quality CMAQ modeling is being conducted at a handful of modeling centers that have the technical and computer-related capabilities to perform this type of analysis. To relieve some of the technical burden on the modeling centers, the Ozone Transport Commission (OTC) sponsored the development of another grid-based photochemical modeling platform. Among the requirements for this new platform were that it be flexible, portable (i.e. PC-based), and easily accessible to agencies that wish to use it.

The CALGRID photochemical model was selected as the basis of the new modeling platform. The CALGRID model originated from a California Air Resources Board (CARB) project to upgrade and modernize the Urban Airshed Model (UAM).[1] CALGRID versions 2.0 and higher were subsequently developed to meet the needs of the OTC and others. Early versions of CALGRID 2.0 were able to take directly as input the UAM-style emissions files that were used in the modeling done by EPA in its Clear Skies Act and Clear Skies Initiative analyses.

An emissions pre-processor, EMSPROC, was developed in a cooperative effort between the New Hampshire Department of Environmental Services (NHDES) and Earth Tech, Inc. of Concord, Massachusetts. EMSPROC is used to adjust and scale the input emissions files, allowing CALGRID users to model a variety of emissions control scenarios. Subsequent versions of the CALGRID 2.0 platform were run with emissions inputs taken from the REMSAD modeling done in support of the Clear Skies Act analysis. Special conversion programs were written to re-format the REMSAD emissions inputs to UAM-style inputs for use with CALGRID. Now, a similar approach has been taken with the current CALGRID modeling platform, which has been updated to CALGRID version 2.45. The input emissions for this platform are the same as those used for the CMAQ SIP-quality modeling platform. Again, special conversion programs and utilities needed to be written to adapt these files for use with CALGRID. The emissions file conversion that was done for the CALGRID version 2.45 platform is the focus of this discussion.

2. Modeling Emissions Inventory

2002 was selected as the base year for the OTC ozone SIP modeling. The 2002 National Emissions Inventory (NEI) served as the basis for the modeling inventory. With contractor assistance, the Regional Planning Organizations (RPOs) developed the necessary files for input to the Sparse Matrix Operator Kernel Emissions (SMOKE) emissions model and subsequent input to CMAQ. Similarly, projected 2009 emissions inventories were developed by the RPOs and their contractors for the On The Way (OTW) and Beyond On The Way (BOTW) emissions scenarios. Ultimately, the OTC SIP-quality modeling platform included modeling emissions inventories developed by:

- ⇒ CENRAP
- ⇒ MANE-VU
- ⇒ MRPO
- ⇒ VISTAS

Year 2000 Canadian emissions were also included in the OTC modeling platform. During the modeling emissions inventory development process, revisions and updates were made to the various RPOs' inventories. These revisions are not discussed in detail here. However, the latest versions of the various RPOs' inventories were recently incorporated into the most recent update of the OTC SIP-quality modeling inventory.

3. Problem Statement and Technical Discussion

As discussed earlier, it was decided that the CALGRID 2.45 modeling platform would be run on a common set of inputs as the OTC SIP-quality CMAQ modeling platform. It was also required that the flexibility of adjusting the input emissions for control strategy analysis be maintained. Thus, the challenge was to convert the pre-merged SMOKE emissions files for direct input into EMSPROC, the emissions pre-processor for the CALGRID modeling system. The 2002 and 2009 pre-merged SMOKE files were obtained from the appropriate modeling centers. These pre-merged files were broken down into the following general emissions categories:

- ⇒ Area
- ⇒ Biogenic
- ⇒ On-Road Mobile
- ⇒ Non-Road Mobile
- ⇒ Point

Each of these emissions categories was further broken down by each of the RPOs that originally developed their inventories. This regional breakout of emissions files was inconsistent with previous CALGRID platforms for which EMSPROC was developed. To preserve the ability to adjust emissions with EMSPROC, the approach was taken to "merge" all of the individual-RPO inventories into a single EMSPROC-ready file for each of the emissions source categories. In this way, EMSPROC could be used in the same manner as in previous versions of the CALGRID modeling system. Please note that much of the following discussion is taken from the user's guide for the most recent version of the EMSPROC emissions processor, EMSPROC6.[2]

During the development of the current version of the CALGRID modeling platform, it was decided that the entire OTC SIP-quality modeling domain would be used. The modeling domain and the associated emissions files were set up on a Lambert Conic Conformal (LCC) projection with a 12-km grid cell resolution. The modeling domain is shown in Figure 1.

As mentioned above, the approach was taken to merge the individual RPOs' emissions files into single files for the area, on- and off-road mobile, and point source categories. Biogenic emissions were not broken down to the RPO level, but they still had to undergo a similar merging and conversion process. A significant difference in file structure exists between the emissions files used in the current CMAQ to CALGRID conversion project and the UAM-style emissions files that were used with earlier versions of CALGRID. Specifically, the point source emissions are now defined on a 3-dimensional grid with elevated emissions being assigned to the appropriate vertical layer. The UAM-style elevated point source emissions were defined by locating each individual point source by its lat/long coordinates and calculating its plume rise with the applicable stack characteristics. This fundamental difference in file structure influenced the way in which the merging and conversion utilities were set up, and it also necessitated changes in the CALGRID model itself, hence version 2.45.

