Final Report

Southeast Michigan Air Quality Modeling Study

Prepared by:
Georgia Institute of Technology

Prepared for:
Lake Michigan Air Directors Consortium

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List of Acronyms

AQM	Air Quality Model
BC	Boundary Conditions
BEIS	Biogenic Emission Inventory System
CAMx	Comprehensive Air quality Model with extension
CB6	Carbon Bond—Version 6
CTM	Chemistry-Transport Model
EBI	Euler Backward Iterative (method)
EGU	Electrical Generating Unit
EGLE	Environment, Great Lakes and Energy
EPA	Environmental Protection Agency
HCHO	Formaldehyde
GIT	Georgia Institute of Technology
IC	Initial Conditions
ID	Identification
I/O API	Input/Output Applications Programming Interface
LADCO	Lake Michigan Air Directors Consortium
NMB	Normalized Mean Bias
NME	Normalized Mean Error
NAAQS	National Ambient Air Quality Standards
netCDF	network Common Data Format
NOx	Nitrogen Oxides
PAMS	Photochemical Assessment Monitoring Stations
PM	Particulate Matter
PM2.5	PM with an aerodynamic diameter less than 2.5 microns.
PPM	Piecewise Parabolic Method
QA	Quality Assurance
QC	Quality Control
RPO	Regional Planning Organization
RRF	Relative Reduction Factor
SEMI	Southeast Michigan
SIP	State Implementation Plan
SLAMS	State and Local Air Monitoring Stations
SMOKE	Sparse Matrix Operator Kernel Emissions
SMAT-CE	Software for the Modeled Attainment Test - Community Edition
TOMS	Total Ozone Mapping Spectrometer
TUV	Total Ultraviolet
US	United States
VOC	Volatile Organic Compounds
VCP	Volatile Chemical Products
WRF	Weather Research and Forecasting model

Document Change Record

Revision	Date	Remarks
1.0	December 15, 2022	Draft version for LADCO and Michigan EGLE review
1.1	February 13, 2023	Revised Final version

Executive Summary

The Southeast Michigan (SEMI) ozone nonattainment area had four regulatory monitors' three-year ozone design value (DV3) for 2020 violating the 2015 ozone National Ambient Air Quality Standards (O3 NAAQS) of 70 ppb. To better assist the Michigan Department of Environment, Great Lakes, and Energy (Michigan EGLE) for their needs to demonstrate attainment of the 2015 O_3 NAAQS for the SEMI nonattainment area (NAA), Georgia Tech team conducted high spatial resolution simulations of current (2016) and future (2023) year air quality in the SEMI region to evaluate emissions control strategies for mitigating surface ozone exceedances. Particularly, we used the Comprehensive Air Quality Model with Extensions (CAMx, Ramboll, 2021) version 7.10 to conduct the ozone simulations for the 2016 ozone season (April 12 -September 25) on a 1.3-km horizontal resolution grid covering the entire SEMI region.

We improved the modeling inventories for the base year by incorporating the addition of undercounted formaldehyde (HCHO) emissions and volatile chemical products (VCP) VOC emissions. We also updated the modeling inventories by switching to the alternative biogenic emissions using the MEGAN program instead of BEIS3. By utilizing the specifically prepared emissions inventories, we conducted nine sensitivity tests for the base year of 2016 to investigate the effect of the changes in the emissions inventory, specifically the enhancements of HCHO and VCP VOCs emissions, on model performance. The performance evaluation indicated that we should include additional HCHO emissions for the optimal base year simulation. We included the addition of VCP VOCs in the optimal configuration as well mainly for its better performance for MDA8 O_3 larger than 60 ppb. The performance evaluation doesn't support the switch to the MEGAN biogenic emissions for the region, mainly due to the simulated lower O_3 levels and worsened performance of isoprene (using the default 2013 LAIv) or too much of terpene emissions (using the GLASS 2016 LAIv). The performance evaluation also demonstrated that the optimal simulation for the base year 2016 is acceptable to the US EPA.

We further prepared the future year base emissions for the 2023 on-the-book (OTB) simulation and the emissions-controlled inventories for control strategies assessment. We conducted four ozone season future year simulations to assess impacts on projected future year ozone design values from 1) the VOC emissions reduction by implementing the Reasonably Available Control Technologies (RACT), especially those that reduce VCP VOC emissions on non-EGU point sources and the Ozone Transport Commission (OTC)-derived rules for Architectural and Industrial Maintenance (AIM) coatings and Consumer and Commercial Products to reduce VOC emissions from non-point VCPs, 2) the NOx emissions reduction by the Good Neighbor-like NOx RACT on non-EGU point sources, 3) the elimination of HCHO emissions from all stationary engines due to the adoption of oxycat or other controls in addition to any NOx emissions reductions obtained from the NOx RACT on the same engines, 4) the NOx and VOC emissions reduction from both the above NOx and VOC control strategies combined together. The results of experiments here in combination with the optimal base year simulation and the future year OTB simulation were then used to investigate the proposed control strategies impacts on projected future year design value (FDV) which can assist demonstration of modeled attainment of ozone NAAQS.

With on-the-book controls, among the ten sites in SEMI NAA, the projected DVF for the East 7 Mile site is 71.8 ppb which is the only one still at nonattainment. The proposed VOC controls would further bring the 2023 DVF at the East 7 Mile site down by 0.3 ppb, while the proposed NOx controls would only bring the DVF down by 0.093 ppb, and the HCHO controls would decrease the DVF by 0.068 ppb, which however are more effective than the NOx controls based on ppb per ton of emissions reduction. Based on the assessment results we recommend VOC controls combined with NOx controls (including the accompanied HCHO control as well) for the SEMI region. This is mainly because the VOC controls have larger impact on reducing ozone concentrations at the nonattainment high ozone sites in the region according to the experiments. At the same time, the experiment results also indicated that the combination of VOCs and NOx controls would enhance each other's impact on ozone reduction, though the enhancement are small.

Section 1: Introduction

The Southeast Michigan (SEMI) ozone nonattainment area has four regulatory monitors with three-year ozone design value (DV3) for 2020 violating the 2015 ozone National Ambient Air Quality Standards (O3 NAAQS) of 70 ppb, and may be reclassified from marginal nonattainment status to moderate nonattainment.

To demonstrate attainment of the 2015 O3 NAAQS for the SEMI nonattainment area in 2023, LADCO initiated the "Southeast Michigan Air Quality Modeling Study". The Georgia Institute of Technology (Georgia Tech) team was awarded the project on September 29, 2021 to perform the tasks to address the high spatial resolution ozone modeling and attainment test needs of the project.

The goal of this project is to evaluate emissions control strategies for mitigating surface ozone exceedances by conducting high spatial resolution simulations of current (2016) and future (2023) year air quality in the SEMI region. The results from this study will assist the Michigan Department of Environment, Great Lakes, and Energy (Michigan EGLE) in submitting to the U.S. EPA a nonattainment area State Implementation Plan (SIP) in early 2023 with an ozone attainment demonstration.

The project objectives are set as follows:

- Provide a 1.3-km resolution ozone simulation of the SEMI region for the base year 2016 that is acceptable to the US EPA based on model performance statistics.
- Improve emission inventories with the addition of undercounted formaldehyde (HCHO) and volatile chemical product (VCP) sources.
- Examine the role of added HCHO and VCP emissions in improving ozone model performance and response to control strategies.
- Assess the impacts of selected emissions control strategies on simulated ozone in 2023 and corresponding relative response factor (RRF) values.

The Georgia Tech team used the Comprehensive Air Quality Model with Extensions (CAMx, Ramboll, 2021) version 7.10 to conduct the ozone simulations for the 2016 ozone season (April 12 -September 25) on a 1.3-km horizontal resolution grid covering the entire SEMI region. In total, nine sensitivity tests were performed for the base year of 2016 to optimize the data and model configurations. Through these runs we investigated the effect of improvements to the emissions inventory, specifically the enhancements of HCHO and VCP VOC emissions, on model performance. Five future year simulations using the 2023 base emission year and four emissions scenarios reflecting potential control strategies were performed. We used results from these runs to assess the control strategy impacts on future year ozone design value projections. We particularly investigated the potential impact of select emissions control strategies on RRF values for future year ozone NAAQS attainment.

In this final report we summarize the results of the ozone simulations and analysis, which includes descriptions of the methods used for the analysis, the results of the analysis, and the interpretation of the results, along with recommendations for the optimal 2015 ozone NAAQS attainment strategies for the SEMI region based on the select emissions control strategies simulations. It also details the data collection, model configurations, modeling approaches, and quality assurance/quality control (QA/QC) processes that have been used in the project. It shows how have we have followed the US EPA guidance documents on air quality modeling and analysis (EPA, 2014; EPA, 2018) for the comprehensive approach to the acquisition, production, assessment, archival, and documentation of all data used for the project.

Section 2: Modeling Setup

This section describes the model configurations of the chosen computational system and the input datasets that were used for the modeling and demonstration tests in the project. The selected air quality model, CAMx, represents the best combination of scientific and computational formulations to satisfy the requirements of the SEMI project. It follows the recommendation in the EPA Modeling Guidance (i.e., Guidance on the Use of Models and Other Analyses for Demonstrating Attainment of Air Quality Goals for Ozone, PM2.5, and Regional Haze) and Appendix W to Part 51 of 40 Code of Federal Regulations: Guideline on Air Quality Models.

2.1 CAMx Model Configuration

The **C**omprehensive **A**ir quality **M**odel with e**x**tensions (CAMx) is an Eulerian photochemical transport model that can track gaseous and particulate air pollutants (ozone, PM2.5, PM10, air toxics, mercury) over multiple scales ranging from urban to continental (Morris et al, 2003a, 2003b, Ramboll 2021). The CAMx model was developed and is supported by Ramboll US Corporation, and its pre- and post-processors are in the public domain. In addition to the ozone and PM simulations for regulatory applications, CAMx also provides extension tools to probe source apportionment and emissions sensitivity problems. The CAMx model version 7.10 is used to conduct the modeling tasks in this project. The model is configured with the Carbon Bond 6 gas-phase chemical mechanism CB6r5 with CF2E Particulate Matter treatment by using the mechanism file CAMx7.1.chemparam.CB6r5_CF2E. It uses the Piecewise Parabolic Method (PPM) as the advection solver and the Eulerian Backward Iterative (EBI) method as the chemistry solver. In addition, the model is configured with ZHANG03 for dry deposition and without bidirectional NH_3 dry deposition (Table 2-1). We use the Intel Fortran Compiler ifort and icc v19.0.5 to compile the CAMx system. The same CAMx executable is used for all the base year and future simulations in this study with the same model configuration choices.

CAMx 7.10 allows multiple emission input files. It supports multiple point, 2-D and 3-D gridded emission files, alleviating the need to merge all sectors into a single file. Point, 2-D, and 3-D emissions files can be listed in any combination of netCDF or Fortran binary format. Although CAMx7.10 supports netCDF format, for this study we chose the Fortran binary format for all the inputs and outputs.

Table 2-1. CAMx configuration

Model Parameter	CAMx_v7.10
Advection Solver	Piecewise Parabolic Method (PPM)
Horizontal Diffusion	Implicit
ACM2_Diffusion	False
Gas Chemistry Mechanism	CB6r5
Gas Chemistry Solver	Euler Backward Iterative (EBI)
Aerosol Mechanism	CF2E
Clouds/Aqueous Chemistry	Implicit
Dry Deposition Model	Zhang03
Bidi_NH3_Drydep	none
Plume in Grid	none
Probing Tool	none

2.2 Modeling Grid

The SEMI1 CAMx modeling grid is defined on a Lambert Conformal Conic projection centered on 40°N and 97°W that covers the SEMI region with a 1.33-km grid resolution. The map projection parameters and horizontal grid definition information for the SEMI1 modeling grid is given in Table 2-2. Figure 3-2 shows the nested LADCO4 and SEMI1 modeling domains. LADCO4 is a 4-km modeling grid, for which a LADCO study has produced CAMx modeling results for year 2016.

Table 2-2. Projection parameters and horizontal grid definition for the SEMI1 modeling grid

Parameter	SEMI1 1.33-km grid
Map Projection	Lambert Conformal Conic
P-alpha	33°N
P-beta	45°N
P-gamma	97°W
X-cent	97°W
Y-cent	40°N
X-orig	1024,000 m
Y-orig	236,000 m
dx	1,333 m
dy	1,333 m
Columns	162
Rows	165
Layers	35

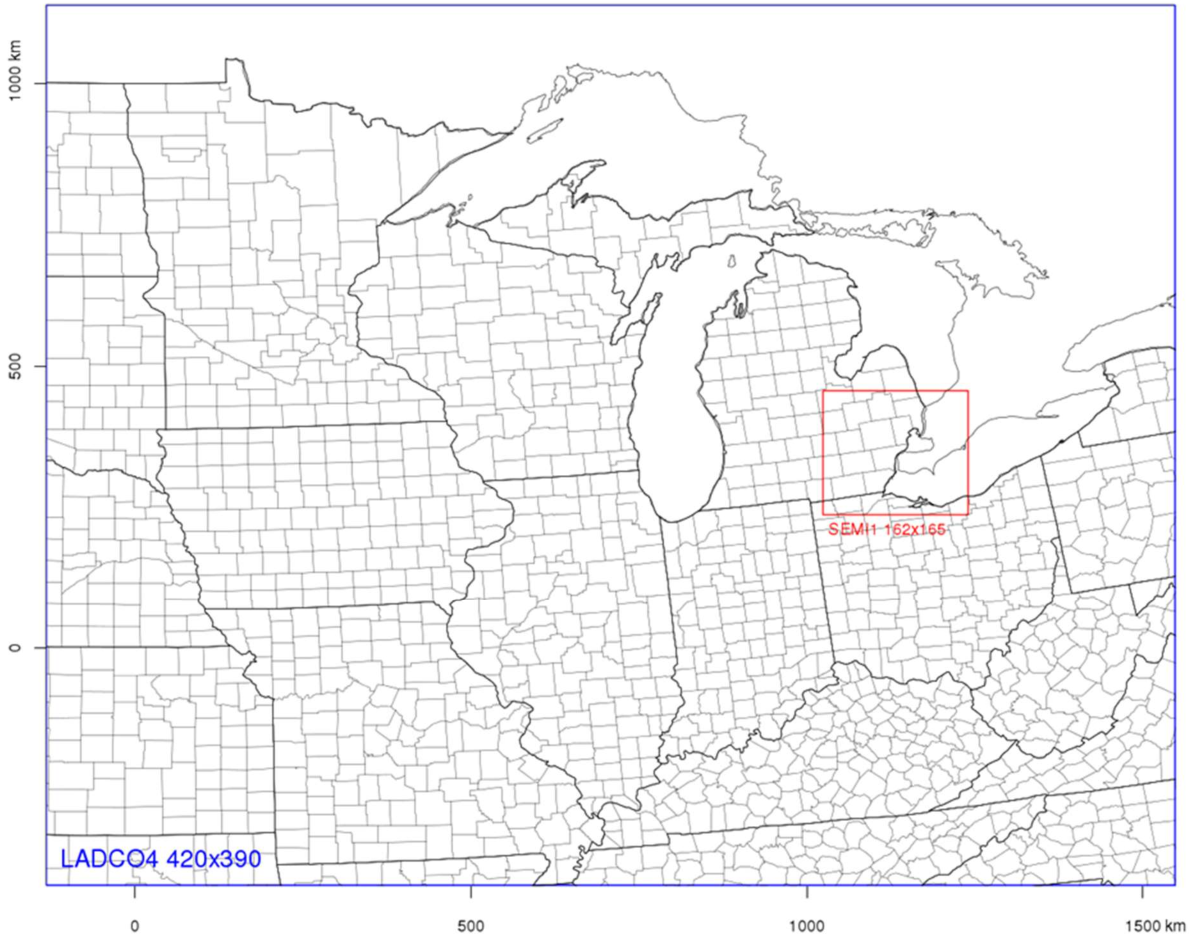


Figure 2-1. The 1.33km modeling domain (the box in red) for the SEMI region, which covers the entire SEMI ozone nonattainment area with 162x165 grid cells).

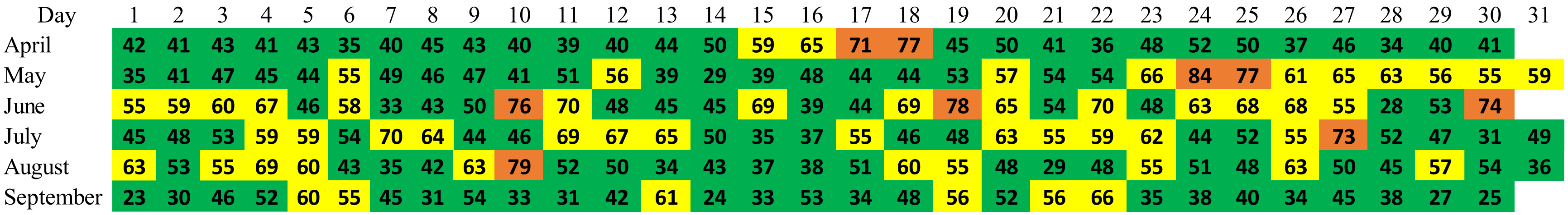
Table 2-3 shows the vertical layer structure of the SEMI1 CAMx modeling grid. It has 35 vertical layers (36 levels) extending from ground to 50 mb at the top.

Table 2-3. SEMI1 CAMx Modeling Grid Vertical Layer Configurations

Level	Sigma	Height (m)	Pressure (pascal)	Depth (m)
36	0.000	17,556	5000	2776
35	0.050	14,780	9750	1958
34	0.100	12,822	14500	1540
33	0.150	11,282	19250	1280
32	0.200	10,002	24000	1101
31	0.250	8,901	28750	969
30	0.300	7,932	33500	868
29	0.350	7,064	38250	789
28	0.400	6,275	43000	722
27	0.450	5,553	47750	668
26	0.500	4,885	52500	621
25	0.550	4,264	57250	581
24	0.600	3,683	62000	547
23	0.650	3,136	66750	517
22	0.700	2,619	71500	393
21	0.740	2,226	75300	285
20	0.770	1,941	78150	276
19	0.800	1,665	81000	180
18	0.820	1,485	82900	177
17	0.840	1,308	84800	174
16	0.860	1,134	86700	170
15	0.880	964	88600	167
14	0.900	797	90500	83
13	0.910	714	91450	82
12	0.920	632	92400	81
11	0.930	551	93350	81
10	0.940	470	94300	80
9	0.950	390	95250	79
8	0.960	311	96200	79
7	0.970	232	97150	78
6	0.980	154	98100	39
5	0.985	115	98575	38
4	0.990	77	99050	39
3	0.995	38	99525	19
2	0.9975	19	99763	19
1	1.000	0	100000	0

2.3 Modeling Period

During the 2016 ozone season, there were 9 ozone exceedance days in the SEMI nonattainment area (NAA), almost evenly distributed among the ozone season months (Figure 2-2). The base and future year modeling period is for the 2016 ozone season (April-September). To remove the impacts from the initial conditions, we chose to model both ozone season simulations with a 3-day spin-up period starting from 4/12/2016 and ending at 09/25/2016. For better initialization, we used initial conditions that are derived from the 4-km LADCO4 CAMx modeling outputs. We chose the same ozone season period as the modeling period for all the testing simulations for the tasks of “Base Year Ozone Model Optimization” and “Future Year Air Quality Modeling Experiments” as well.