Another significant challenge to re-formatting and converting the SMOKE files for use with the EMSPROC/CALGRID system was the data format of the files.

All of the SMOKE files were provided in Unidata's Network Common Data Form (NetCDF) format. Unidata is a National Science Foundation-sponsored program that provides universities and other institutions with innovative means to analyze earth science-related data. The intent of NetCDF was to provide a common data format among Unidata's applications, and it functions as an I/O library callable by FORTRAN and other programming languages.[3] As a first step in the conversion process, the NetCDF utility, ncdump, was used to convert the binary NetCDF data files into ASCII representations of the data in network Common data form Description Language (CDL). The resulting CDL files could be quite large, exceeding 100 MB in some instances. Further, since there was one pre-merged SMOKE file for each RPO and each emissions category, many CDL files were created for each modeling episode day.

Once the NetCDF-formatted SMOKE files were converted to CDL, a specially-written processor called MERGE was used to merge the various RPOs' inventories into a single emissions file for each emissions component. As mentioned earlier, the biogenic emissions files went through a similar CDL conversion and merging process, since the MERGE program has the dual functions of merging the separate RPO files and creating an output emissions file in the format suitable for input into the EMSPROC6 emissions processor. Two-dimensional and three-dimensional versions of the MERGE program were written to handle the 2-D surface and 3-D elevated point source components of the inventory. Further, a separate specialty processor, ADDER, was written to address the fact that MRPO provided two separate area source inventories – one for ammonia and one for the other pollutants. The ADDER program took these two inventory files at the CDL level and blended them to create a resulting CDL file that included all pollutants. This CDL file was then input into the MERGE routine described above.

Once the merging process was complete, the resulting converted emissions files by component were ready for input into the EMSPROC6 processor. Although the user inputs for the EMSPROC6 emissions processor have remained unchanged since previous versions, significant changes were made to the underlying core of the program to accommodate the new file structures encountered by using the SMOKE pre-merged emissions files versus the UAM-style emissions files used in previous CALGRID platforms. Similar to the MERGE program, two-dimensional and three-dimensional versions of EMSPROC6 were written to accommodate the 2-D surface emissions and the 3-D point source emissions. However, as mentioned, the EMSPROC6 input file structure, which allows the user to scale emissions by hour, pollutant species, emissions component, geographic area, or any combination thereof, were kept consistent between the 2-D and 3-D versions as well as with previous versions of EMSPROC.

An overview of the process used to create CALGRID model-ready emissions from the pre-merged SMOKE emissions files is shown in Figure 2.

4. Data Processing and Quality Assurance

Once the ADDER, MERGE, and EMSPROC6 programs were developed and fully tested, the full set of pre-merged SMOKE emissions files were obtained from the CMAQ modeling centers. The conversion programs were then put into production to convert all of the SMOKE files for use with the OTC CALGRID 2.45 modeling platform. Because of the large amount of data and the number of processing steps involved, batch files were used to automate the processing and to eliminate the error involved with performing each part of the process individually. In summary, batch files were set up to:

- ⇒ Decompress (gunzip) the NetCDF pre-merged SMOKE files, which were provided by the modeling centers in compressed format.
- ⇒ Convert, using ncdump, the decompressed NetCDF files into ASCII CDL format.
- ⇒ Run the ADDER program to combine the MANE-VU with- and without-ammonia area source inventories into a single MANE-VU area source CDL file with all pollutants.
- ⇒ Run the 2-D and 3-D versions of MERGE to combine the separate RPO CDL files into single EMSPROC-ready emissions files for the area, on-road mobile, non-road mobile, and point source emissions categories.
- ⇒ Run the 2-D version of MERGE on the biogenic CDL file to create an EMSPROC-ready biogenic emissions file.
- ⇒ Run the 2-D and 3-D versions of EMSPROC6 to create model-ready merged 2-D surface emissions and 3-D point source emissions for direct input into the CALGRID 2.45 air quality model.

Fortunately, all of the processing steps outlined above only needed to be performed on a one-time basis. Once the gunzip, ncdump, ADDER, and MERGE processing was complete for a given modeling episode day, the resulting EMSPROC-ready files by emissions component were retained for subsequent input into EMSPROC6. In this manner, all the necessary emissions files were created to either run CALGRID directly (i.e. run the base cases with the 2-D surface and 3-D point emissions) or run EMSPROC6 to scale the base case emissions and create adjusted model-ready 2-D surface and 3-D point emissions for input into CALGRID.

Processing time and data storage were two additional challenges encountered during this project. It took over four hours of processing time to convert a single episode day's worth of emissions files on a machine with a 2.4 GHz processor and 785 MB of RAM. Similarly, it took just over 800 MB of storage to preserve a single episode day's worth of the necessary EMSPROC-ready emissions component files required for emissions scaling purposes. Data storage capabilities were expanded for this project with the purchase of relatively inexpensive external hard drives, generally of 250 to 300 GB capacity.