Day	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31
April	42	41	43	41	43	35	40	45	43	40	39	40	44	50	59	65	71	77	45	50	41	36	48	52	50	37	46	34	40	41	
May	35	41	47	45	44	55	49	46	47	41	51	56	39	29	39	48	44	44	53	57	54	54	66	84	77	61	65	63	56	55	59
June	55	59	60	67	46	58	33	43	50	76	70	48	45	45	69	39	44	69	78	65	54	70	48	63	68	68	55	28	53	74	
July	45	48	53	59	59	54	70	64	44	46	69	67	65	50	35	37	55	46	48	63	55	59	62	44	52	55	73	52	47	31	49
August	63	53	55	69	60	43	35	42	63	79	52	50	34	43	37	38	51	60	55	48	29	48	55	51	48	63	50	45	57	54	36
September	23	30	46	52	60	55	45	31	54	33	31	42	61	24	33	53	34	48	56	52	56	66	35	38	40	34	45	38	27	25	

Figure 2-2. Heat map of 2016 daily MDA8 O_3 ***concentrations (ppb) in ozone season observed in the SEMI NAA***

2.4 Meteorological Inputs

The meteorological input data (as WRF outputs in netCDF format) required for the CAMx modeling were provided by LADCO. The LADCO-provided WRF outputs are on the LADCO D04 WRF modeling grid, which has the same 1.33 km horizontal resolution and same vertical layers as the SEMI1 grid (Figure 2-3 shows both the LADCO D04 and SEMI1 domains). All the necessary meteorological variables were processed through the WRFCAMx program along with the other support programs KVPATCH and WATERMASK.

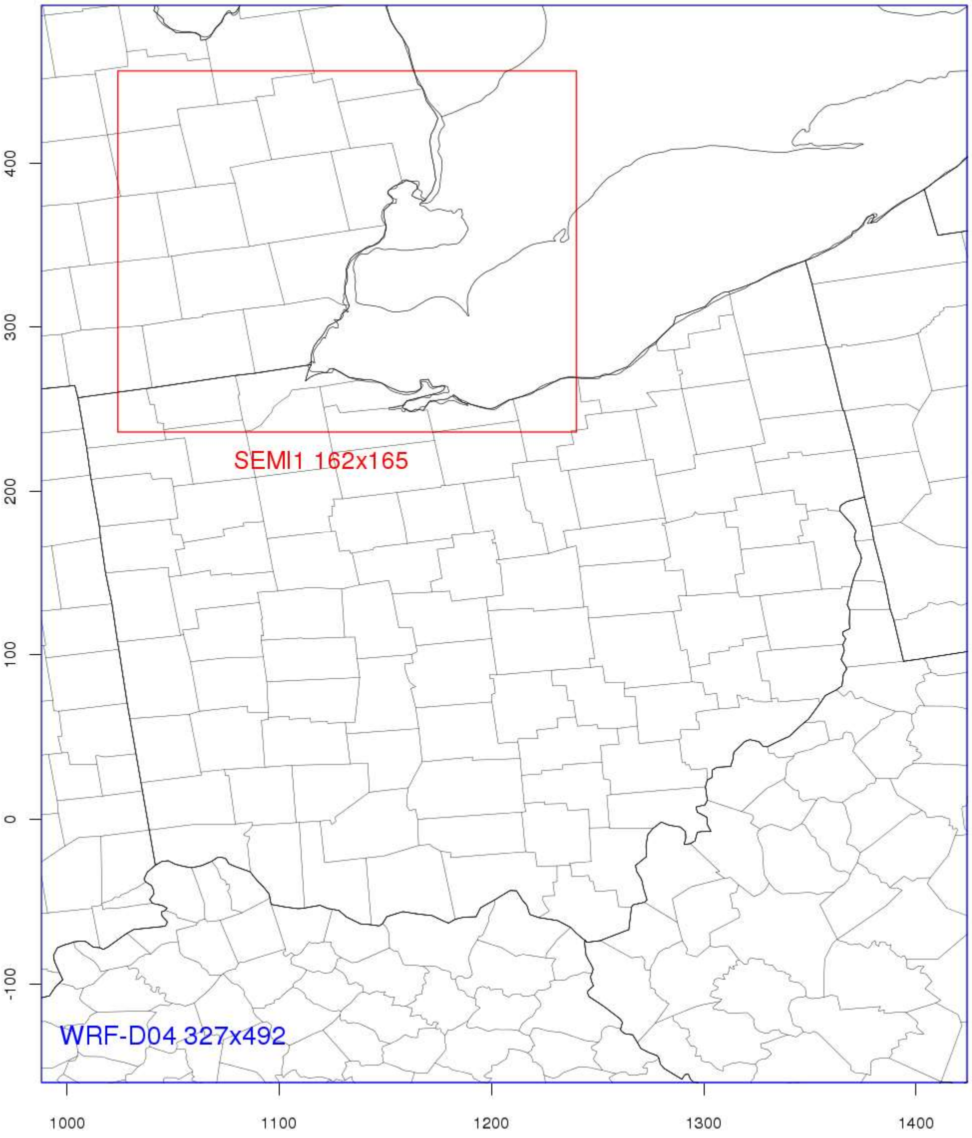


Figure 2-3. The 1.33 km horizontal resolution CAMx modeling grid (the inner box in red) for the SEMI region, which covers the entire SEMI ozone nonattainment area with 162x165 grid cells. Also shown on the map is the 1.33 km horizontal resolution LADCO D04 Weather Research and Forecasting (WRF) modeling grid (the outer box in blue).

We used the wrfcamx v4.8.1 (14Dec20) and kvpatch v6 (8may14) to prepare meteorological inputs to CAMx. The WRFCAMx program generates CAMx meteorological input files from WRF (ARW core) hourly output files. The program generates the FORTRAN binary files for each single day with 25 hours of meteorology (midnight through midnight, inclusive). The CAMx layer structure was kept the same as the WRF layers. We also conducted KVPATCH program to apply minimum Kv (vertical diffusivity) values to layers below 200 m height based on input land use fields and surface layer stability. Finally, the WATERMASK program was used to convert the CAMx land use file containing all water coverage in index=1 to a new land use file that differentiates between salt/ocean water coverage (index=1) and fresh water coverage (index=3). WATERMASK program operates only on FORTRAN binary files.

WRF outputs were also processed through MCIP program to prepare meteorological fields that needed by the SMOKE, BEIS and MEGAN programs for emissions modeling. We reviewed the MCIP files by plotting the major meteorological variables such as winds, temperature, rain, cloud cover, PBL heights etc. to visually verify the ranges.

Meteorological input files were prepared for the months of April through September covering the ozone season period from 4/12/2016 through 09/25/2016, and used for both the base year and future year simulations.

2.5 Initial and Boundary Conditions

The CAMx modeling requires initial and boundary conditions (IC/BC) for the air quality fields. The IC/BC for the air quality were provided by LADCO and derived from the 3D outputs from LADCO4 4-km CAMx simulations.

The IC file is prepared for 4/12/2016, the starting day of the modeling period. The BC files are prepared for the modeling period from 4/12/2016 through 09/25/2016. The same IC/BC files are used for all the base year and future year simulations.

We reviewed the initial and boundary conditions files by plotting them to visually verify the ranges of IC and BCs.

2.6 Emissions Inputs

Emissions input files were prepared by the Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system (version 4.7) through the U.S. EPA 2016v1 Emissions Modeling platform (https://www.epa.gov/air-emissions-modeling/2016v1-platform.). Emissions input files for CAMx include the gridded emissions (emis2d/emis3d files) and point emissions (ptsr files) for all sectors of anthropogenic and biogenic emissions.

The SMOKE modeling system is a set of programs that is used by the U.S. EPA, Regional Planning Organizations (RPOs), and State environmental agencies to prepare emissions inventory data for input to an air quality model such as CMAQ and CAMx. SMOKE has strict requirements for the nature and formats of the inventory data that it can use. SMOKE integrates annual (or daily) estimates of county-level emissions inventories (or individual point-level emissions inventories) with source-based temporal, spatial, and chemical allocation profiles to create hourly emissions fluxes on a predefined model grid. In general, SMOKE requires an emissions inventory, temporal allocation, spatial allocation, and chemical allocation data to prepare emissions estimates for an air quality model. For some source categories, such as on-road mobile, fugitive dust and stationary point sources, SMOKE also requires meteorology data to calculate emissions. In addition to its capacity to simulate emissions from stationary area, stationary point, and on-road mobile sectors, SMOKE is also instrumented with the Biogenic Emissions Inventory System, version 3 (BEIS3) for estimating biogenic emissions fluxes (U.S. EPA, 2004). BEIS3 calculates biogenic emissions estimates with gridded land use, vegetative emissions factors, and meteorology data. SMOKE is designed with flexible QA capabilities to generate standard and custom reports for checking the emissions modeling process. After modeling all the emissions source categories individually, SMOKE creates two types of files per day for input into CMAQ or CAMx: (1) a set of elevated point source files for large stationary sources, and (2) a set of pre-merged gridded source files and a merged gridded source file of low-level point, mobile, non-road, area, and biogenic emissions.

We processed the emissions inventories for base year 2016 (inventory version 2016fh_16j) and future year 2023 (inventory version 2023fh_16j), by using SMOKE through the EPA 2016v1Platform for the 1.33km SEMI1 domain and the entire 2016 ozone season period. Table 2-4 2016v1 Platform Emissions Source Sectors List for 2016 and 2023

2016fh_16j sector ID	2023fh_16j sector ID	Source Category
afdust_adj	afdust_adj	US area fugitive dust sources
ag	ag	US agricultural sources
airports	airports	US airport sources
nonpt	nonpt	US non-point sources
nonroad	nonroad	US off-road mobile sources
np_oilgas	np_oilgas	US non-point oil&gas sources
onroad	onroad	US on-road mobile sources
onroad_can	onroad_can	Canada on-road mobile sources
othafdust_adj	othafdust_adj	Canada&Mexico area fugitive dust sources
othar	othar	Canada&Mexico area sources
othptdust_adj	othptdust_adj	Canada&Mexico point dust sources
rail	rail	US railroad sources
rwc	rwc	US residential wood combustion sources
cmv_c1c2_4*	cmv_c1c2_4*	US commercial marine vessels class 1&2
cmv_c3_4*	cmv_c3_4*	US commercial marine vessels class 3
ptagfire3d	-	US agricultural fire sources
ptfire3d	-	US biomass fire sources
ptfire_othna3d	-	Canada&Mexico biomass fire sources
othpt	othpt	Canada&Mexico point sources
pt_oilgas	pt_oilgas	US point oil&gas sources
ptegu	ptegu**	US EGU point sources
ptnonipm	ptnonipm	US Non-IPM point sources
beis	-	Biogenic sources

*These are 4-km resolution commercial marine vessels emissions inventories produced by EPA specifically for the LADCO region, which replaced the original 12-km resolution inventories that came with the 2016v1Platform.

** The updated 2023fh1_16j version of the ptegu sector inventory is used, instead of 2023fh_16j.

While for most of sectors we used the default inventories that came with the 2016v1Platform, we did replace the original 12-km resolution commercial marine vessels emissions inventories (sectors cmv_c1c2_12 and cmv_c3_12 for both 2016 and 2023) that came with the 2016v1Platform with the 4-km resolution inventories that were specifically produced by EPA for the LADCO region. Figures 2-4 and 2-5 show, respectively, how the 12-km resolution inventories of cmv_c1c2_12 and cmv_c3_12 would mislocate the emissions released from vessels that should travel on water to over the land.

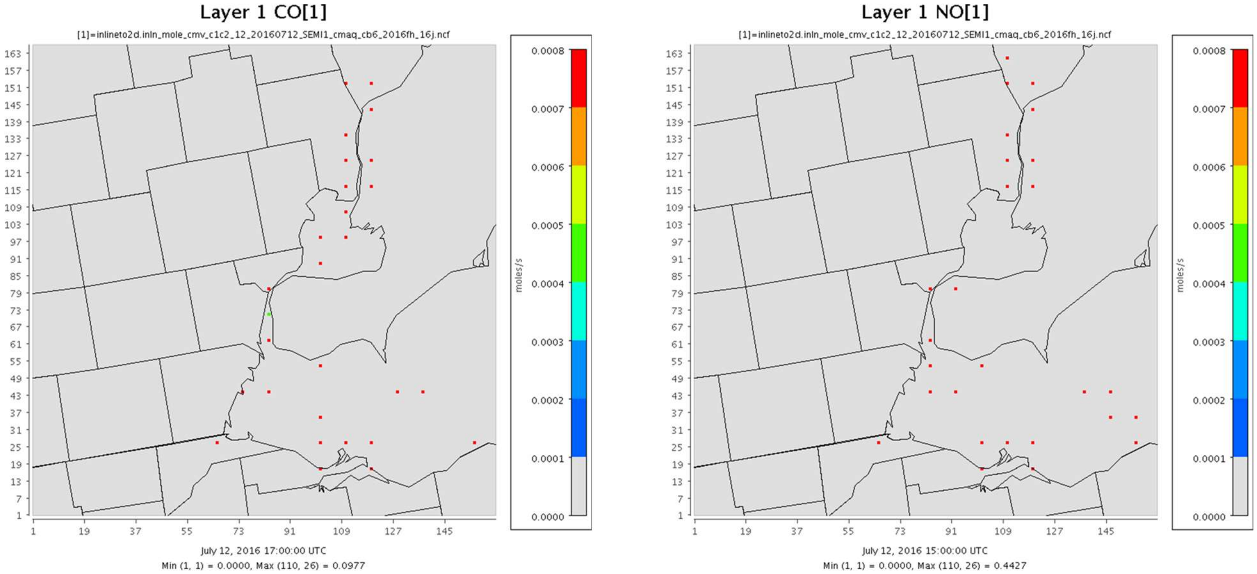


Figure 2-4. Emissions visual check on 2016fh_16j cmv_c1c2_12 sector, July 12th 15Z hourly CO (left) and NO (right) emissions rates spatial distribution on the SEMI1 grid.

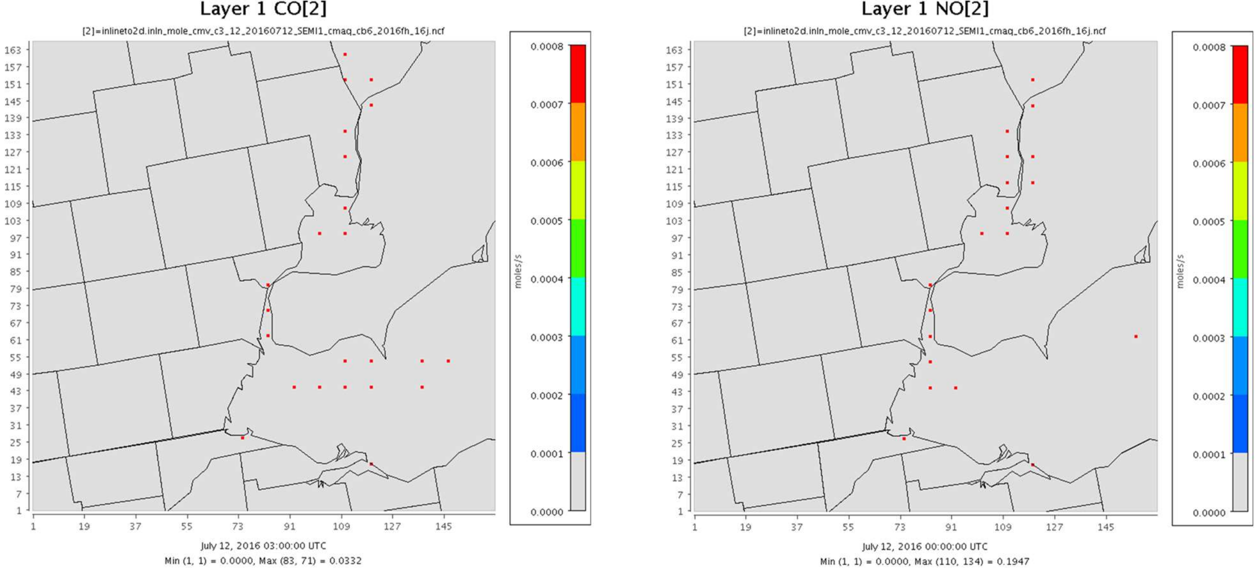


Figure 2-5. Emissions visual check on 2016fh_16j cmv_c3_12 sector, July 12th 00Z hourly CO (left) and NO (right) emissions rates spatial distribution on the SEMI1 grid.

The spatial surrogates database that came with the 2016v1Platform are only available at 4-km, 12-km and 36-km resolutions. We used the 1.33-km U.S. spatial surrogates provided by LADCO covering the entire LADCO region, including the SEMI1 domain. We used the Spatial Allocator program to prepare Canadian spatial surrogates at 1.33 km resolution for the SEMI1 grid.

The inputs to the Spatial Allocator program are the Canadian shape files from the "Canadian shapefile catalog 2015" that are compiled for the 2017Platform and recommended by EPA (Correspondence with Alison Eyth on April 26, 2022).

Through the 2016v1Platform (with the updates) we generated in-line emissions files for point sources and pre-merged gridded emissions files for low-level point, mobile, non-road, area, and biogenic sources. We kept these emissions files separated for each sector. We further used the CMAQ2CAMx interface program to generate CAMx ready emissions inputs as in CAMx FORTRAN binary formats. The CAMx ready emissions files are still kept separated for each sector mainly for the convenience of updating emission files at the individual sector's level.

We performed a rigorous check on the generated emissions files (in IOAPI format). The examination included reviewing the SMOKE-generated reports for checking each step of the emissions modeling process and graphical visualization of the files to verify if the spatial distribution patterns are reasonable for the sector and the minimums and maximums lie within reasonable bounds for the entire modeling period. Sample visual check plots are shown in Figures 2-6, 2-7, 2-8, 2-9, for verification of select species' emission rates on the SEMI1 grid for the sectors of onroad, nonroad, nonpt, and beis respectively.

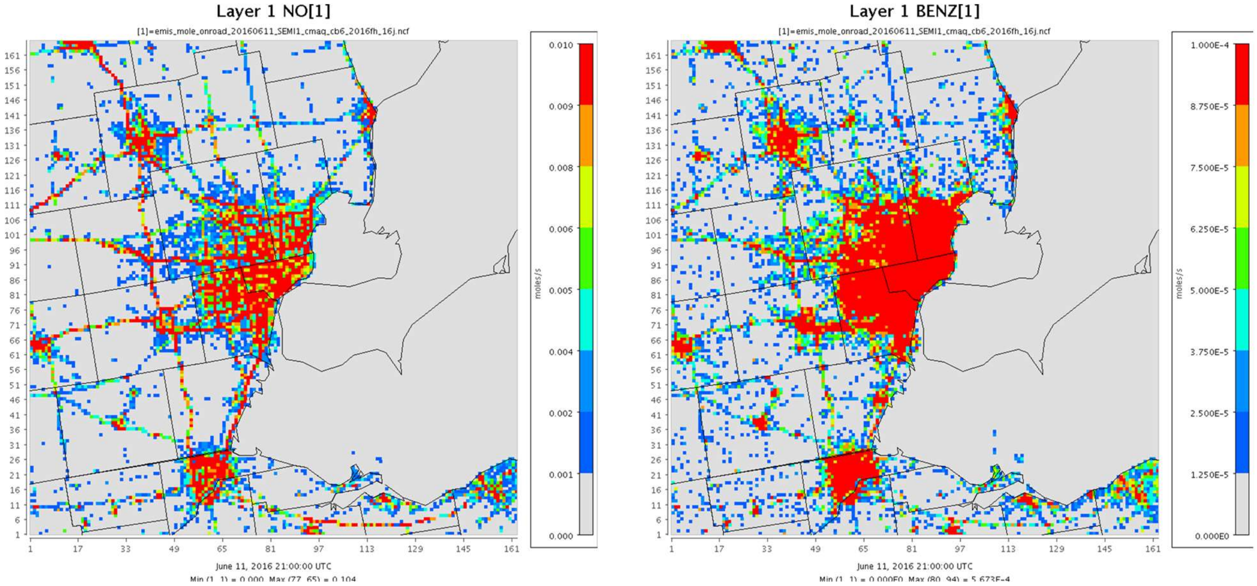


Figure 2-6. Emissions visual check on 2016fh_16j onroad sector, June 11th 21Z hourly NO (left) and BENZ (right) emissions rates spatial distribution on the SEMI1 grid.