Quality Assurance and Quality Control (QA/QC) measures were employed during the data processing to ensure that an accurate and high-quality CALGRID-ready modeling inventory was being created from the SMOKE files. The MERGE programs include user inputs to generate QA/QC plots for a desired hour and pollutant species. The graphical output of the MERGE program is in a format suitable for plotting with a package such as Golden Software's SURFER software. Figure 3 provides an example plot from the 2-D MERGE program; this example shows the on-road mobile source CO emissions for hour 12 of the August 6th episode day. The EMSPROC emissions pre-processor has always incorporated features for QA/QC of the emissions processing, including easy-to-read emissions tabulations and graphical output. These features were retained in the EMSPROC6 systems. With EMSPROC, graphical outputs can be produced for plotting with SURFER or the Center for Ocean-Land-Atmosphere Studies' Grid Analysis and Display System (GrADS). Figures 4 though 10 show examples of 2-D merged surface and 3-D point source emissions plots. QA/QC plots such as these provide confidence that the user has created a high-quality modeling inventory for input into CALGRID; they are also useful for analyzing the data and revealing the limitations of the underlying inventories (e.g. Figure 7 for primary fine particle emissions). Figure 11 provides an example of the tabular QA/QC output provided by the EMSPROC processor.

5. Summary and Conclusions

The CALGRID photochemical air quality modeling system provides the air quality community with a means of performing screening-level modeling for purposes of SIP planning, control strategy assessment, and weight-of-evidence (WOE) analysis. By using the CALGRID modeling system, multiple emissions scenarios can be run relatively easily, thus relieving the burden on the very resource-intensive SIP-quality CMAQ platform. Further, the CALGRID modeling system is highly transportable and allows a high throughput of additional modeling beyond the traditional Unix-based SIP modeling platforms.

To make the CALGRID 2.45 system the best tool possible for supplementing the CMAQ SIP-quality platform, it was designed to be run on a common set of inputs. Using the processing steps outlined above, the pre-merged SMOKE emissions files that were provided by the CMAQ modeling centers were converted into a useable, quality-assured modeling inventory for the CALGRID system. The CALGRID 2.45 model has been successfully run on this modeling inventory and has exhibited acceptable model performance. Because the EMSPROC/CALGRID modeling system is designed to be run in a PC-based environment, this CALGRID modeling emissions inventory development project has provided the air quality community with the benefit of taking a SIP-quality modeling inventory and making it more accessible to a wider variety of users.

6. References

1. G.R. Carmichael, Y.S. Chang, J.S. Scire, and R.J. Yamartino, *CALGRID: A Mesoscale Photochemical Grid Model, Volume II: User's Guide*, 1989.

2. Earth Tech, Inc., *Technical Memorandum: Documentation for the MERGE-EMSPROC6 Processing System for CMAQ to CALGRID Emissions Processing*, 2006.

3. Harvey Davies, Glenn Davis, Steve Emmerson, Ed Hartner, and Russ Rew, *The NetCDF Users Guide: Data Model, Programming Interfaces, and Format for Self-Describing, Portable Data*, 2006.