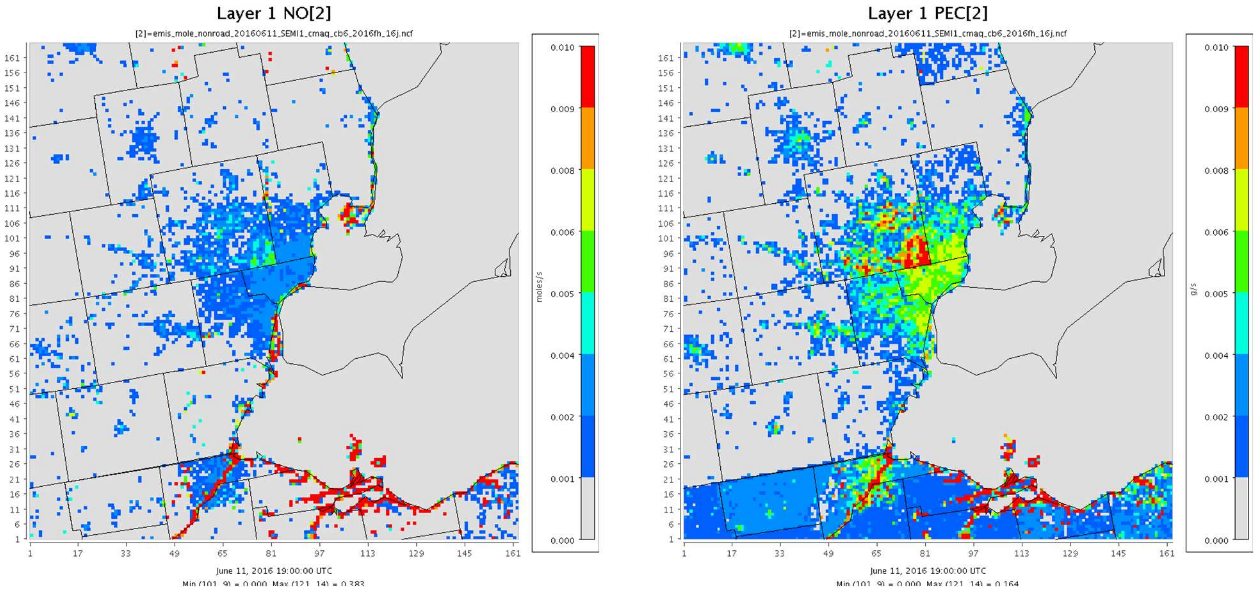


Figure 2-7. Emissions visual check on 2016fh_16j nonroad sector, June 11th 19Z hourly NO (left) and PEC (right) emissions rates spatial distribution on the SEMI1 grid.

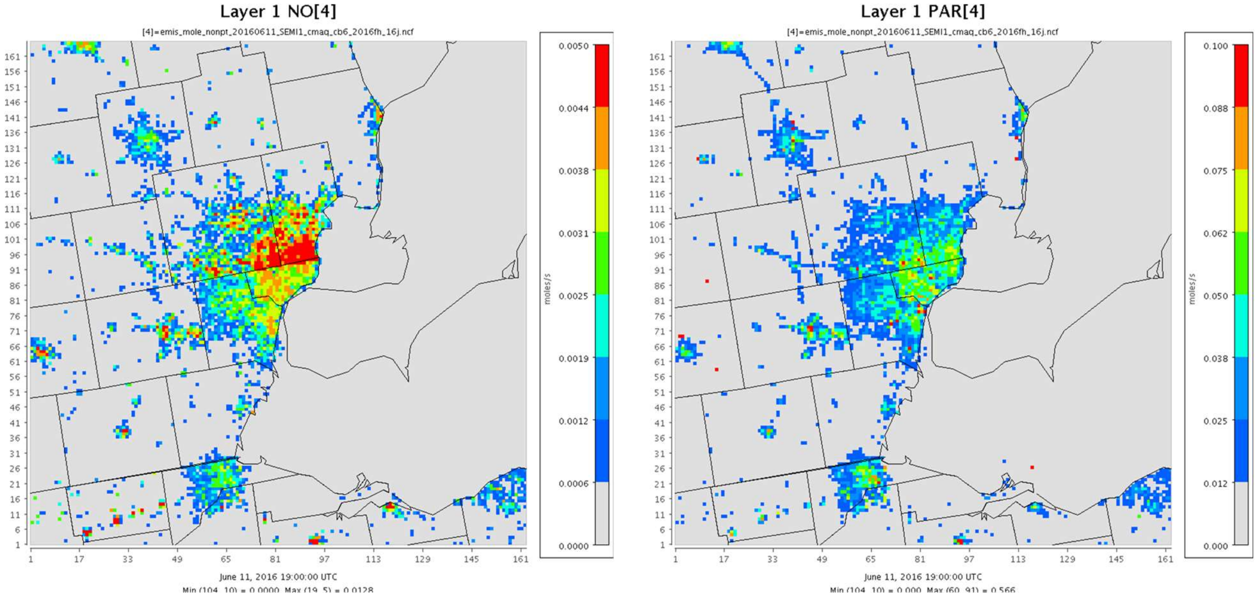


Figure 2-8. Emissions visual check on 2016fh_16j nonpt sector, June 11th 19Z hourly NO (left) and PAR (right) emissions rates spatial distribution on the SEMI1 grid.

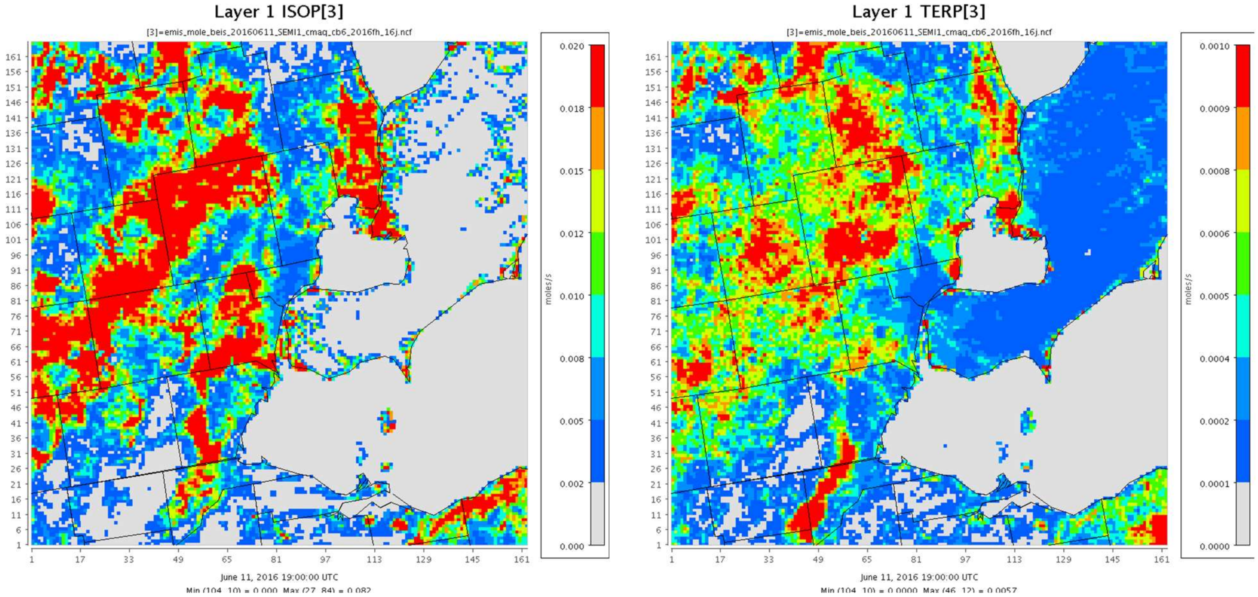


Figure 2-9. Emissions visual check on 2016fh_16j beis sector, June 11th 21Z hourly ISOP (left) and TERP (right) emissions rates spatial distribution on the SEMI1 grid.

We also updated the emissions estimates for a few sectors from the default 2016 inventories for the purpose of sensitivity tests for optimizing the performance of the base year simulation, and from the default 2023 inventories for the purpose of future year control scenario experiments. The preparation of such emissions updates on individual specific sectors are described in later chapters.

Emissions input files for each sector, for either 2016 or 2023, and either default or updated emissions, were all prepared for the months of April through September, which covers the ozone season period from 4/12/2016 through 09/25/2016. Depending on the simulation, a specific set of sectorized emissions input files were used for that simulation, either a base year 2016 simulation or a future year 2023 simulation as further specified and discussed in later chapters.

lists the detailed emissions source inventories separated for each sector for 2016 and 2023 from the EPA 2016v1 platform. Note that all the anthropogenic sectors have 2016 level and 2023 level emissions inventories, but emissions inventories for biomass burning sectors, i.e., ptagfire3d, ptfire3d, and ptfire_othna3d, are only available for 2016. The biogenic emissions sector (beis) is also only available for 2016 as well. When conducting BEIS3 modeling, the seasonal variable SUMMER_YN=Y was set for April 16 and later days and SUMMER_YN=N was set for April 15 and earlier days. The biogenic land use input data to BEIS3 was prepared using the beld4smk and beld4_water_fix programs with the BELD4.1 dataset.

Table 2-4 2016v1 Platform Emissions Source Sectors List for 2016 and 2023

2016fh_16j sector ID	2023fh_16j sector ID	Source Category
afdust_adj	afdust_adj	US area fugitive dust sources
ag	ag	US agricultural sources
airports	airports	US airport sources
nonpt	nonpt	US non-point sources
nonroad	nonroad	US off-road mobile sources
np_oilgas	np_oilgas	US non-point oil&gas sources

onroad	onroad	US on-road mobile sources
onroad_can	onroad_can	Canada on-road mobile sources
othafdust_adj	othafdust_adj	Canada&Mexico area fugitive dust sources
othar	othar	Canada&Mexico area sources
othptdust_adj	othptdust_adj	Canada&Mexico point dust sources
rail	rail	US railroad sources
rwc	rwc	US residential wood combustion sources
cmv_c1c2_4*	cmv_c1c2_4*	US commercial marine vessels class 1&2
cmv_c3_4*	cmv_c3_4*	US commercial marine vessels class 3
ptagfire3d	-	US agricultural fire sources
ptfire3d	-	US biomass fire sources
ptfire_othna3d	-	Canada&Mexico biomass fire sources
othpt	othpt	Canada&Mexico point sources
pt_oilgas	pt_oilgas	US point oil&gas sources
ptegu	ptegu**	US EGU point sources
ptnonipm	ptnonipm	US Non-IPM point sources
beis	-	Biogenic sources

*These are 4-km resolution commercial marine vessels emissions inventories produced by EPA specifically for the LADCO region, which replaced the original 12-km resolution inventories that came with the 2016v1Platform.

** The updated 2023fh1_16j version of the ptegu sector inventory is used, instead of 2023fh_16j.

While for most of sectors we used the default inventories that came with the 2016v1Platform, we did replace the original 12-km resolution commercial marine vessels emissions inventories (sectors cmv_c1c2_12 and cmv_c3_12 for both 2016 and 2023) that came with the 2016v1Platform with the 4-km resolution inventories that were specifically produced by EPA for the LADCO region. Figures 2-4 and 2-5 show, respectively, how the 12-km resolution inventories of cmv_c1c2_12 and cmv_c3_12 would mislocate the emissions released from vessels that should travel on water to over the land.

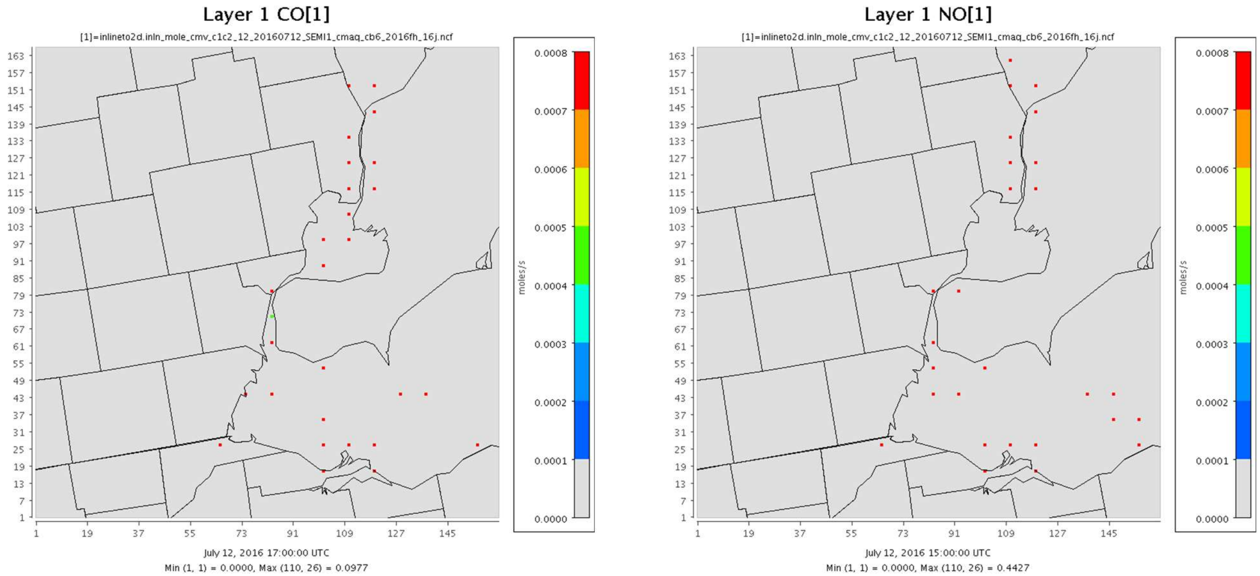


Figure 2-4. Emissions visual check on 2016fh_16j cmv_c1c2_12 sector, July 12th 15Z hourly CO (left) and NO (right) emissions rates spatial distribution on the SEMI1 grid.

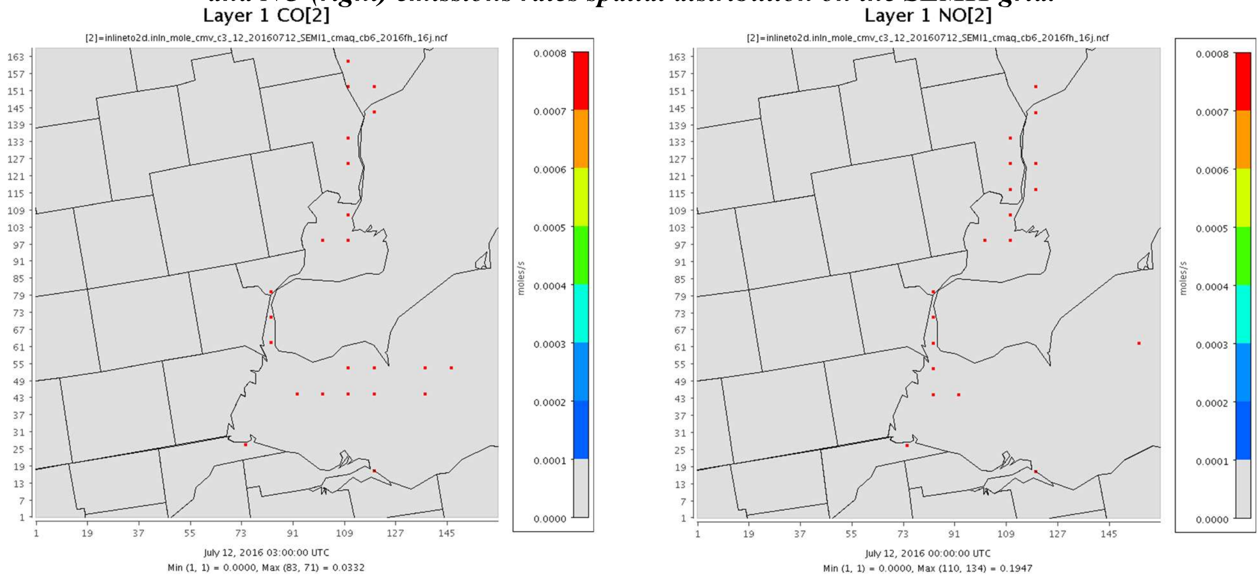


Figure 2-5. Emissions visual check on 2016fh_16j cmv_c3_12 sector, July 12th 00Z hourly CO (left) and NO (right) emissions rates spatial distribution on the SEMI1 grid.

The spatial surrogates database that came with the 2016v1Platform are only available at 4-km, 12-km and 36-km resolutions. We used the 1.33-km U.S. spatial surrogates provided by LADCO covering the entire LADCO region, including the SEMI1 domain. We used the Spatial Allocator program to prepare Canadian spatial surrogates at 1.33 km resolution for the SEMI1 grid. The inputs to the Spatial Allocator program are the Canadian shape files from the "Canadian shapefile catalog 2015" that are compiled for the 2017Platform and recommended by EPA (Correspondence with Alison Eyth on April 26, 2022).

Through the 2016v1Platform (with the updates) we generated in-line emissions files for point sources and pre-merged gridded emissions files for low-level point, mobile, non-road, area, and biogenic sources. We kept these emissions files separated for each sector. We further used the CMAQ2CAMx interface program to generate CAMx ready emissions inputs as in CAMx

FORTRAN binary formats. The CAMx ready emissions files are still kept separated for each sector mainly for the convenience of updating emission files at the individual sector's level.

We performed a rigorous check on the generated emissions files (in IOAPI format). The examination included reviewing the SMOKE-generated reports for checking each step of the emissions modeling process and graphical visualization of the files to verify if the spatial distribution patterns are reasonable for the sector and the minimums and maximums lie within reasonable bounds for the entire modeling period. Sample visual check plots are shown in Figures 2-6, 2-7, 2-8, 2-9, for verification of select species' emission rates on the SEMI1 grid for the sectors of onroad, nonroad, nonpt, and beis respectively.

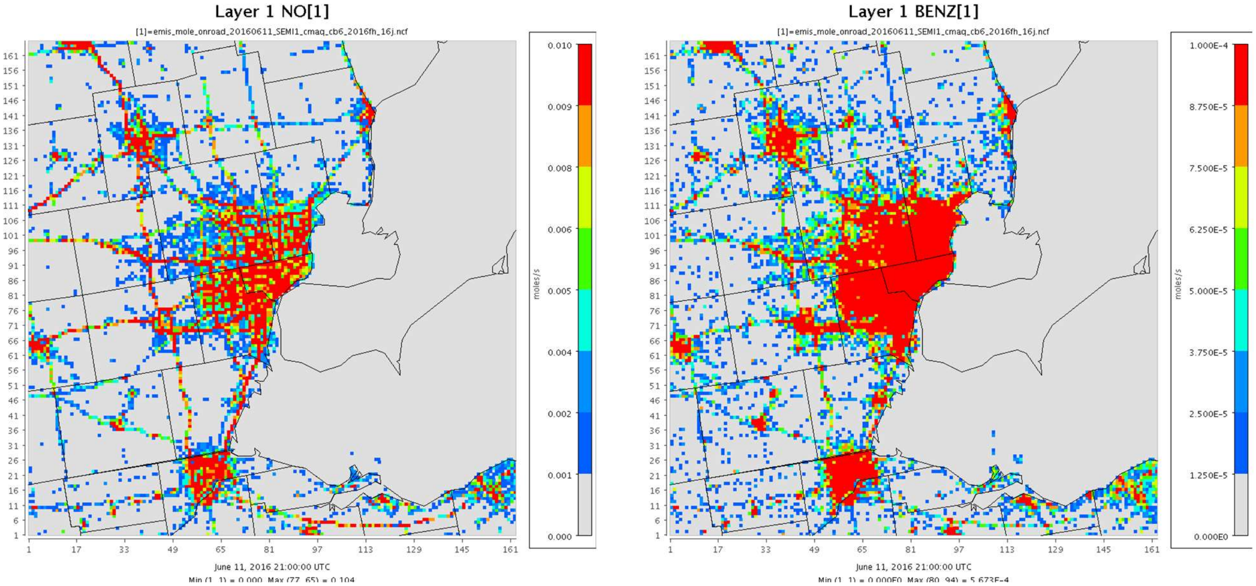


Figure 2-6. Emissions visual check on 2016fh_16j onroad sector, June 11th 21Z hourly NO (left) and BENZ (right) emissions rates spatial distribution on the SEMI1 grid.

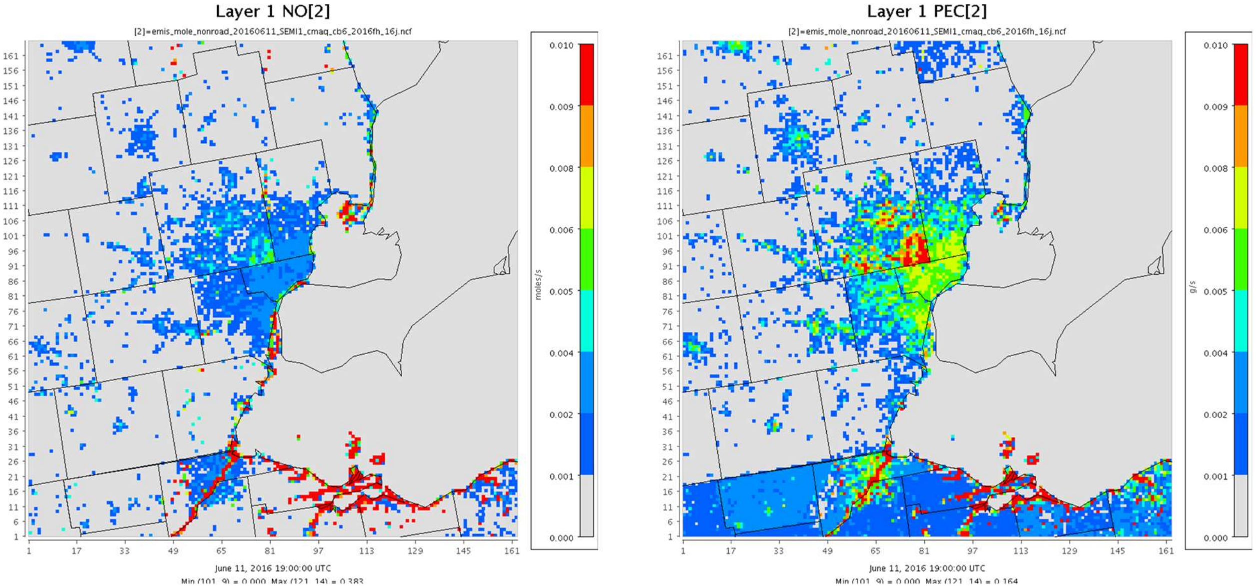


Figure 2-7. Emissions visual check on 2016fh_16j nonroad sector, June 11th 19Z hourly NO (left) and PEC (right) emissions rates spatial distribution on the SEMI1 grid.

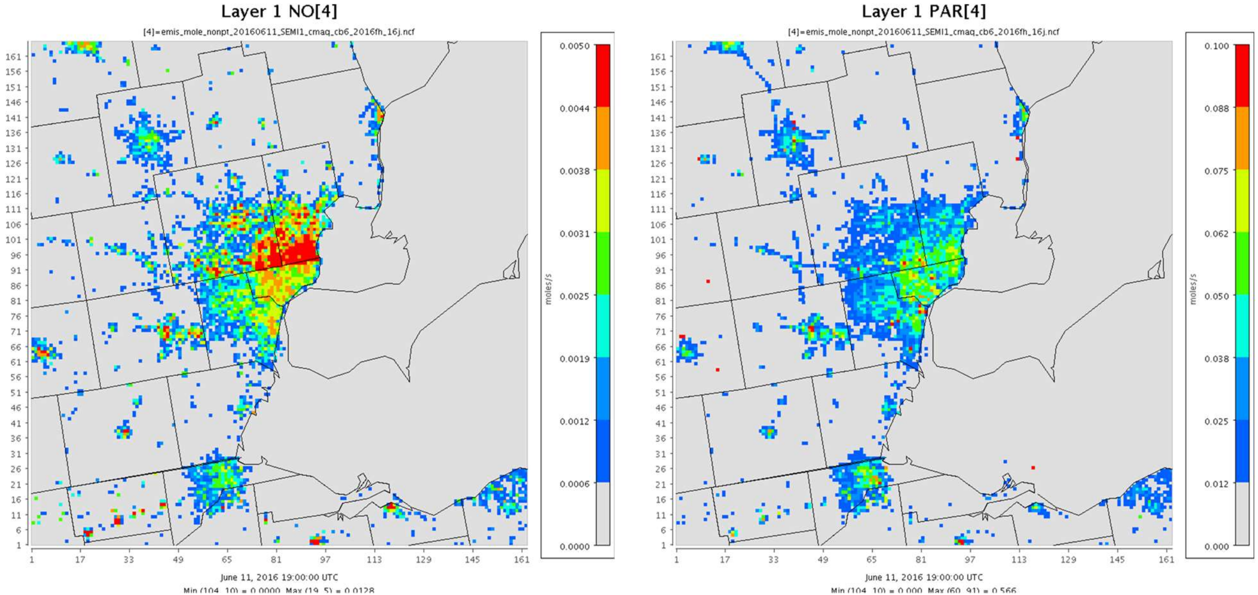


Figure 2-8. Emissions visual check on 2016fh_16j nonpt sector, June 11th 19Z hourly NO (left) and PAR (right) emissions rates spatial distribution on the SEMI1 grid.

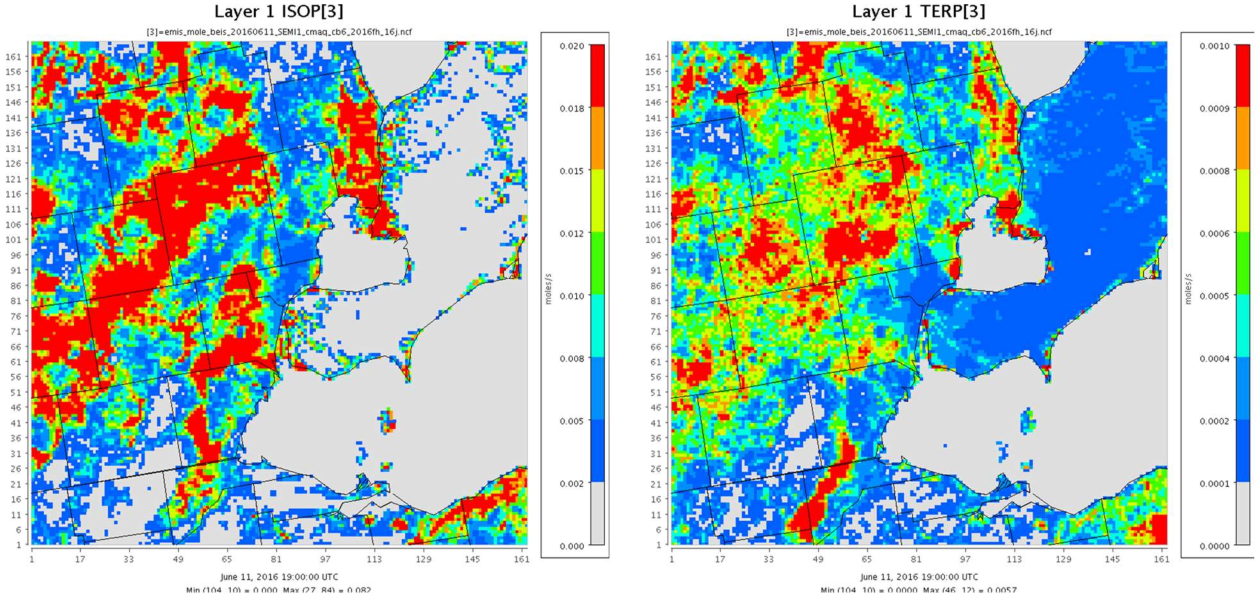


Figure 2-9. Emissions visual check on 2016fh_16j beis sector, June 11th 21Z hourly ISOP (left) and TERP (right) emissions rates spatial distribution on the SEMI1 grid.

We also updated the emissions estimates for a few sectors from the default 2016 inventories for the purpose of sensitivity tests for optimizing the performance of the base year simulation, and from the default 2023 inventories for the purpose of future year control scenario experiments. The preparation of such emissions updates on individual specific sectors are described in later chapters.

Emissions input files for each sector, for either 2016 or 2023, and either default or updated emissions, were all prepared for the months of April through September, which covers the ozone season period from 4/12/2016 through 09/25/2016. Depending on the simulation, a specific set of sectorized emissions input files were used for that simulation, either a base year 2016 simulation or a future year 2023 simulation as further specified and discussed in later chapters.

2.7 Other Inputs

Other necessary input files required for the CAMx runs are ozone column and photolysis rate files. We used the O3MAP program (version 31may20 for CAMx v7.0+) with the total integrated ozone column (TOMS) data to prepare ozone column input files for CAMx. We used the Total Ultraviolet (TUV) radiative transfer model, TUV program versions 4.8 for CAMx7.10, to prepare look-up table of photolysis rates to be used in CAMx. The table defines photolysis rates for all the CB6 photolytic reactions over a range of solar zenith angles, altitudes, ozone column, surface UV albedo, and haze turbidity. CAMx internally adjusts the photolysis rates for cloud cover according to the cloud inputs provided to CAMx.

The ozone column and photolysis rate files are all prepared for the modeling period from 4/12/2016 through 09/25/2016. The same ozone column and photolysis rate files are used for both the base year and future year simulations.

Section 3: Emissions Updates for Sensitivity Tests of Base Year Simulation

This section describes the efforts to prepare the updated emissions files for the sensitivity tests for the base year simulation optimization. These efforts include improving the HCHO and VCP VOC emissions and using alternative biogenic emissions estimates from MEGAN.

3.1 HCHO emissions improvement

We worked with Michigan EGLE and LADCO to update HCHO emission in the 2016 base year inventories for counties in the SEMI region. The updates were derived from measured ratios of HCHO to CO in stack tests and prior field campaigns. Michigan EGLE maintains a platform that currently includes emissions reported to EGLE by regulated facilities as tabulated in the Michigan Air Emissions Reporting System (MAERS). This platform enables the automatic estimation of HCHO emissions by assuming different HCHO/CO mass ratios for different source categories, especially those associated with stationary engines, flares, and other combustion sources. These mass ratios are based on stack tests, air quality field campaigns, and other reputable sources of information that provide assurance of the HCHO emission estimates.

Michigan EGLE provided a spreadsheet ("GT HCHO ss v4.xlsx") containing the calculated emissions of HCHO by SCC code from facilities in SE Michigan (in seven counties in the SEMI NAA). These are 1533 records extracted from MAERS are from 2017. Michigan EGLE also provided a spreadsheet that contains a list of all relevant SCC (in total 150 SCCs) each being assigned with a HCHO to CO mass ratio that were used to scale the HCHO emissions from CO emissions. These SCC's were selected to attribute HCHO-to-CO mass ratios to specific SCCs for the purpose of estimating more realistic HCHO emissions. Among them, the SCCs related to flares, stationary engines and Landfill Gas (LFG) engines are assigned a specific molar ratio (5%, 10% and 15%, respectively) hence the similar mass ratios due to the very close molecular weights of HCHO and CO (Table 3-1). Other combustion SCCs were assigned a default 2% ratio.

Table 3-1 Mass ratios of HCHO to CO assignments to combustion categories

Molar ratio (%)	Tag	Mass ratio	Note
2	Default	0.02	Default
5	Jay5	0.05	Default for Flares
10	Jay10	0.1	Default for stationary engines (non-LFG)
15	Jay15	0.15	Default for LFG engines

Due to the difficulty of matching the 1533 HCHO/CO emissions records directly to the records in the EPA 2016fh_16j inventories, we decided to adopt the MAERS method by using mass ratios to recalculate the individual facility's HCHO emissions from the same facility's 2016fh_16j inventory CO emissions for all the inventory records that with a relevant SCC.

In practice, in terms of SMOKE modeling, we updated both the speciation profiles file "GSPRO" and the SCC-profile reference file "GSREF" from the 2016v1platform for adding new HCHO emissions estimates and removing the old HCHO emissions at the same time.

The to-be-updated GSREF file is “gsref_cmaq_cb6_2016fh_16j_nf.txt” and the to-be-updated GSPRO file is “gspro_cmaq_cb6_2016fh_16j_nf.txt”.

Among the 150 relevant SCCs, we got rid of 4 SCCs 30301510 40600141 40600162, 40688801. The SCC 30301510 is missing from the GSREF file, and SCCs 40600141 40600162, 40688801 are all for Chemical Evaporation fugitive sources with no associated CO emissions.

The updating procedure includes the following 7 steps:

Step 1: From the GSREF file, take out the “VOC” profile reference entries for the 146 SCCs that has a HCHO/CO ratio assigned. These 146 SCC uses 27 unique profiles.

Step 2: Replace the 146 SCCs’ “VOC” profile reference entries in the GSREF file with the new entries that using the newly named 27 profiles (Table 3-2).

Step 3: Add the 27 new “VOC” profiles in the GSPRO file, by revising the original 27 profiles’ entries from FORM to UNK and FORM_PRIMARY to UNK_PRIMARY. The new profile’s ID is named as by adding “S” to the old ID (Table 3-3).

Step 4: Add the 4 new “CO” profiles in the GSPRO file, speciating emissions pollutant of CO to species CO and FORM (HCHO) . Table 3-4 shows these new CO profiles.

Step 5: Add the 146 SCCs’s “CO” profile reference entries in the GSREF file, assigning each of these SCC with one of the four “CO” profiles (Table 3-2).

Step 6: Add the entries of TOG to VOC conversion ratios for the 27 new VOC profiles in the GSCNV file “gscnv_Create_Speciate4_5_CB6CMAQ_04jan2018_nf_v1.txt”, by keeping the ratios as the same as the old profiles.

Table 3-2 List of the relevant SCCs with their assignments of the new CO and VOC profiles

SCC	New CO_profile_id	New VOC_profile_id
"10100222"	"S002"	"S1178"
"10100226"	"S002"	"S1178"
"10100401"	"S002"	"S0001"
"10100501"	"S002"	"S0002"
"10100601"	"S002"	"S0003"
"10100602"	"S002"	"S0003"
"10100604"	"S002"	"S0003"
"10101302"	"S002"	"S0001"
"10200204"	"S002"	"S1185"
"10200401"	"S002"	"S0001"
"10200402"	"S002"	"S0001"
"10200501"	"S002"	"S0002"
"10200502"	"S002"	"S0002"
"10200601"	"S002"	"S0003"
"10200602"	"S002"	"S0003"
"10200603"	"S002"	"S0003"

"10200604"	"S002"	"S0003"
"10200701"	"S002"	"S0004"
"10200704"	"S002"	"S0004"
"10200707"	"S002"	"S0005"
"10200711"	"S005"	"S0202"
"10200799"	"S002"	"S0004"
"10201001"	"S002"	"S0003"
"10201002"	"S002"	"S0003"
"10201303"	"S002"	"S0001"
"10201401"	"S002"	"S0003"
"10300401"	"S002"	"S0001"
"10300501"	"S002"	"S0002"
"10300502"	"S002"	"S0002"
"10300503"	"S002"	"S0002"
"10300601"	"S002"	"S0003"
"10300602"	"S002"	"S0003"
"10300603"	"S002"	"S0003"
"10300811"	"S002"	"S0003"
"10301002"	"S002"	"S0003"
"10500106"	"S002"	"S0003"
"10500114"	"S002"	"S0001"
"10500206"	"S002"	"S0003"
"20100101"	"S002"	"S0009"
"20100102"	"S002"	"S0009"
"20100201"	"S010"	"S0007"
"20100202"	"S010"	"S1001"
"20100801"	"S015"	"S0007"
"20100802"	"S015"	"S1001"
"20200102"	"S002"	"S0009"
"20200103"	"S002"	"S0009"
"20200104"	"S002"	"S0009"
"20200107"	"S002"	"S0009"
"20200201"	"S010"	"S0007"
"20200202"	"S010"	"S1001"
"20200203"	"S010"	"S0007"
"20200207"	"S010"	"S1001"
"20200252"	"S010"	"S1001"
"20200253"	"S010"	"S1001"
"20200254"	"S010"	"S1001"
"20200301"	"S002"	"S3150"
"20200401"	"S002"	"S0008"
"20200402"	"S002"	"S0008"
"20201001"	"S002"	"S1001"
"20300101"	"S002"	"S0009"
"20300102"	"S002"	"S0009"
"20300106"	"S002"	"S0009"

"20300201"	"S010"	"S1001"
"20300202"	"S010"	"S0007"
"20300203"	"S010"	"S0007"
"20300206"	"S002"	"S1001"
"20300301"	"S002"	"S3150"
"20301001"	"S002"	"S1001"
"20400110"	"S002"	"S5565"
"20400301"	"S010"	"S0007"
"20400399"	"S002"	"S0007"
"20400401"	"S002"	"S3150"
"20400402"	"S002"	"S0008"
"20400404"	"S002"	"S1001"
"20400406"	"S002"	"S0008"
"20400407"	"S002"	"S0009"
"20400409"	"S002"	"S0003"
"20400499"	"S002"	"S3150"
"30107101"	"S002"	"S95325"
"30181003"	"S002"	"S2462"
"30190013"	"S002"	"S0003"
"30190014"	"S002"	"S0004"
"30190099"	"S002"	"S0079"
"30203803"	"S002"	"S0000"
"30290003"	"S002"	"S0003"
"30300302"	"S002"	"S0011"
"30300303"	"S002"	"S0011"
"30300308"	"S002"	"S0011"
"30300317"	"S002"	"S0000"
"30300399"	"S002"	"S0011"
"30301511"	"S002"	"S0000"
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"30301513"	"S002"	"S0000"
"30301526"	"S002"	"S0000"
"30301544"	"S002"	"S0000"
"30301581"	"S002"	"S0000"
"30301587"	"S002"	"S0000"
"30301599"	"S002"	"S0000"
"30390003"	"S002"	"S0003"
"30390004"	"S002"	"S0004"
"30390023"	"S005"	"S0051"
"30390024"	"S002"	"S0079"
"30400360"	"S002"	"S0000"
"30490003"	"S002"	"S0003"
"30500209"	"S002"	"S0025"
"30500213"	"S002"	"S0025"
"30500214"	"S002"	"S0025"
"30500255"	"S002"	"S0025"

"30500258"	"S002"	"S0025"
"30500716"	"S002"	"S0000"
"30501403"	"S002"	"S0000"
"30501613"	"S002"	"S0000"
"30501618"	"S002"	"S0000"
"30599999"	"S002"	"S0000"
"30600105"	"S002"	"S0003"
"30600106"	"S002"	"S0004"
"30600201"	"S002"	"S0029"
"30600401"	"S002"	"S2485"
"30600905"	"S002"	"S0003"
"30609903"	"S002"	"S0003"
"30890003"	"S002"	"S0003"
"30900198"	"S002"	"S2466"
"30999999"	"S002"	"S2466"
"31000302"	"S002"	"S0003"
"31000404"	"S002"	"S0003"
"31000414"	"S002"	"S0003"
"31000415"	"S002"	"S0004"
"31499999"	"S002"	"S0000"
"39000699"	"S002"	"S0000"
"39900601"	"S002"	"S0003"
"39990003"	"S002"	"S0003"
"40201001"	"S002"	"S0003"
"40290013"	"S002"	"S0003"
"40400153"	"S002"	"S8869"
"40400154"	"S002"	"S2489"
"50100103"	"S002"	"S0122"
"50100410"	"S005"	"S0051"
"50100515"	"S002"	"S0122"
"50100516"	"S002"	"S0122"
"50200101"	"S002"	"S0122"
"50290006"	"S002"	"S0000"
"50300203"	"S002"	"S0000"
"50300601"	"S005"	"S0079"
"50300702"	"S002"	"S0000"
"50300899"	"S002"	"S0000"
"50400320"	"S002"	"S0000"

Table 3-3 Example of the original VOC profiles versus the revised VOC profile that excluding HCHO (species name FORM)

Original profile 0003 for VOC (TOG)	New profile S0003 for VOC (TOG)
0003;"TOG";"FORM_PRIMARY";0.08;30.026;0.08 0003;"TOG";"SOAALK";0.17;73.469;0.17	S0003;"TOG";"UNK_PRIMARY";0.08;30.026;0.08 S0003;"TOG";"SOAALK";0.17;73.469;0.17

0003;"TOG";"BENZ";0.04;78.1118;0.04	S0003;"TOG";"BENZ";0.04;78.1118;0.04
0003;"TOG";"CH4";0.56;16.0425;0.56	S0003;"TOG";"CH4";0.56;16.0425;0.56
0003;"TOG";"FORM";0.08;30.026;0.08	S0003;"TOG";"UNK";0.08;30.026;0.08
0003;"TOG";"PAR";0.2597;14.446;0.2597	S0003;"TOG";"PAR";0.2597;14.446;0.2597
0003;"TOG";"PRPA";0.04;44.0956;0.04	S0003;"TOG";"PRPA";0.04;44.0956;0.04
0003;"TOG";"TOL";0.02;92.1384;0.02	S0003;"TOG";"TOL";0.02;92.1384;0.02
0003;"TOG";"UNR";2.7779E-4;14.3633;2.7779E-4	S0003;"TOG";"UNR";2.7779E-4;14.3633;2.7779E-4

Table 3-1 New CO profile that scale CO emissions to HCHO (FORM) emissions

Profile ID	Profile for CO	HCHO to CO Mass ratio
S002	S002;"CO";"FORM";0.02;30.026;0.02 S002;"CO";"CO";1.0;28.0;1.0	0.02
S005	S005;"CO";"FORM";0.05;30.026;0.05 S005;"CO";"CO";1.0;28.0;1.0	0.05
S010	S010;"CO";"FORM";0.10;30.026;0.10 S010;"CO";"CO";1.0;28.0;1.0	0.1
S015	S015;"CO";"FORM";0.15;30.026;0.15 S015;"CO";"CO";1.0;28.0;1.0	0.15

For the base year optimization sensitivity tests for HCHO improvements, we processed the EPA 2016v1 base emissions inventories for point sources to update the HCHO emissions. By using the revised GSPRO, GSREF and GSCNV files, we conducted the SMOKE modeling for the point source sectors of ptnonipm and ptegu through the EPA 2016v1Platform and prepared emissions files for the months of April through September for the 1.33km SEMI1 grid. The pre-merged CAMx ready emissions files are kept separated for these sectors for easy combination for specific sensitivity tests.