Figure 1: Map of the OTC 12-km, 172 x 172 Grid Cell Modeling Domain

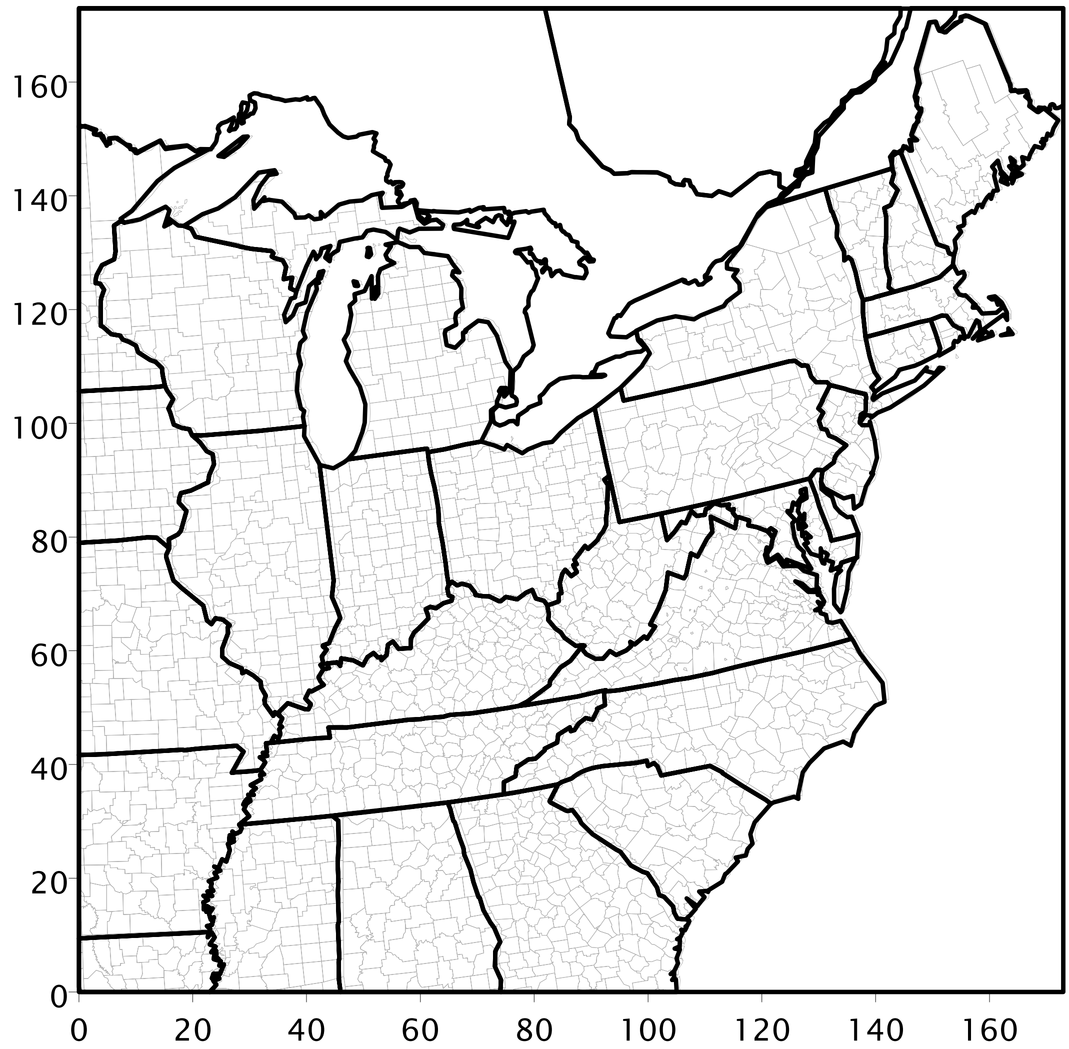

Figure 2: Overview of the Process Used to Create CALGRID Model-Ready Emissions from the Pre-Merged SMOKE Emissions Files