The model-ready emissions files of the default HCHO emissions and the updated HCHO emissions were compared for QA/QC of the updating procedure. The HCHO-excluded VOC emissions and the CO emissions from the HCHO updated sources were also compared to check for mass conservation between the default and the updated emissions. For easier comparison, the SMOKE inlineto2d program was used to convert the inline format of elevated point source emissions file to the 2-d column total emissions.

Figures 3-1 shows side by side the updated (left panel) and the default (right panel) ptnonipm sector HCHO (FORM) hourly emission rates on the SEMI1 grid at 19Z on July 12th. Figures 3-2 show the spatial distributions of the difference (left panel) and the ratio (right panel, ratio of the updated over the default, a small number of 0.000001 was used to prevent dividing by zero) between the updated and the default ptnonipm sector HCHO emissions. Figures 3-3 and 3-4 demonstrate that the supposed-to-be emissions-unchanged species of CO and VOC species are kept absolutely the same between the updated and the default ptnonipm sector. We refer to the updated ptnonipm sector as ptnonipm_semihcho hereafter.

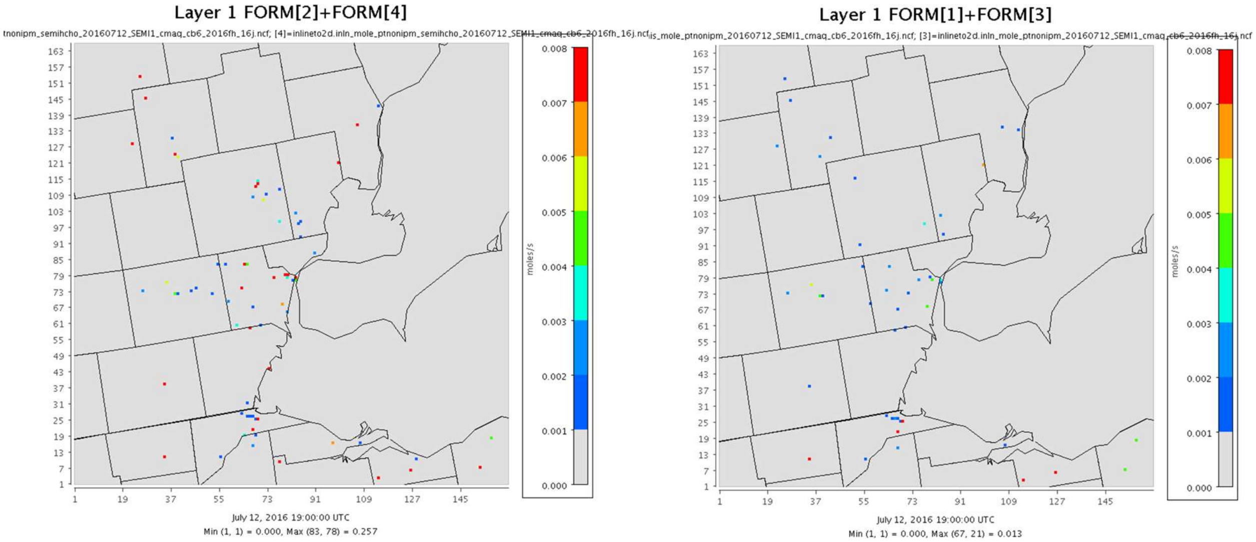


Figure 3-1. Emissions visual check on comparison of the spatial distribution of HCHO (FORM) hourly emission rates on the SEMI1 grid at 19Z on July 12th between the updated (left) and the default 2016fh_16j (right) ptnonipm sector

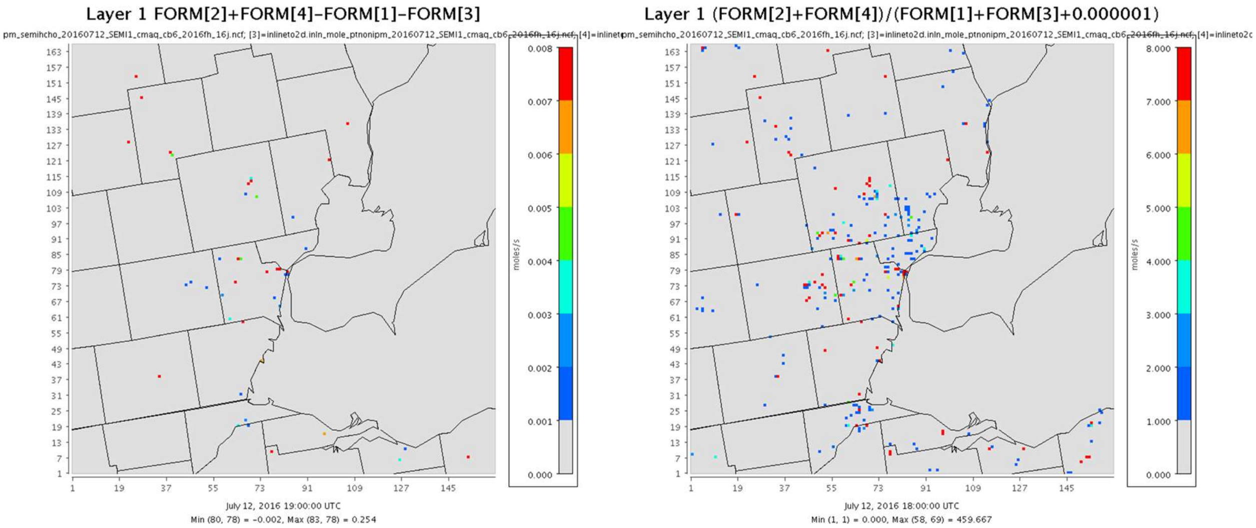


Figure 3-2. Emissions visual check on the spatial distribution of the difference (left) and the ratio (right) between the updated and the default 2016fh_16j ptnonipm sector of HCHO (FORM) hourly emission rates on the SEMI1 grid at 19Z on July 12th.

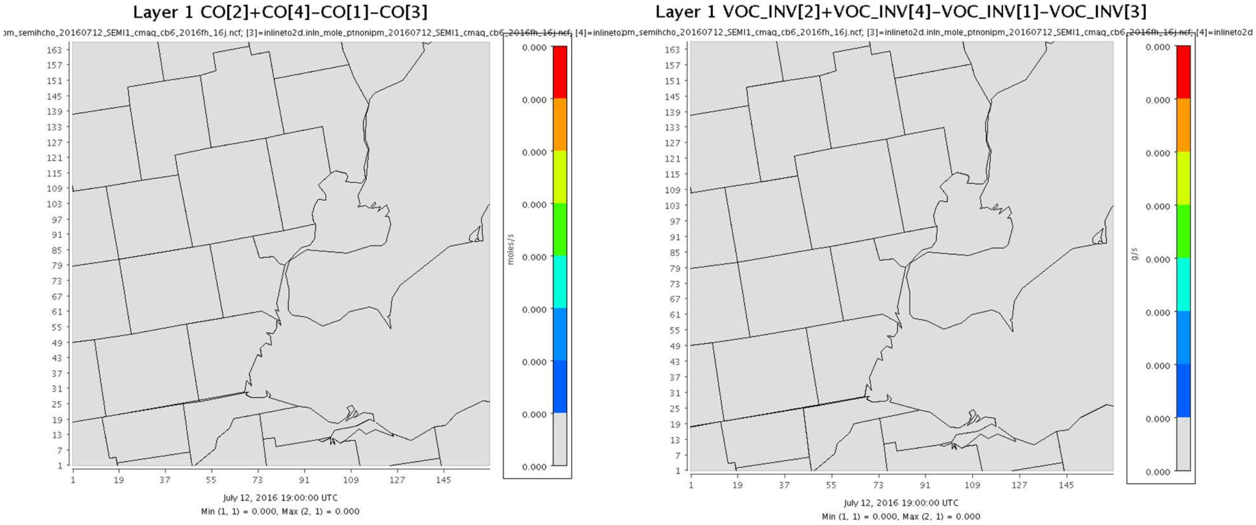


Figure 3-3. Emissions visual check on the emissions-unchanged species of CO (left) and VOC_INV (right) between the updated and the default 2016fh_16j ptnonipm sector.

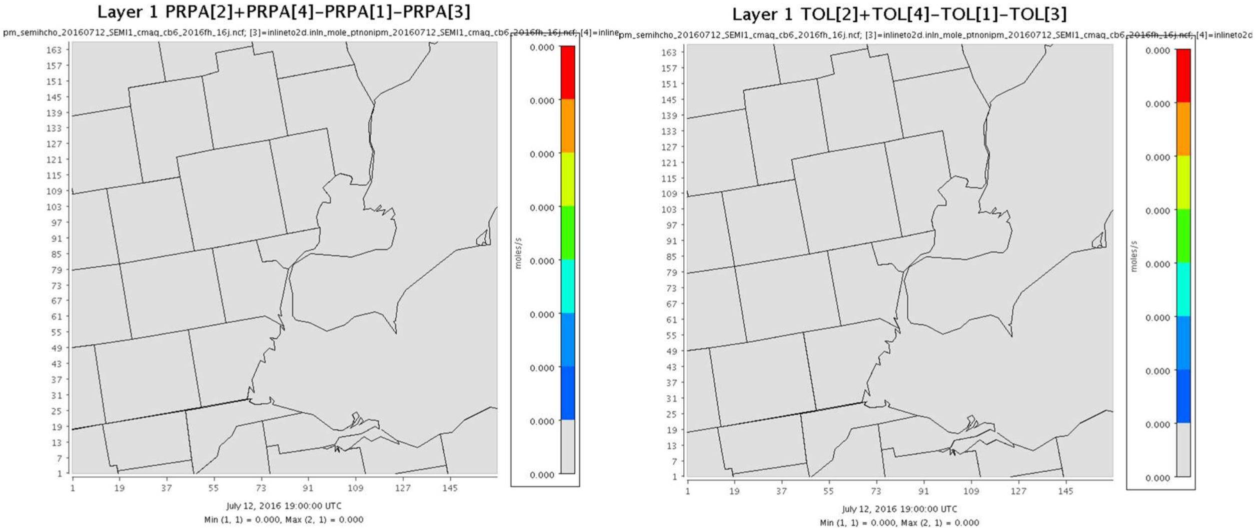


Figure 3-4. Emissions visual check on the emissions-unchanged species of PRPA (left) and TOL (right) between the updated and the default 2016fh_16j ptnonipm sector.

Figures 3-5 shows side by side the updated (left panel) and the default (right panel) ptegu sector HCHO (FORM) hourly emission rates on the SEMI1 grid on at 19Z July 12th. Figures 3-6 show the spatial distributions of the difference (left panel) and the ratio (right panel, ratio of the updated over the default, a small number of 0.000001 was used to prevent dividing by zero) between the updated and the default ptegu sector HCHO emissions. Figures 3-7 and 3-8 demonstrate that the supposed-to-be emissions-unchanged species of CO and VOC species are kept absolutely the same between the updated and the default ptegu sector. We refer to the updated ptegu sector as ptegu_semihcho hereafter.

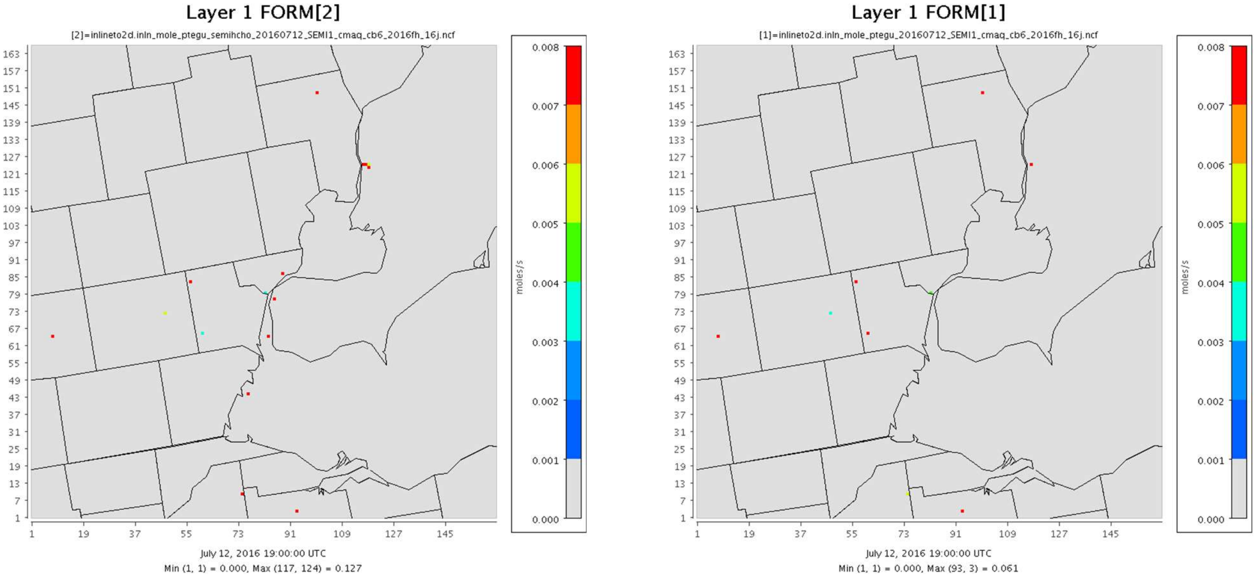


Figure 3-5. Emissions visual check on comparison of the spatial distribution of HCHO (FORM) hourly emission rates on the SEMI1 grid at 19Z on July 12th between the updated (left) and the default 2016fh_16j (right) ptegu sector.

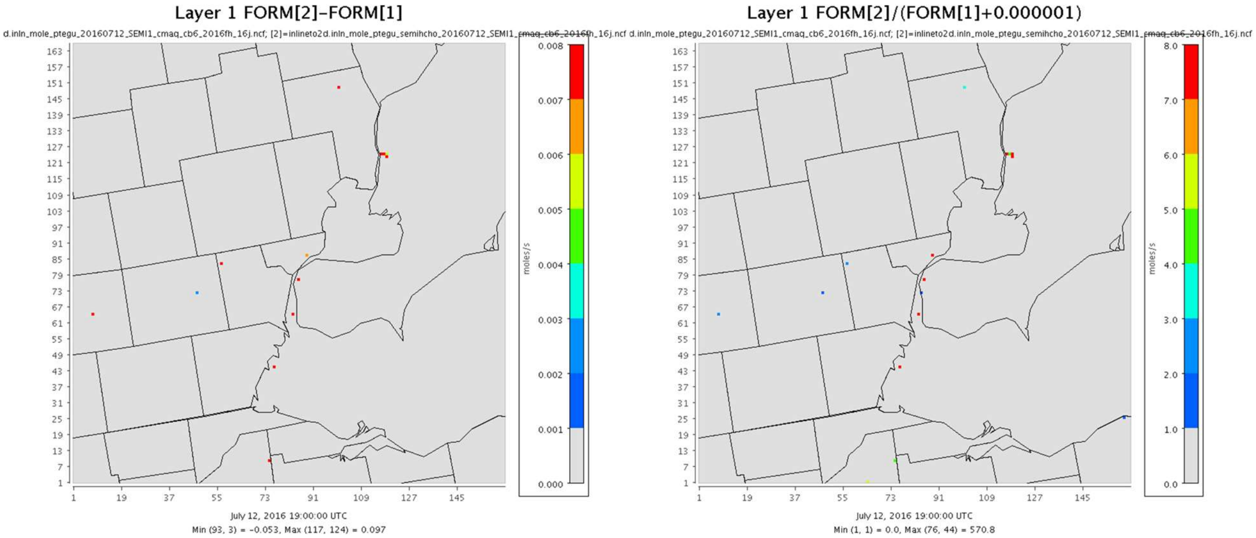


Figure 3-6. Emissions visual check on the spatial distribution of the difference (left) and the ratio (right) between the updated and the default 2016fh_16j ptegu sector of HCHO (FORM) hourly emission rates on the SEMI1 grid at 19Z on July 12th.

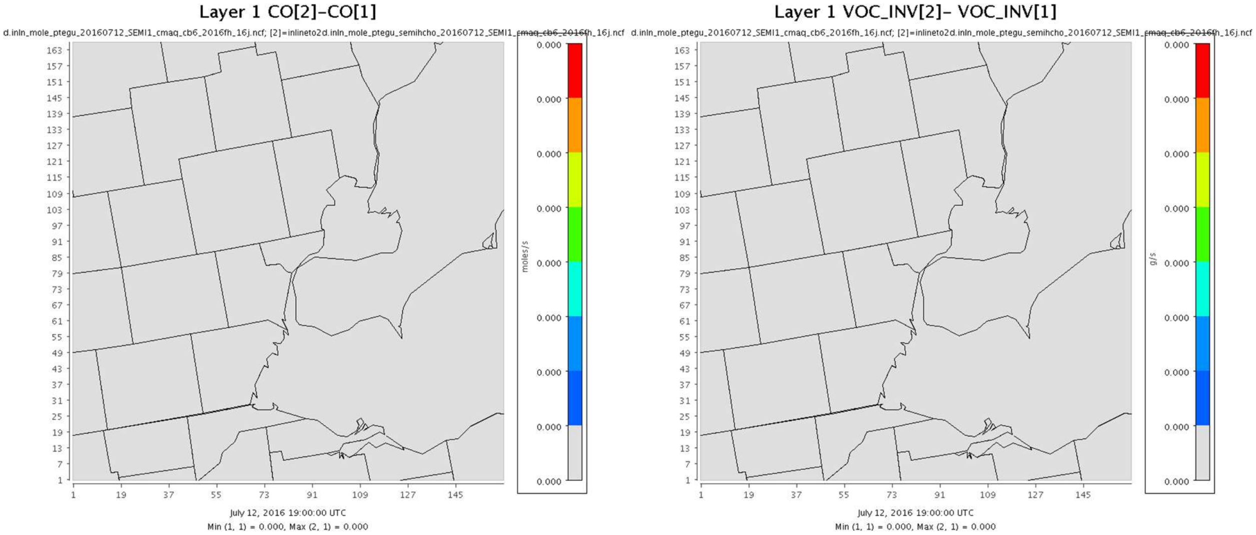


Figure 3-7. Emissions visual check on the emissions-unchanged species of CO (left) and VOC_INV (right) between the updated and the default 2016fh_16j ptegu sector.

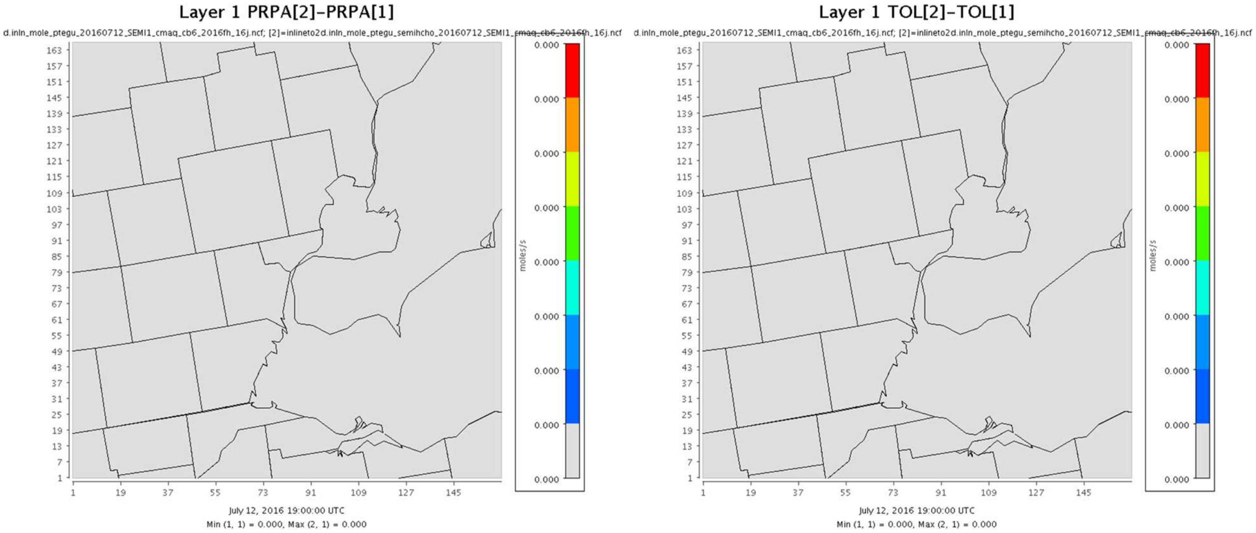


Figure 3-8. Emissions visual check on the emissions-unchanged species of PRPA (left) and TOL (right) between the updated and the default 2016fh_16j ptegu sector.

Among the total default HCHO emissions of 121 tpy from non-EGU sources (sector ptnonipm) in SE Michigan within the SEMI1 grid, 77 tpy HCHO emissions from the relevant facilities were adjusted to 1034 tpy, by an average ratio of 13.4 (Table 3-5). The adjusting ratio of facilities in the Ohio portion inside the grid is however much lower at 4.7. Meanwhile all the default HCHO emissions of 44.5 tpy from EGU sources (sector ptegu) in SE Michigan within the SEMI1 grid were adjusted to 169 tpy, by an average ratio of 3.8, significantly lower than the adjusting ratio to non-EGU sources. The adjusting ratio of EGU sources in the Ohio portion inside the grid is 0.2, i.e. a reduction in HCHO emissions (Table 3-5). Reasons for this might be none or too little associated CO emission reported in the inventory for these sources.

Table 3-5 Sector default (2016fh_16j) versus updated emissions of HCHO in short tons per year (tpy) in Michigan and Ohio grid cells within the SEMI1 molding domain

HCHO(tons/yr)	**default ptnonipm**	**updated ptnonipm_semihcho**	**Updated portion default**	**Updated**	**Adjusting Ratio**
Michigan	121	1,078	77	1,034	13.4
Ohio	77	192	31	146	4.7
HCHO(tons/yr)	**default ptegu**	**updated ptegu_semihcho**	**Updated portion default**	**Updated**	**Adjusting Ratio**
Michigan	44.5	169	44.5	169	3.8
Ohio	27.6	5.9	27.6	5.9	0.2

Figures 3-9 shows the distribution of the ratio between the updated and the default HCHO emissions from all the point sources (ptegu and ptnonipm together) on the SEMI1 grid at 19Z on July 12th. All the non-EGU and EGU point sources together, 121.5 tpy HCHO emissions from the relevant facilities in SE Michigan within the SEMI1 grid, were adjusted to 1203 tpy by an average ratio of 9.9 (Table 3-6). The updated total amount of HCHO emissions of 1203 tpy from all the relevant point sources is slightly larger than the EGLE MAERS estimated total of 1180 tpy.

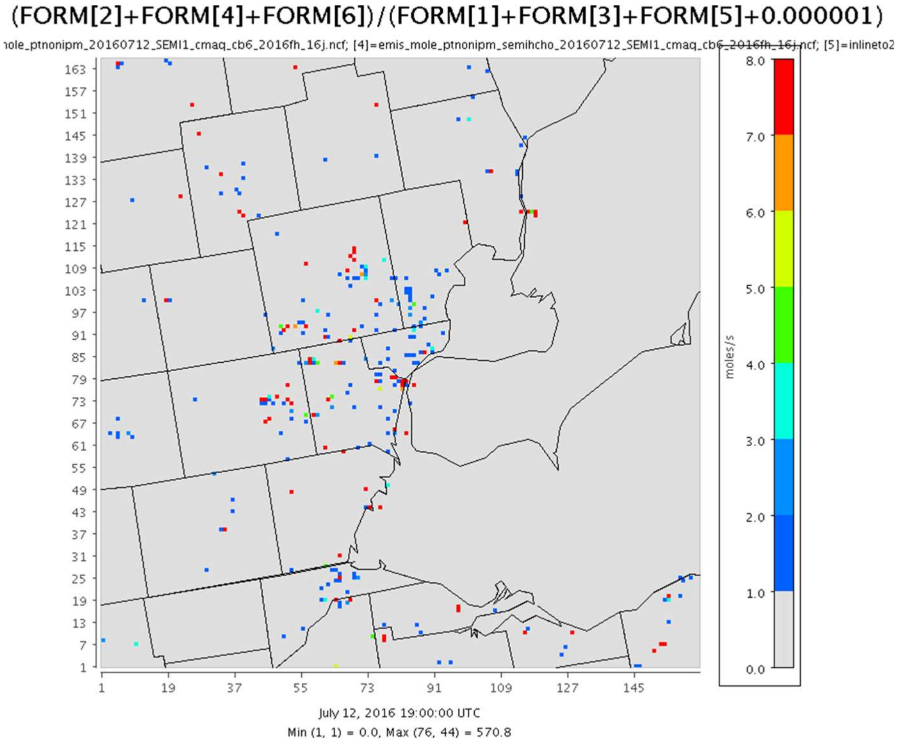


Figure 3-9. Spatial distribution of the ratio of the updated over the default 2016fh_16j HCHO (FORM) hourly emission rates from the ptegu and ptnonipm sectors together on the SEMI1 grid at 19Z on July 12th.

Table 3-6 Point sources total default (2016fh_16j) versus updated emissions of HCHO in short tons per year (tpy) in SE Michigan compared to the EGLE MAERS inventory

FORM(tons/yr)	Updated portion Default total	Updated total	Adjusting Ratio	EGLE MAERS 2017 Estimated Total
SE Michigan	121.5	1,203	9.9	1,180
North Ohio	58.6	151.9	2.6	

3.2 VCP VOCs Emissions Improvement

To improve the VCP VOC emissions, we followed the work performed by Ramboll in a separate LADCO project that scaled 2016 emissions to account for the deficiency of VCP emissions in the inventories (Ramboll, 2020), as advised by LADCO. By using the Ramboll method, VCP emissions are directly updated by scaling the original VOC emissions amount for identified sources in the specific 2016fh_16j default emissions inventories mainly the nonpt and ptnonipm sectors. The adjustment factors for individual sources and/or source categories are directly adopted from the Ramboll study as listed in Table 3-7. The relevant sources to be scaled by certain factors are identified by searching through the inventory records for SCC codes that matched with the specific leading digits (Table 3-7). In the table, the SCCs with leading digits in red are sources from the ptnonipm sector, while other SCCs are all from the nonpt sector.

Table 3-7 List of adjustment factors for VCP VOCs emissions by VCP category and the relevant SCCs

VCP category	SCC (with leading digits only)	VOC Adjustment factor
Pesticides	24608, 24618, 24658	1.69
Coatings	2401, 24605, 402	2.70
Printing inks	2425, 405	4.80
Adhesives	244002, 24606, 24656, 24612	18.00
Cleaning products	2402, 2415, 2420, 401	1.12
Personal care products	24601, 24602, 24604, 24651, 24652, 24654	5.19

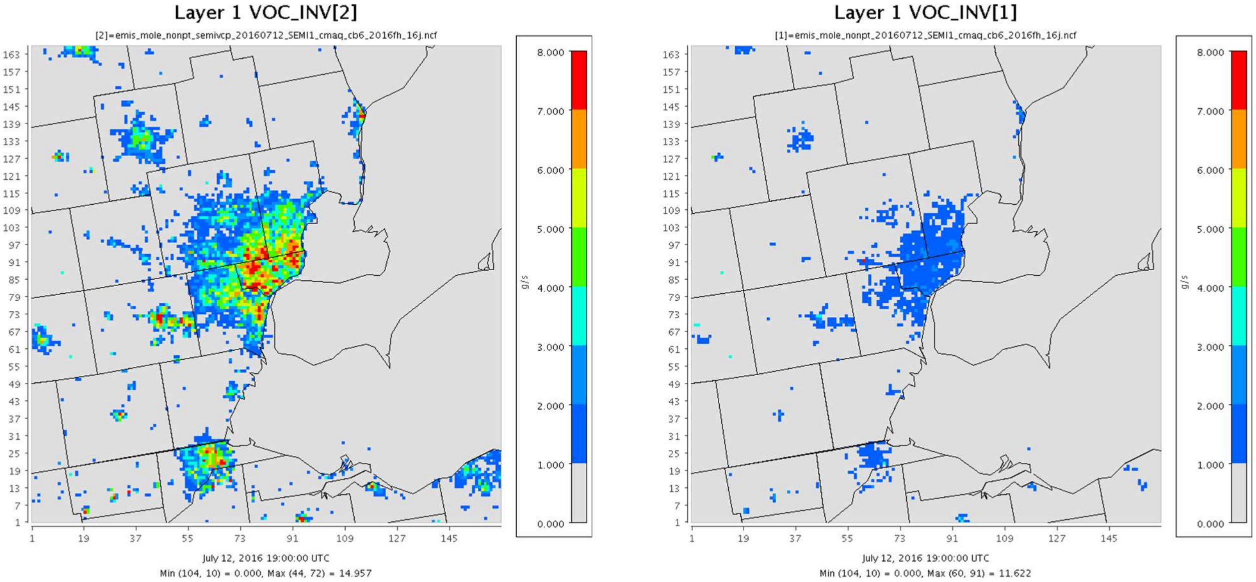
For the base year optimization sensitivity test for VCP emissions improvements, by using the relevant VCP VOC emissions scaled inventories, we conducted SMOKE modeling for both the area source sector nonpt and the non-EGU point source sector ptnonipm through the EPA 2016v1Platform and prepared emissions files for the months of April through September for the 1.33km SEMI1 grid. The pre-merged CAMx ready emissions files are kept separated for these sectors for easy combination for specific sensitivity tests. These updated sectors are referred to as nonpt_semivcp and ptnonipm_semivcp hereafter. We also conducted the SMOKE modeling for the ptnonipm sector by using the VCP VOC emissions scaled inventories with the updated GSPRO, GSREF and GSCNV files updated for HCHO improvements. We refer to the HCHO and VCP VOC updated sectors as ptnonipm_semihchovcp hereafter.

The model-ready emissions files of the default VOC emissions and the updated VOC emissions from these two sectors were compared for QA/QC of the updating procedure. For easier comparison, the SMOKE inlineto2d program was used to convert the inline format of elevated non-EGU point source emissions file to the 2-d column total emissions.

Figures 3-10 shows side by side the updated (left panel) and the default (right panel) nonpt sector total VOC hourly emission rates on the SEMI1 grid at 19Z on July 12th. While Figures 3-

11 show the spatial distributions of the difference (left panel) and the ratio (right panel, ratio of the updated over the default, a small number of 0.000001 was used to prevent dividing by zero) between the updated and the default nonpt sector total VOC emissions.

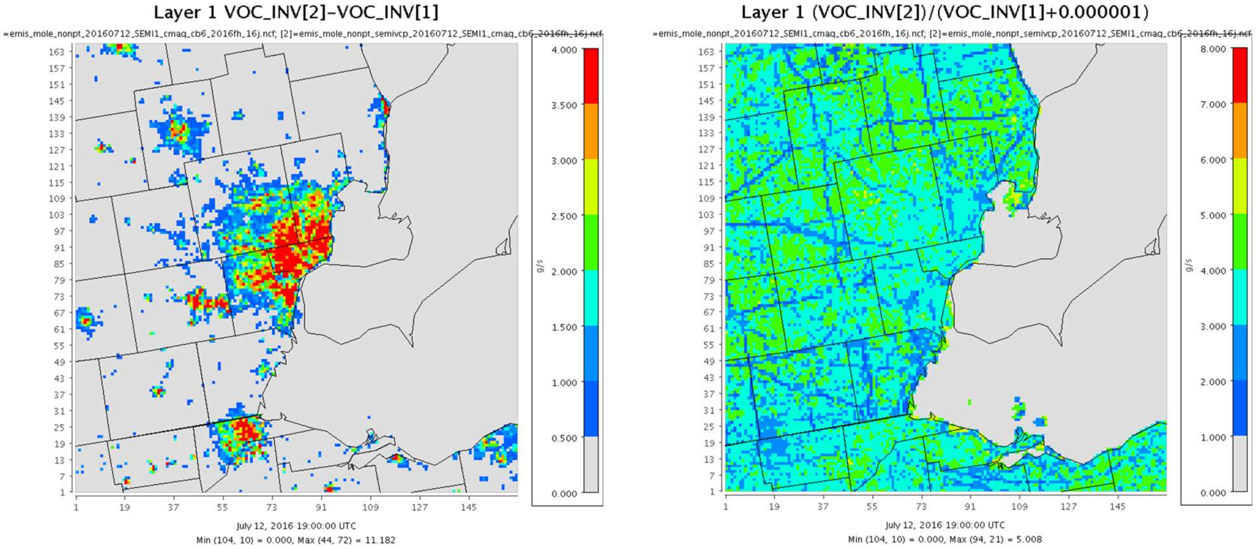
Figures 3-12 shows side by side the updated (left panel) and the default (right panel) ptnonipm sector total VOC hourly emission rates on the SEMI1 grid at 19Z on July 12th. While Figures 3-13 show the spatial distributions of the difference (left panel) and the ratio (right panel, ratio of the updated over the default, a small number of 0.000001 was used to prevent dividing by zero) between the updated and the default ptnonipm sector total VOC emissions.



Layer 1 VOC_INV[2]

Layer 1 VOC_INV[1]

Figure 3-10. Emissions visual check on comparison of the spatial distribution of VOC (VOC_INV, non-speciated VOC) hourly emission rates on the SEMI1 grid on at 19Z on July 12th between the updated (left) and the default 2016fh_16j (right) nonpt sector.



Layer 1 VOC_INV[2]-VOC_INV[1]

Layer 1 (VOC_INV[2])/(VOC_INV[1]+0.000001)

Figure 3-11. Emissions visual check on the spatial distribution of the difference (left) and the ratio (right) between the updated and the default 2016fh_16j nonpt sector of VOC hourly emission rates on the SEMI1 grid at 19Z on July 12th.

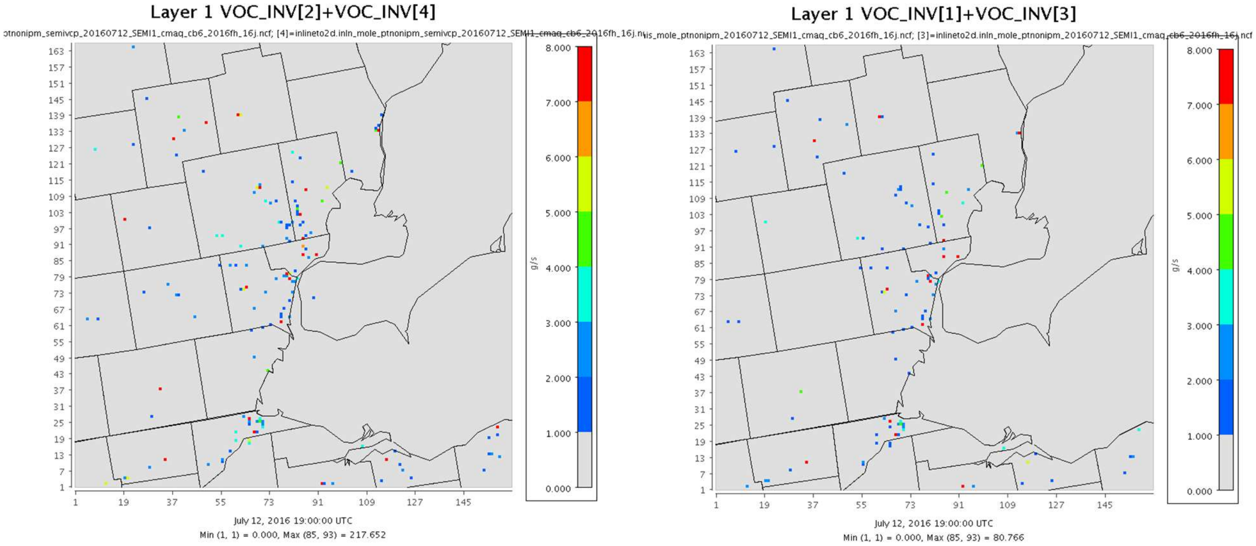


Figure 3-12. Emissions visual check on comparison of the spatial distribution of VOC (VOC_INV, non-speciated VOC) hourly emission rates on the SEMI1 grid on at 19Z on July 12th between the updated (left) and the default 2016fh_16j (right) ptnonipm sector.

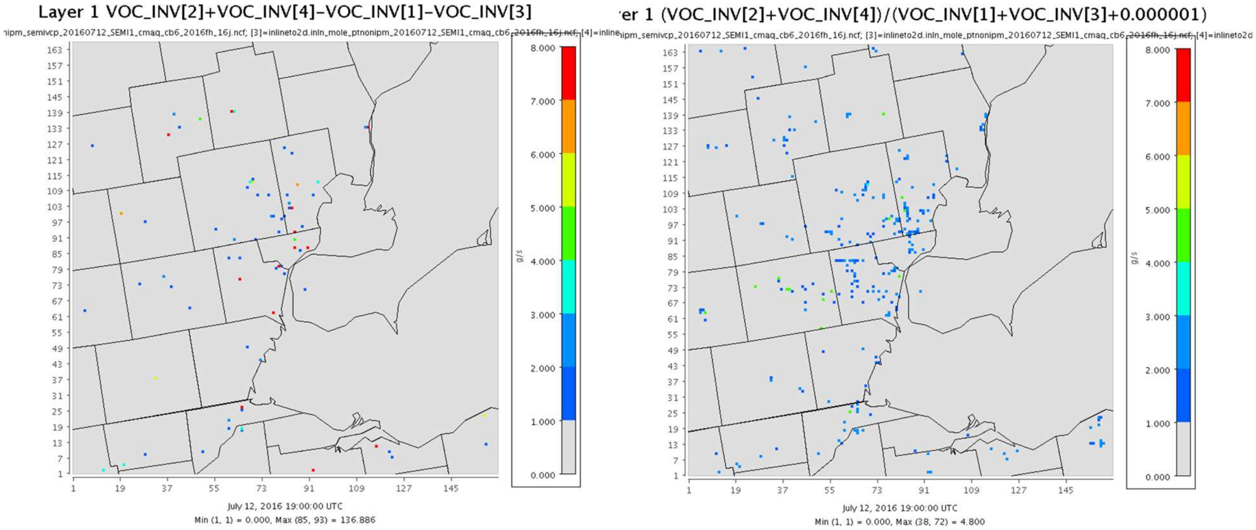


Figure 3-13. Emissions visual check on the spatial distribution of the difference (left) and the ratio (right) between the updated and the default 2016fh_16j ptnonipm sector of VOC hourly emission rates on the SEMI1 grid at 19Z on July 12th.