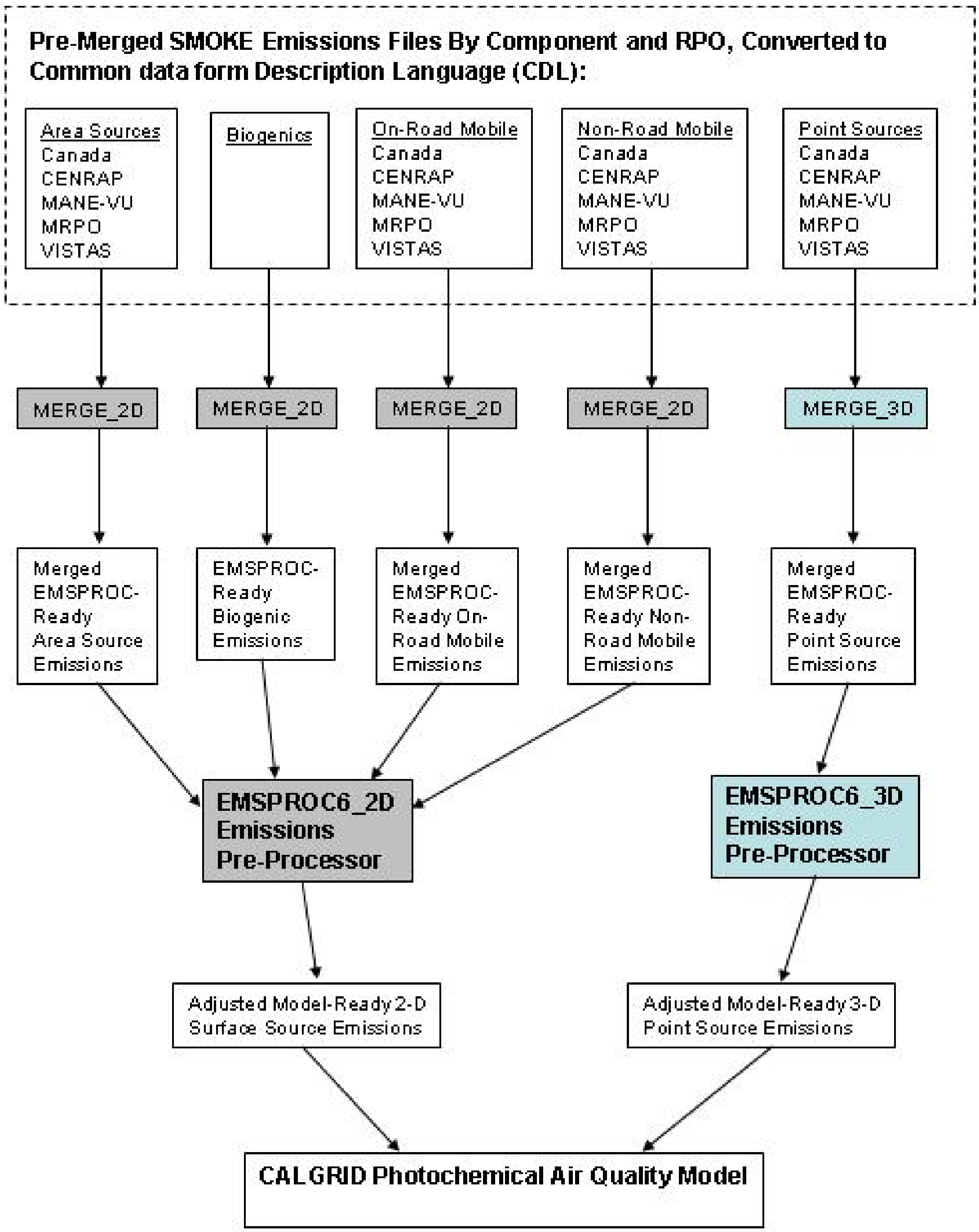

Figure 3: QA/QC Plot from the 2-D MERGE Processor

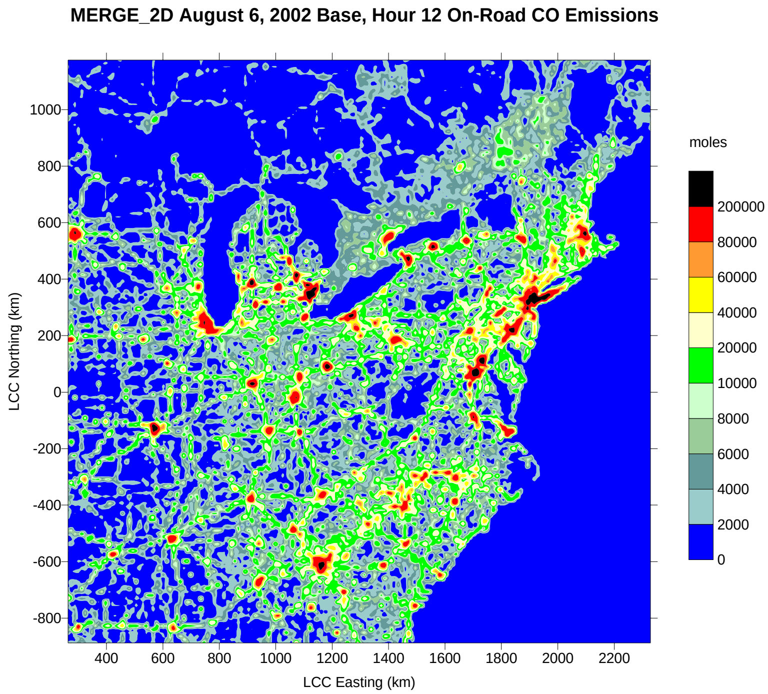

Figure 4: QA/QC Plot of 2-D EMSPROC6 Surface CO Emissions

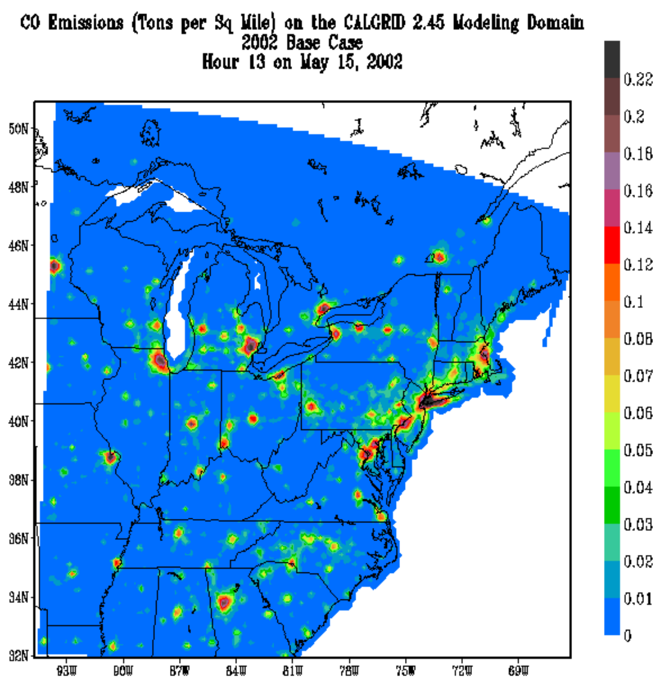

Figure 5: QA/QC Plot of 2-D EMSPROC6 Surface NOx Emissions

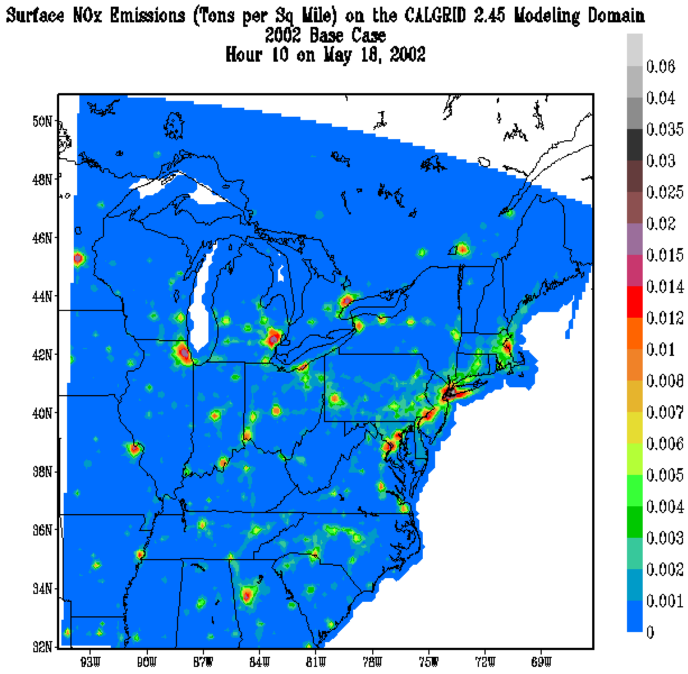

Figure 6: QA/QC Plot of 2-D EMSPROC6 Surface VOC Emissions

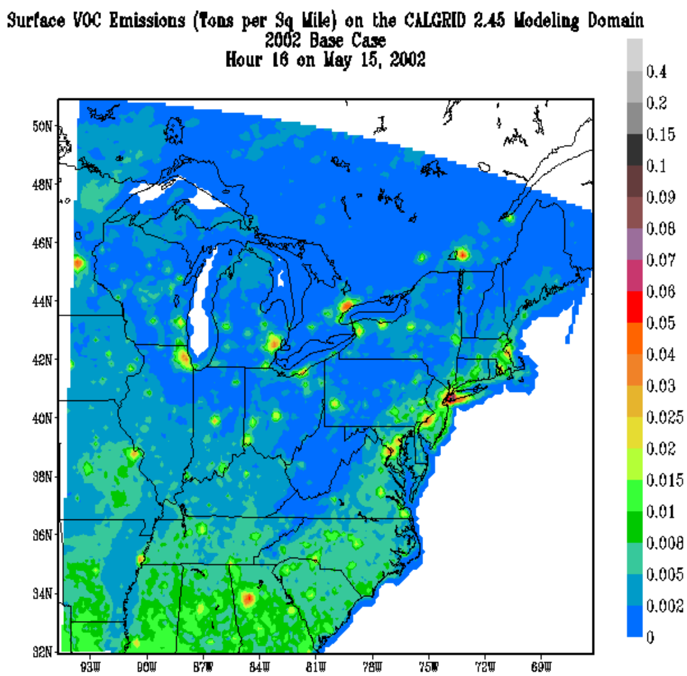

Figure 7: QA/QC Plot of 2-D EMSPROC6 Surface Primary Fine Particle Emissions