Among the total default VOC emissions of 66,239 tpy from the nonpt sector in SE Michigan within the SEMI1 grid, 53,116 tpy VCP VOC emissions were adjusted to 20,9230 tpy, by an average ratio of 3.94 (Table 3-8). The adjusting ratio of nonpt VCP VOC emissions in the Ohio portion inside the grid is almost the same at 3.92. Among the total default VOC emissions of 12,223 tpy from the ptnonipm sector in SE Michigan within the SEMI1 grid, 7,990 tpy VCP VOC emissions were adjusted to 21,547 tpy, by an average ratio of 2.70 (Table 3-8). The adjusting ratio of ptnonipm VCP VOC emissions in the Ohio portion inside the grid is also very similar at 2.68. In comparison, the Ramboll estimated average adjusting ratio of all VCP VOC emissions in

Michigan state is 3.27, while in this study the estimated average adjusting ratio of all VCP VOC emissions in SE Michigan is 3.78, which is slightly higher.

Table 3-8 Sector default (2016fh_16j) versus updated emissions of VCP VOC in short tons per year (tpy) in Michigan and Ohio grid cells within the SEMI1 molding domain

VOC(tons/yr)	Sector	Sector default	Sector updated	VCP portion Default	VCP updated	Adjusting Ratio
Michigan	nonpt	66,239	222,353	53,116	209,230	3.94
	ptnonipm	12,223	25,780	7,990	21,547	2.70
Ohio	nonpt	13,215	45,911	11,213	43,909	3.92
	ptnonipm	4,599	7,736	1,863	5,000	2.68
Ramboll-Michigan	Statewide			116,836	382,014	3.27

According to the Ramboll's estimate, the adjustment would increase the total VOC emissions in Michigan state by about 265,178 tpy. That would increase the VCP VOC portion of the total anthropogenic VOC emissions from the current 37% (according to Table 3-8) up to about 66%.

Table 3-8 EPA 2016NEI annual VOC emissions in Michigan State by Tier 1 Categories

Emissions Category (Tier1)	VOC emissions (tons/yr)
FUEL COMB. ELEC. UTIL.	1,310
FUEL COMB. INDUSTRIAL	1,804
FUEL COMB. OTHER	15,096
CHEMICAL & ALLIED PRODUCT MFG	1,248
METALS PROCESSING	1,098
PETROLEUM & RELATED INDUSTRIES	20,612
OTHER INDUSTRIAL PROCESSES	5,153
SOLVENT UTILIZATION	116,900
STORAGE & TRANSPORT	17,877
WASTE DISPOSAL & RECYCLING	6,027
HIGHWAY VEHICLES	63,809
OFF-HIGHWAY	55,294
MISCELLANEOUS	2,343
PRESCRIBED FIRES	7,055
Total	**315,626**

To make further improvement of VCP VOC emissions, we collected the newly revised VOC speciation profiles for VCP sources from the recently released EPA 2017platform (https://www.epa.gov/air-emissions-modeling/2017-emissions-modeling-platform). The implementation of these new speciation profiles would promote the improvement on the composition hence the reactivity of the VCP VOC emissions. The EPA 2017platform updated 8 VCP VOC speciation profiles; the IDs of these profiles are 95507, 95508, 95509, 95510, 95511, 95512, 95513 and CARB3103. We identified the VCP SCCs that are associated with these new profiles and revised the GSPRO files to update the reference entries for these SCCs according to Table 3-9. We also added the 8 new profiles into the GSREF file and revised the GSCNV files accordingly for these profiles. The SCCs listed in Table 3-9 are all for sources from the nonpt sector.

For the base year optimization sensitivity test for composition improvement of VCP VOC emissions, by using the relevant VCP VOCs emissions scaled nonpt sector inventories with the updated GSPRO, GSREF and GSCNV files, we conducted SMOKE modeling for the area source sector nonpt through the EPA 2016v1Platform and prepared emissions files for the months of April through September for the 1.33km SEMI1 grid. The pre-merged CAMx-ready emissions files are kept separated for these sectors for easy combination for specific sensitivity tests. This sector with both the amount and composition updated for VCP VOC emissions is referred to as nonpt_semivcpgspro hereafter. Note that the VOC emissions amount of this sector doesn't change from the nonpt_semivcp sector. Only some of the VOC species swapped portions of their emissions to other species and hence the reactivity of the total VOC emissions has changed. But by reviewing and comparing the new profiles to the old ones, the changes of the composition are quite small.

Table 3-9 List of the VCP SCCs with updated assignment of new VOC speciation profiles

SCC	Old VOC profile	Updated VOC profile	Note on Updates (from the 2017Paltform's speciation profiles reference file)
2460800000	3145	95511	! Updated for 2017 per M. Strum. Profile name: Consumer and Commercial Products All FIFRA Related Products Composite CARB 2010 Survey Update
2461800000	3001	CARB3103	! Updated for 2017 per M. Strum. Profile name: CONS PRD- OTHER PESTICIDES AND INSECTICIDES (2010 UPDATE)
2461850000	3001	CARB3103	! Updated for 2017 per M. Strum. Profile name: CONS PRD- OTHER PESTICIDES AND INSECTICIDES (2010 UPDATE)
2461850001	3001	CARB3103	! Updated for 2017 per M. Strum. Profile name: CONS PRD- OTHER PESTICIDES AND INSECTICIDES (2010 UPDATE)
2461850004	3001	CARB3103	! Updated for 2017 per M. Strum. Profile name: CONS PRD- OTHER PESTICIDES AND INSECTICIDES (2010 UPDATE)
2461850005	3001	CARB3103	! Updated for 2017 per M. Strum. Profile name: CONS PRD- OTHER PESTICIDES AND INSECTICIDES (2010 UPDATE)
2461850006	3001	CARB3103	! Updated for 2017 per M. Strum. Profile name: CONS PRD- OTHER PESTICIDES AND INSECTICIDES (2010 UPDATE)
2461850009	3001	CARB3103	! Updated for 2017 per M. Strum. Profile name: CONS PRD- OTHER PESTICIDES AND INSECTICIDES (2010 UPDATE)
2461850051	3001	CARB3103	! Updated for 2017 per M. Strum. Profile name: CONS PRD- OTHER PESTICIDES AND INSECTICIDES (2010 UPDATE)

2461850054	3001	CARB3103	! Updated for 2017 per M. Strum. Profile name: CONS PRD- OTHER PESTICIDES AND INSECTICIDES (2010 UPDATE)
2461850055	3001	CARB3103	! Updated for 2017 per M. Strum. Profile name: CONS PRD- OTHER PESTICIDES AND INSECTICIDES (2010 UPDATE)
2461850056	3001	CARB3103	! Updated for 2017 per M. Strum. Profile name: CONS PRD- OTHER PESTICIDES AND INSECTICIDES (2010 UPDATE)
2461850099	3001	CARB3103	! Updated for 2017 per M. Strum. Profile name: CONS PRD- OTHER PESTICIDES AND INSECTICIDES (2010 UPDATE)
2461870999	3001	CARB3103	! Updated for 2017 per M. Strum. Profile name: CONS PRD- OTHER PESTICIDES AND INSECTICIDES (2010 UPDATE)
2461800001	3001	CARB3103	! Updated for 2017 per M. Strum. Profile name: CONS PRD- OTHER PESTICIDES AND INSECTICIDES (2010 UPDATE)
2461800002	3001	CARB3103	! Updated for 2017 per M. Strum. Profile name: CONS PRD- OTHER PESTICIDES AND INSECTICIDES (2010 UPDATE)
2461850002	3001	CARB3103	! Updated for 2017 per M. Strum. Profile name: CONS PRD- OTHER PESTICIDES AND INSECTICIDES (2010 UPDATE)
2461850003	3001	CARB3103	! Updated for 2017 per M. Strum. Profile name: CONS PRD- OTHER PESTICIDES AND INSECTICIDES (2010 UPDATE)
2461850052	3001	CARB3103	! Updated for 2017 per M. Strum. Profile name: CONS PRD- OTHER PESTICIDES AND INSECTICIDES (2010 UPDATE)
2461850053	3001	CARB3103	! Updated for 2017 per M. Strum. Profile name: CONS PRD- OTHER PESTICIDES AND INSECTICIDES (2010 UPDATE)
2465800000	3001	CARB3103	! Updated for 2017 per M. Strum. Profile name: CONS PRD- OTHER PESTICIDES AND INSECTICIDES (2010 UPDATE)
2401001000	8744	95513	! Updated for 2017 per M. Strum. Profile name: Architectural Coatings Solvent and Waterborne Composite CARB 2005 Survey
2460500000	3144	95512	! Updated for 2017 per M. Strum. Profile name: Consumer and Commercial Products Composite CARB 2010 Survey Update
2460520000	3144	95512	! Updated for 2017 per M. Strum. Profile name: Consumer and Commercial Products Composite CARB 2010 Survey Update
2440020000	3142	95507	! Updated for 2017 per M. Strum. Profile name: Consumer and Commercial Products Adhesives and Sealants Composite CARB 2010 Survey Update

2460600000	3142	95507	! Updated for 2017 per M. Strum. Profile name: Consumer and Commercial Products Adhesives and Sealants Composite CARB 2010 Survey Update
2460610000	3142	95507	! Updated for 2017 per M. Strum. Profile name: Consumer and Commercial Products Adhesives and Sealants Composite CARB 2010 Survey Update
2465600000	3142	95507	! Updated for 2017 per M. Strum. Profile name: Consumer and Commercial Products Adhesives and Sealants Composite CARB 2010 Survey Update
2460100000	3147	95509	! Updated for 2017 per M. Strum. Profile name: Consumer and Commercial Products Personal Care Composite CARB 2010 Survey Update
2460110000	3147	95509	! Updated for 2017 per M. Strum. Profile name: Consumer and Commercial Products Personal Care Composite CARB 2010 Survey Update
2460120000	3147	95509	! Updated for 2017 per M. Strum. Profile name: Consumer and Commercial Products Personal Care Composite CARB 2010 Survey Update
2460130000	3147	95509	! Updated for 2017 per M. Strum. Profile name: Consumer and Commercial Products Personal Care Composite CARB 2010 Survey Update
2460150000	3147	95509	! Updated for 2017 per M. Strum. Profile name: Consumer and Commercial Products Personal Care Composite CARB 2010 Survey Update
2460160000	3147	95509	! Updated for 2017 per M. Strum. Profile name: Consumer and Commercial Products Personal Care Composite CARB 2010 Survey Update
2460180000	3147	95509	! Updated for 2017 per M. Strum. Profile name: Consumer and Commercial Products Personal Care Composite CARB 2010 Survey Update
2460190000	3147	95509	! Updated for 2017 per M. Strum. Profile name: Consumer and Commercial Products Personal Care Composite CARB 2010 Survey Update
2460200000	3146	95508	! Updated for 2017 per M. Strum. Profile name: Consumer and Commercial Products Household Composite CARB 2010 Survey Update
2460220000	3146	95508	! Updated for 2017 per M. Strum. Profile name: Consumer and Commercial Products Household Composite CARB 2010 Survey Update

2460400000	8520	95510	! Updated for 2017 per M. Strum. Profile name: Consumer and Commercial Products Automotive Aftermarket Composite CARB 2010 Survey Update
2465100000	3147	95509	! Updated for 2017 per M. Strum. Profile name: Consumer and Commercial Products Personal Care Composite CARB 2010 Survey Update
2465200000	3146	95508	! Updated for 2017 per M. Strum. Profile name: Consumer and Commercial Products Household Composite CARB 2010 Survey Update
2465400000	8520	95510	! Updated for 2017 per M. Strum. Profile name: Consumer and Commercial Products Automotive Aftermarket Composite CARB 2010 Survey Update

The model-ready emissions files of the nonpt_semivcpgspro sector and the nonpt_semivcp sector were compared for emissions rates of total VOC and the major VOC species for QA/QC of the updating procedure. The emissions rates of the VOC totals are kept the same between the two sectors while small differences were found for major VOC species that reflect the changes of the VOC composition of the VCP VOC emissions.

3.3 Alternative Biogenic Emissions using MEGAN

The 2016v1platform uses BEIS3 integrated into the SMOKE system for preparing biogenic emissions. BEIS3 estimates emissions of VOCs from biological activity from land-based vegetative species and nitric oxide emissions from microbial activity in certain soil types. BEIS3 uses land use data projected to an air quality modeling grid to compute normalized gridded biogenic emissions for different land use categories. The normalized emissions are adjusted for temporal variability using gridded, hourly meteorology data and speciated using precomputed VOC profiles for different photochemical mechanisms. BEIS3 outputs CMAQ model-ready hourly, gridded biogenic emissions files which can be converted to binary format for CAMx modeling system using the CMAQ2CAMx program. Overall, BEIS3 uses spatially and temporally resolved meteorology data to estimate hourly emissions factors of NO and VOCs using species-specific Leaf Area Index (LAI) for each land use type.

The model of Emissions of Gases and Aerosols from Nature (MEGAN) was developed to estimate biogenic emissions of reactive gases and aerosols needed for both regional air quality models and global chemistry transport models (Guenther et al., 2006). MEGAN uses an approach similar to BEIS3 but is easier to update, use, and expand to other compounds. The user can easily update some of the input datasets such as LAIv for vegetated surfaces from the latest MODIS LAI and Fractional Vegetation Coverage (FVC) products. One of the biggest changes in MEGAN as compared to the BEIS3 is in its treatment of plant species area coverage. In the BEIS3, plant species are mostly treated explicitly (e.g., California live oak, corn row crop, loblolly pine) through the BELD (BELD4, BELD5 etc.) datasets where in MEGAN plants are grouped by the following six plant functional types (PFTs): 1) broadleaf trees, 2) fine leaf evergreen trees, 3) fine leaf deciduous trees, 4) shrubs, 5) grass, and non-vascular plants and other ground cover and 6) crops.

We use the latest version of MEGAN, i.e., version 3.2 that was released in October 2021 (https://sites.google.com/uci.edu/bai/megan/data-and-code) for biogenic emissions estimates alternative to the BEIS3 method. In addition to the input datasets to MEGAN that came with the MEGAN V3.2 release which include the landcover (LAIv and Growth form and ecotypes) and soil data, we used the MCIP meteorological inputs prepared by this study for the SMOKE modeling. We also prepared alternative LAIv inputs by using the recommended GLASS LAI products (http://www.glass.umd.edu) specifically for year 2016 (http://www.glass.umd.edu) to replace the default 2013 LAIv data that came with MEGAN. We also obtained the GLASS LAI products to produce 2013 LAIv to directly compare with the default 2013 LAIv data.

Figures 3-14 and 3-15 show the example GLASS MODIS LAI and FVC data that covers the SEMI1 domain in the beginning of April for 2013 and for 2016 in different resolutions. Figures 3-16 and 3-17 show the example GLASS MODIS LAI and FVC data in the beginning of July.

Figure 3-14. GLASS MODIS LAI in April starting on the 89th day of the year : 2013 500m resolution (left), 2016 500m resolution (middle), and 2016 0.05Degree resolution (right).

Figure 3-15. GLASS MODIS FVC in April starting on the 89th day of the year : 2013 500m resolution (left), 2016 500m resolution (middle), and 2016 0.05Degree resolution (right).

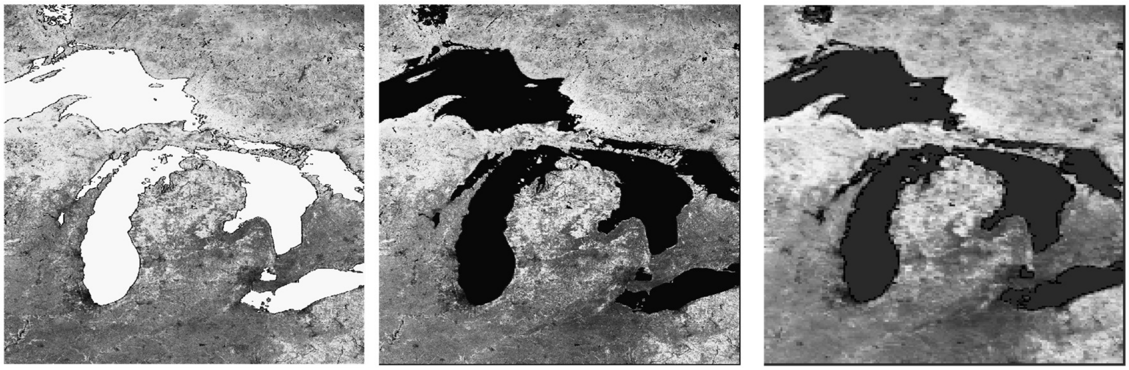


Figure 3-16. GLASS MODIS LAI in July starting on the 177th day of the year : 2013 500m resolution (left), 2016 500m resolution (middle), and 2016 0.05Degree resolution (right).

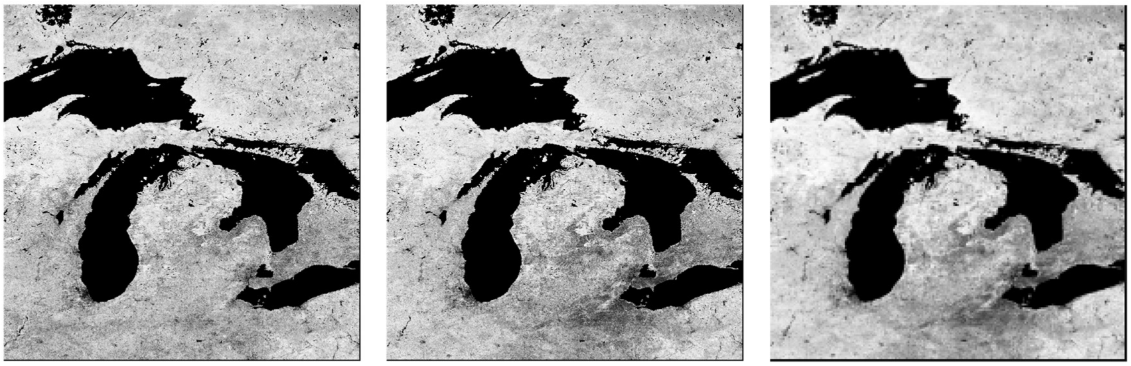


Figure 3-17. GLASS MODIS FVC in July starting on the 177th day of the year : 2013 500m resolution (left), 2016 500m resolution (middle), and 2016 0.05Degree resolution (right).

We utilized the GLASS MODIS LAI and FVC data to calculate the MEGAN required LAIv values on the SEMI1 grid every 8 days over the entire ozone season. Figures 3-18 and 3-19 show the LAIv distribution on the SEMI1 grid from using different GLASS LAI products compared to the MEGAN default 2013 data, and comparison of their changes between the beginning of April and the beginning of July. The MEGAN default 2013 LAIv data, in a very coarse resolution, show the largest and reasonable differences between the spring and the summer. The three GLASS-derived LAIv show similar but much less change from spring to summer. The GLASS-derived 2013 LAIv differs significantly from the default 2013 LAIv. By using these four different LAIv datasets as inputs we further ran MEGAN programs to generate 4 sets of the biogenic files for the entire 2016 ozone season for the SEMI1 grid.