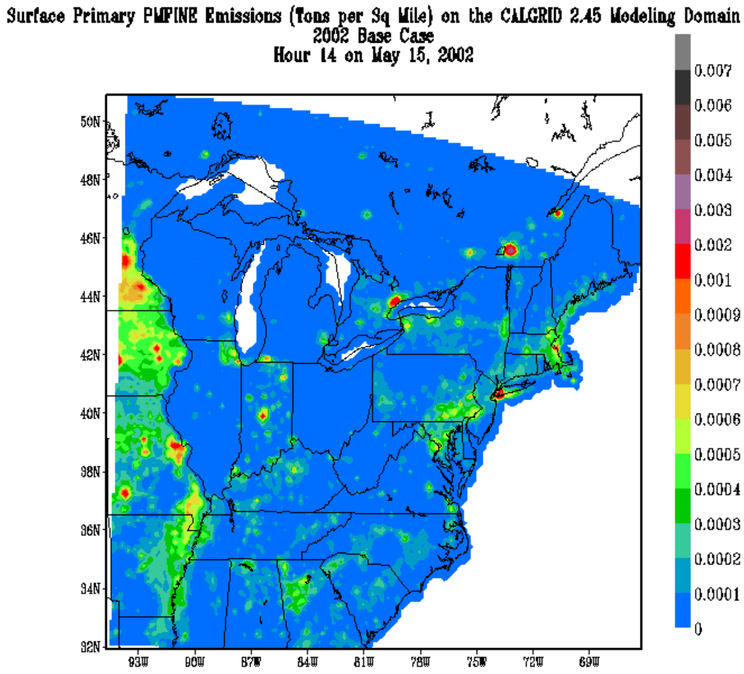

Figure 8: QA/QC Plot of 3-D EMSPROC6 Point Source NOx Emissions

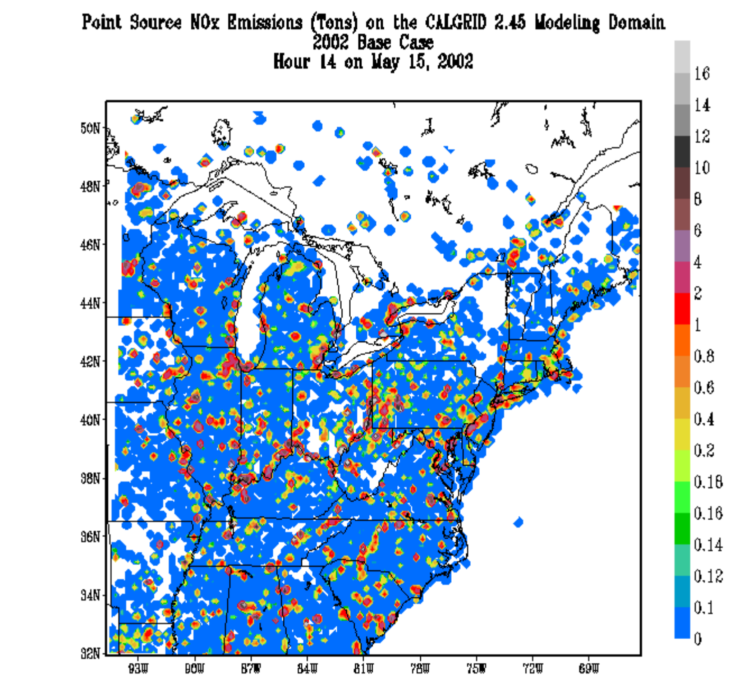

Figure 9: QA/QC Plot of 3-D EMSPROC6 Point Source SO2 Emissions

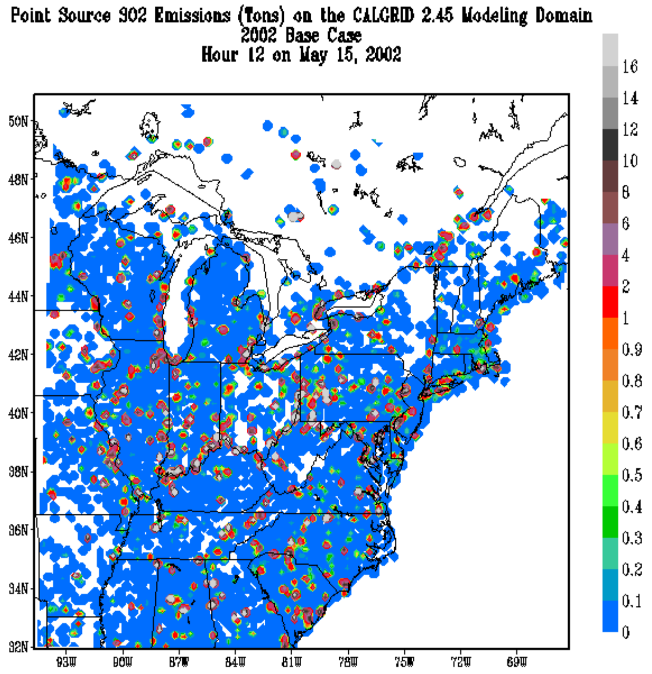

Figure 10: QA/QC Plot of 3-D EMSPROC6 Point Source VOC Emissions

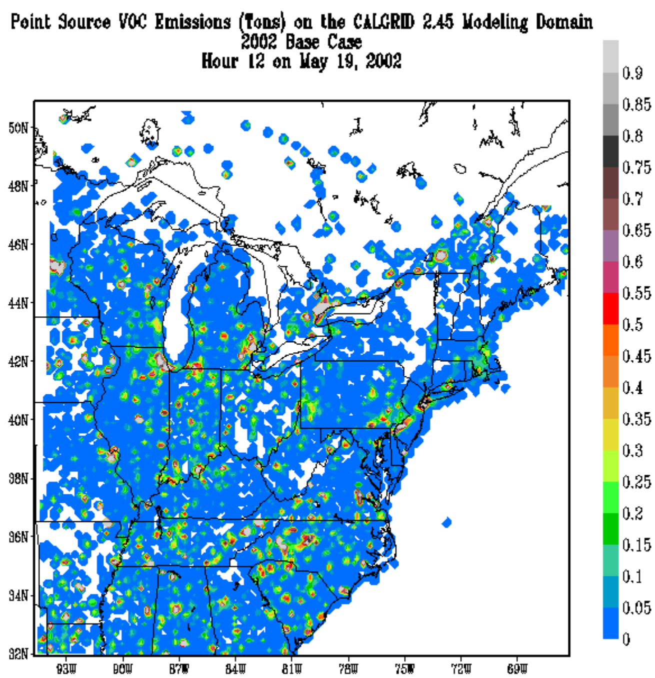

Figure 11: Example of 2-D EMSPROC6 Tabular QA/QC Output (in Tons per Day)

EMSPROC Emissions Processing: Create 2-D Emissions for 2002 Base Case Day 05/15/02

Total Emissions for the Day by Sector:

Sector	NOx Before	NOx After	Delta NOx	VOC Before	VOC After	Delta VOC	SO2 Before	SO2 After	Delta SO2
Biogenic	1639.99	1639.99	0.00	41381.60	41381.60	0.00	0.00	0.00	0.00
Area	2058.89	2058.89	0.00	12148.05	12148.05	0.00	2430.64	2430.64	0.00
Nonroad	4130.89	4130.89	0.00	5551.31	5551.31	0.00	612.04	612.04	0.00
Mobile	10210.26	10210.26	0.00	8445.54	8445.54	0.00	500.15	500.15	0.00
Total Em	18040.03	18040.03	0.00	67526.51	67526.51	0.00	3542.83	3542.83	0.00

Strategy NOx Emissions

Zone	Biogenic	Area	Nonroad	Mobile
AL	33.36	17.25	105.47	253.15
AR	81.54	37.39	112.48	274.66
CT	3.11	21.40	44.29	136.61
DE	3.92	2.78	25.87	40.43
DC	0.06	2.10	5.64	18.32
GA	62.65	61.57	195.59	561.35
IL	203.75	255.07	257.38	534.40
IN	99.95	135.93	159.82	413.22
IA	143.41	13.17	187.71	176.38
KY	71.98	78.93	171.60	286.46
LA	15.78	78.25	36.40	95.41
ME	6.98	12.87	18.49	110.28
MD	11.42	28.07	67.88	261.86
MA	3.69	52.99	70.82	275.99
MI	70.68	118.46	158.98	614.88
MN	36.21	89.65	106.04	241.29
MS	44.01	6.95	103.51	147.07
MO	113.52	54.57	138.48	319.89
NH	1.74	20.43	19.39	76.97
NJ	6.98	62.71	125.96	339.40

Figure 11, Continued

NY	44.04	155.98	179.89	614.55
NC	32.04	59.16	173.24	556.14
OH	115.43	174.83	205.96	582.34
PA	51.49	89.99	203.56	769.15
RI	0.63	6.68	8.92	36.67
SC	39.18	32.71	96.55	258.41
TN	93.67	28.98	193.56	449.05
TX	0.52	3.89	3.32	9.35
VT	5.13	6.84	8.80	42.64
VA-OTR	1.55	12.29	27.79	90.77
VA-NOTR	24.93	68.06	91.56	305.18
WV	12.57	19.36	50.33	114.71
WI	75.07	80.69	110.55	270.98
Other	128.94	169.21	665.85	934.11

Strategy VOC Emissions

Zone	Biogenic	Area	Nonroad	Mobile
AL	4037.04	290.05	138.38	249.05
AR	3206.74	158.23	113.44	117.15
CT	58.44	213.77	93.60	87.68
DE	72.54	41.46	20.12	28.36
DC	1.37	15.24	4.89	15.63
GA	4678.74	653.93	222.91	618.81
IL	1424.97	591.91	243.82	396.40
IN	648.72	359.73	141.70	356.36
IA	875.01	185.04	93.91	156.60
KY	1581.47	212.60	111.82	228.73
LA	1325.33	56.75	40.23	54.71
ME	457.48	263.99	88.41	71.79
MD	302.76	301.52	138.65	205.92
MA	76.24	414.67	138.52	153.91
MI	641.89	436.26	371.58	481.82
MN	929.78	302.62	65.45	165.68
MS	2992.85	234.49	76.66	189.87
MO	3127.12	289.30	244.06	208.39
NH	82.38	193.00	68.71	59.52
NJ	262.63	482.45	226.58	309.05
NY	283.95	1329.26	423.90	595.90
NC	2516.99	416.43	224.12	635.71
OH	424.52	465.90	221.58	492.39
PA	346.58	696.46	319.61	596.24
RI	22.06	98.75	19.83	41.41
SC	2254.29	295.61	147.21	241.24
TN	2369.07	360.62	185.45	389.67
TX	99.59	8.11	1.49	3.53
VT	68.94	76.84	31.36	41.89
VA-OTR	64.51	70.03	38.75	64.44
VA-NOTR	1331.20	249.81	141.77	244.46
WV	151.98	141.92	44.20	96.72
WI	694.14	580.02	241.17	199.79
Other	3973.80	1662.97	868.63	648.21

Strategy SO2 Emissions

Zone	Biogenic	Area	Nonroad	Mobile
AL	0.00	112.48	13.03	15.28
AR	0.00	58.14	15.79	11.60
CT	0.00	29.28	5.15	4.18
DE	0.00	2.16	9.21	1.24
DC	0.00	2.58	0.80	0.70

Figure 11, Continued

GA	0.00	153.23	26.60	28.13
IL	0.00	34.98	37.03	24.13
IN	0.00	177.98	25.47	23.48
IA	0.00	7.57	28.01	7.34
KY	0.00	105.90	29.48	15.59
LA	0.00	84.53	6.73	3.95
ME	0.00	33.56	2.49	4.26
MD	0.00	32.74	17.30	10.44
MA	0.00	128.32	8.93	7.98
MI	0.00	109.08	21.49	36.14
MN	0.00	32.68	13.82	6.49
MS	0.00	1.25	16.34	8.35
MO	0.00	97.99	19.94	13.49
NH	0.00	19.95	2.48	2.05
NJ	0.00	40.57	35.39	10.42
NY	0.00	316.06	27.88	27.64
NC	0.00	14.45	23.31	32.52
OH	0.00	49.86	28.77	39.49
PA	0.00	169.56	30.90	33.57
RI	0.00	11.99	0.97	1.07
SC	0.00	33.25	13.37	15.21
TN	0.00	86.22	29.69	23.90
TX	0.00	1.65	0.19	0.36
VT	0.00	12.17	1.11	1.93
VA-OTR	0.00	27.71	4.85	3.74
VA-NOTR	0.00	233.33	18.65	14.41
WV	0.00	28.16	5.18	6.40
WI	0.00	24.35	15.11	15.02
Other	0.00	157.80	76.69	49.71