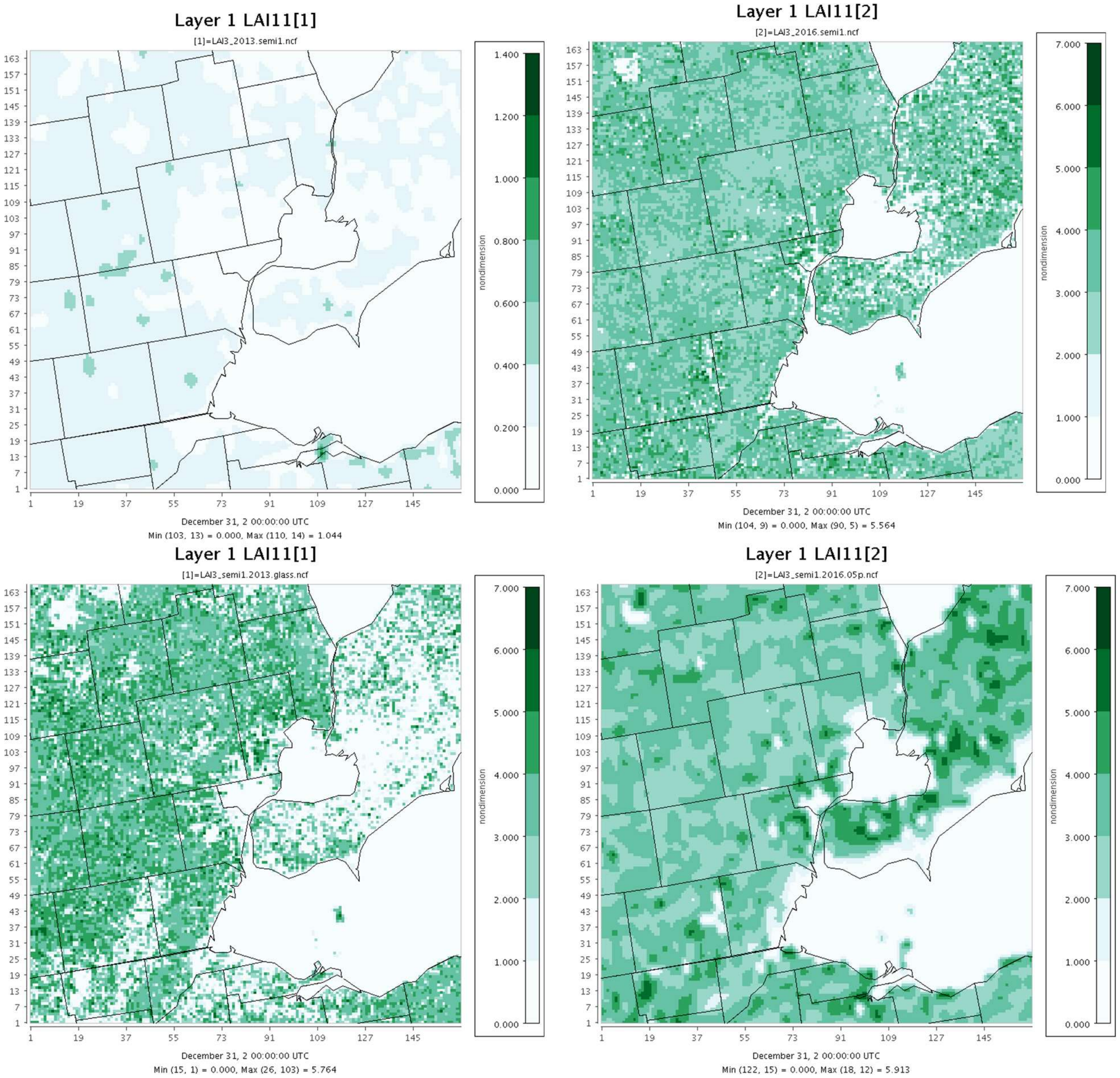


Figure 3-18. LAIv distribution on the SEMI1 grid for the 11th 8-day period of the year: Default 2013 (top left), using GLASS 2013 500m resolution data (bottom left), using GLASS 2016 500m data (top right), and using GLASS 2016 0.05Degree data (bottom right).

Figure 3-19. LAIv distribution on the SEMI1 grid for the 22th 8-day period of the year : Default 2013 (top left), using GLASS 2013 500m resolution data (bottom left), using GLASS 2016 500m data (top right), and using GLASS 2016 0.05Degree data (bottom right).

Figures 3-20 and 3-21 show side by side comparisons of the hourly emissions rates for isoprene (ISOP) generated by the five methods on a spring (April 1) and a summer day (July 1). In spring, the isoprene emissions estimated from BEIS3 and MEGAN Default 2013 are in general several times lower than from the other three MEGAN GLASS methods, with BEIS3 showing further lower emissions within the US portion in the domain. In summer, the isoprene emissions from the five methods are all at similar levels, with BEIS3 yielding higher emissions rates than other four methods. Note that the scale of the plots for summer are 10 times larger than for spring. The isoprene emissions rates in summer are generally about 10 times higher than in spring for all the MEGAN methods with the BEIS3 method yielding even larger difference between summer and spring.

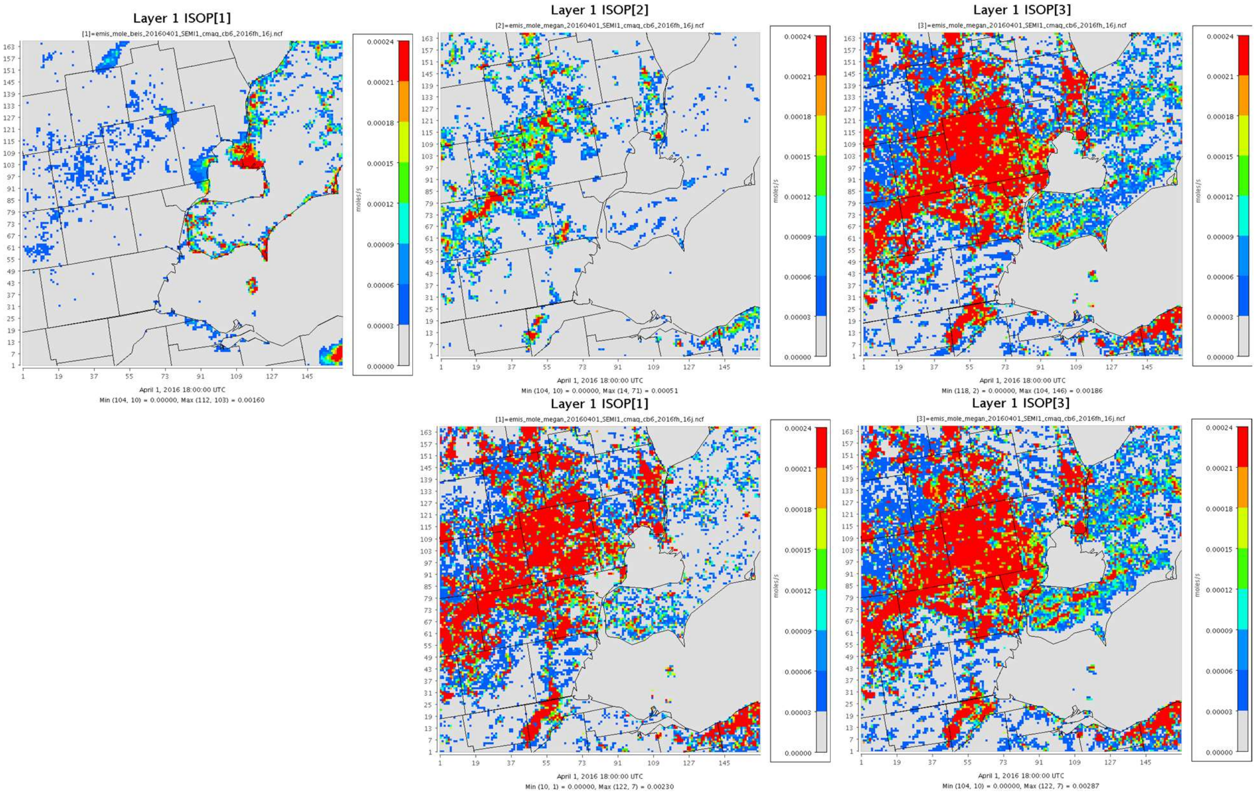


Figure 3-20. ISOP emissions rates distribution on the SEMI1 grid at 18Z on April 1, 2016, generated by BEIS3 (top left), MEGAN using Default 2013 LAIv (top middle), MEGAN using GLASS 2013 500m LAIv (bottom left), MEGAN using GLASS 2016 500m LAIv (top right), and MEGAN using GLASS 2016 0.05Degree LAIv (bottom right).

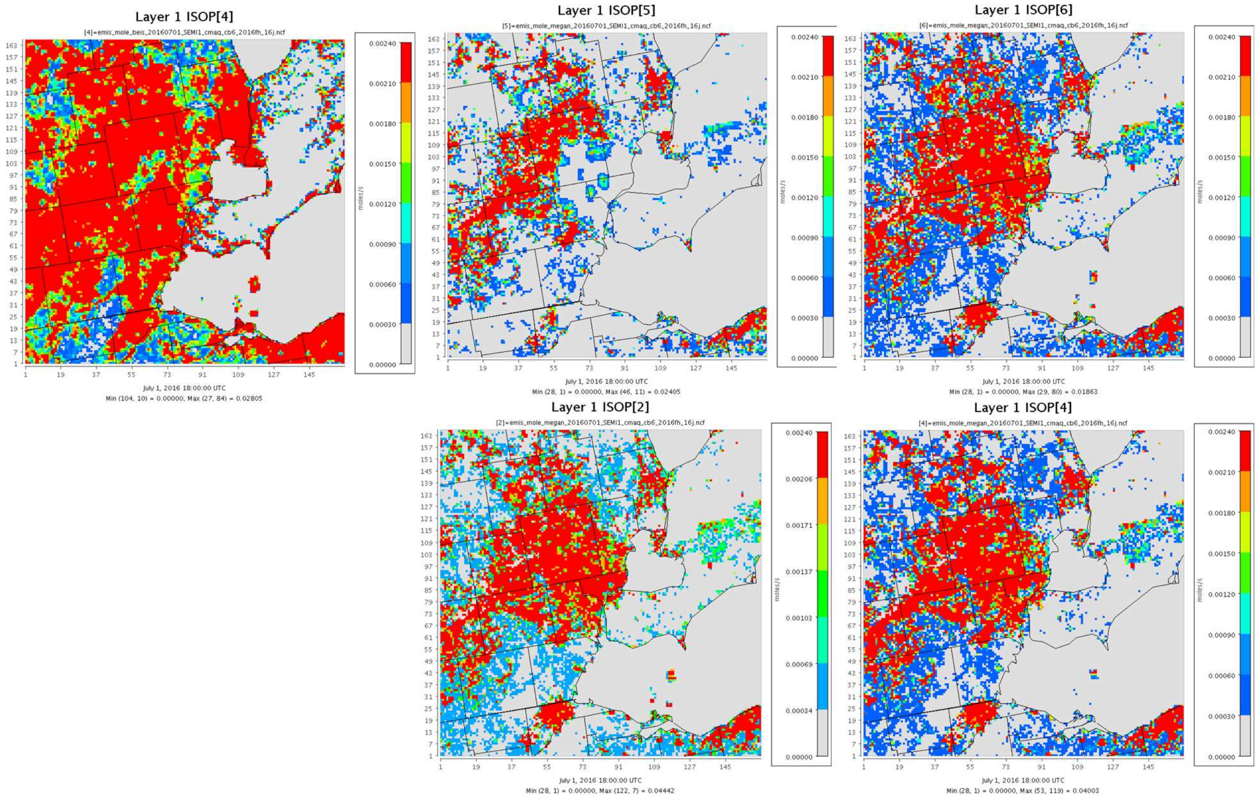


Figure 3-21. ISOP emissions rates distribution on the SEMI1 grid at 18Z on July 1, 2016, generated by BEIS3 (top left), MEGAN using Default 2013 LAIv (top middle), MEGAN using GLASS 2013 500m LAIv (bottom left), MEGAN using GLASS 2016 500m LAIv (top right), and MEGAN using GLASS 2016 0.05Degree LAIv (bottom right).

Figures 3-22 and 3-23 show side by side comparisons of the hourly emissions rates of species PAR generated by the five methods on a spring (April 1) and a summer day (July 1). In spring, like isoprene, the PAR emissions estimated from BEIS3 and MEGAN Default 2013 are several times lower than from the other three MEGAN GLASS methods (note that the plot scale of BEIS3 and MEGAN Default 2013 are 10 times lower than the other three), with MEGAN Default 2013 showing even lower PAR emissions domain wide. In summer, the PAR emissions from BEIS3 and MEGAN Default 2013 are several times higher than their spring estimates, while the other three methods yielded 3-4 times higher emissions than their spring estimates. Again, note that the scale of the plots for summer are 10 times larger than for spring. But in summer, the PAR emissions estimates from BEIS3 and MEGAN Default 2013 are still much lower than the other three MEGAN methods.

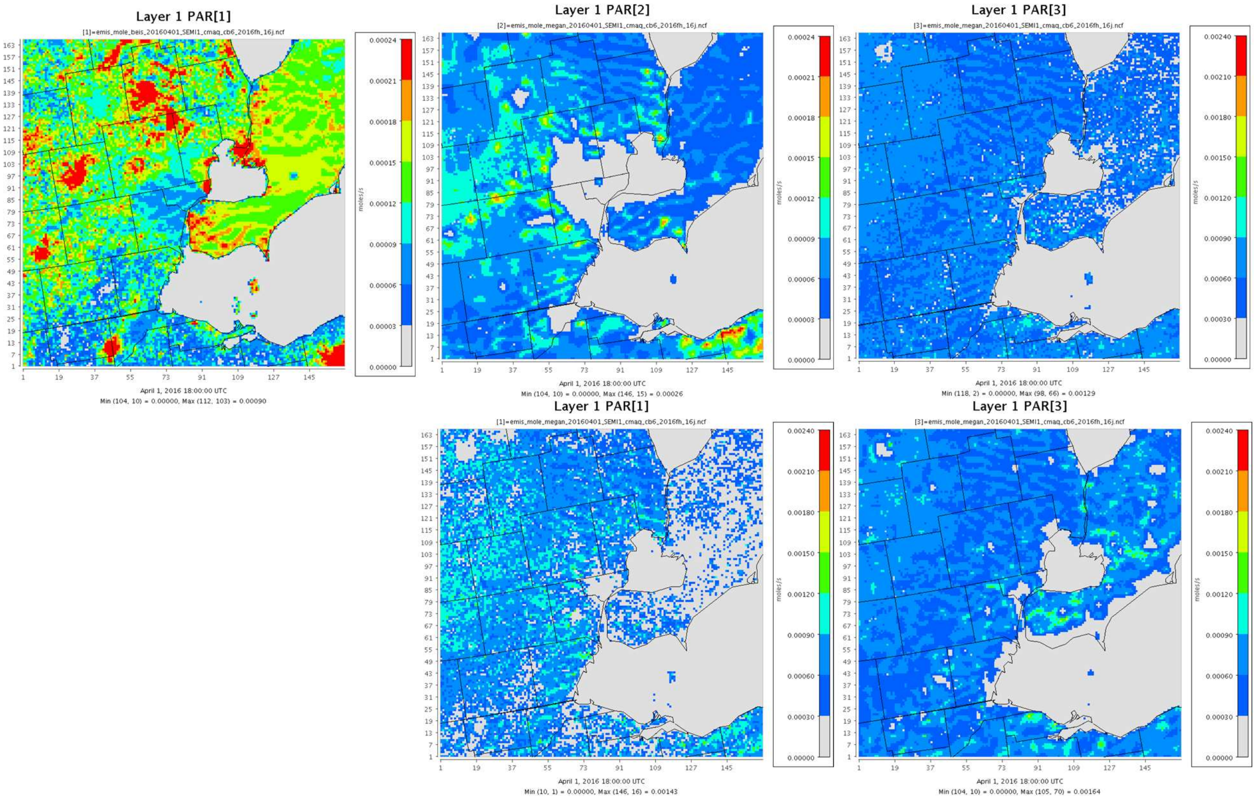


Figure 3-22. PAR emissions rates distribution on the SEMI1 grid at 18Z on April 1, 2016, generated by BEIS3 (top left), MEGAN using Default 2013 LAIv (top middle), MEGAN using GLASS 2013 500m LAIv (bottom left), MEGAN using GLASS 2016 500m LAIv (top right), and MEGAN using GLASS 2016 0.05Degree LAIv (bottom right).

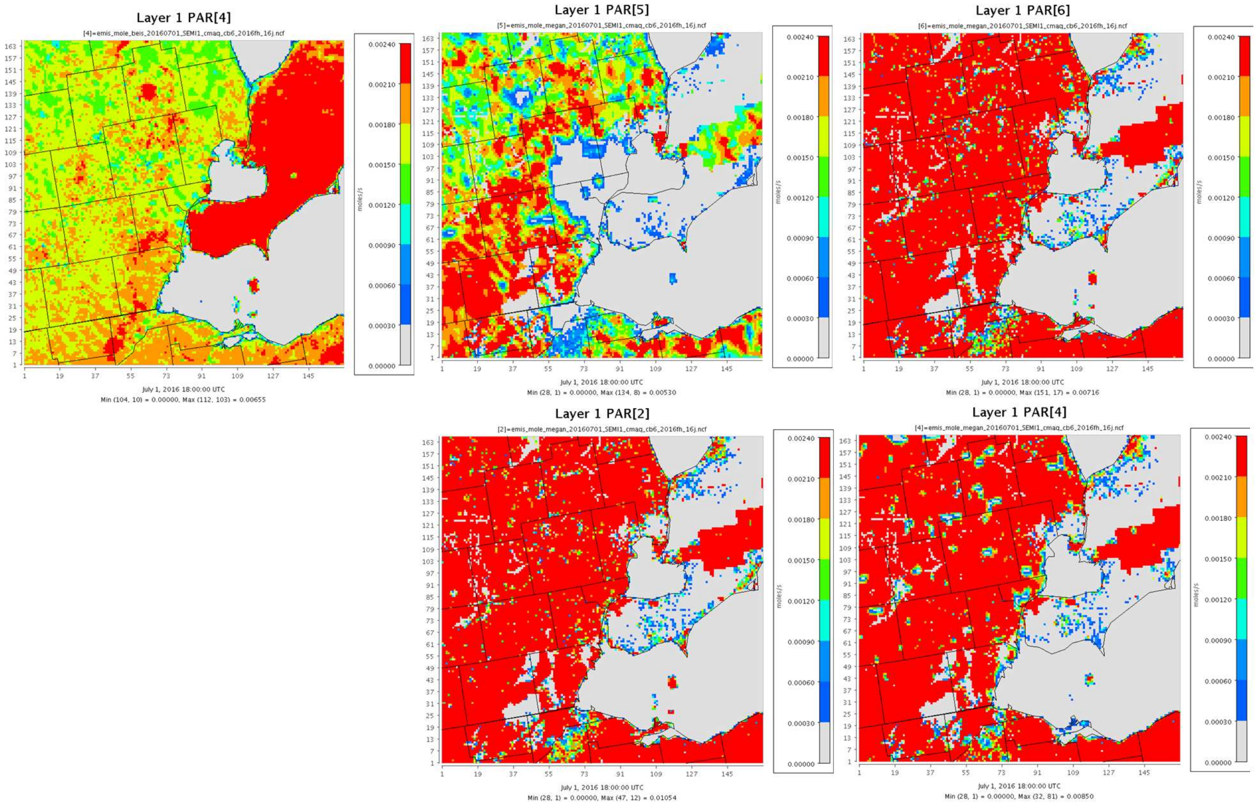


Figure 3-23. PAR emissions rates distribution on the SEMI1 grid at 18Z on July 1, 2016, generated by BEIS3 (top left), MEGAN using Default 2013 LAIv (top middle), MEGAN using GLASS 2013 500m LAIv (bottom left), MEGAN using GLASS 2016 500m LAIv (top right), and MEGAN using GLASS 2016 0.05Degree LAIv (bottom right).

Figures 3-24 and 3-25 show side by side comparisons of the hourly emissions rates of species terpene (TERP) generated by the five methods on a spring (April 1) and a summer day (July 1). In spring, the terpene emissions estimated from BEIS3 and MEGAN default 2013 are several times lower than from the other three MEGAN methods, with MEGAN Default 2013 yielding even lower emissions than BEIS3. In summer, the terpene emissions from BEIS3 and MEGAN default 2013 are still several times lower than the other three methods that use GLASS products. BEIS3 yields even lower emissions than MEGAN default 2013. Note that the scale of the plots for summer are 10 times larger than for spring. Comparing the summer emissions to spring, the estimates from BEIS3 and MEGAN Default 2013 are several times higher, but the other three MEGAN GLASS methods yield much smaller differences in their estimates, being only 2-3 times higher in summer than in spring.

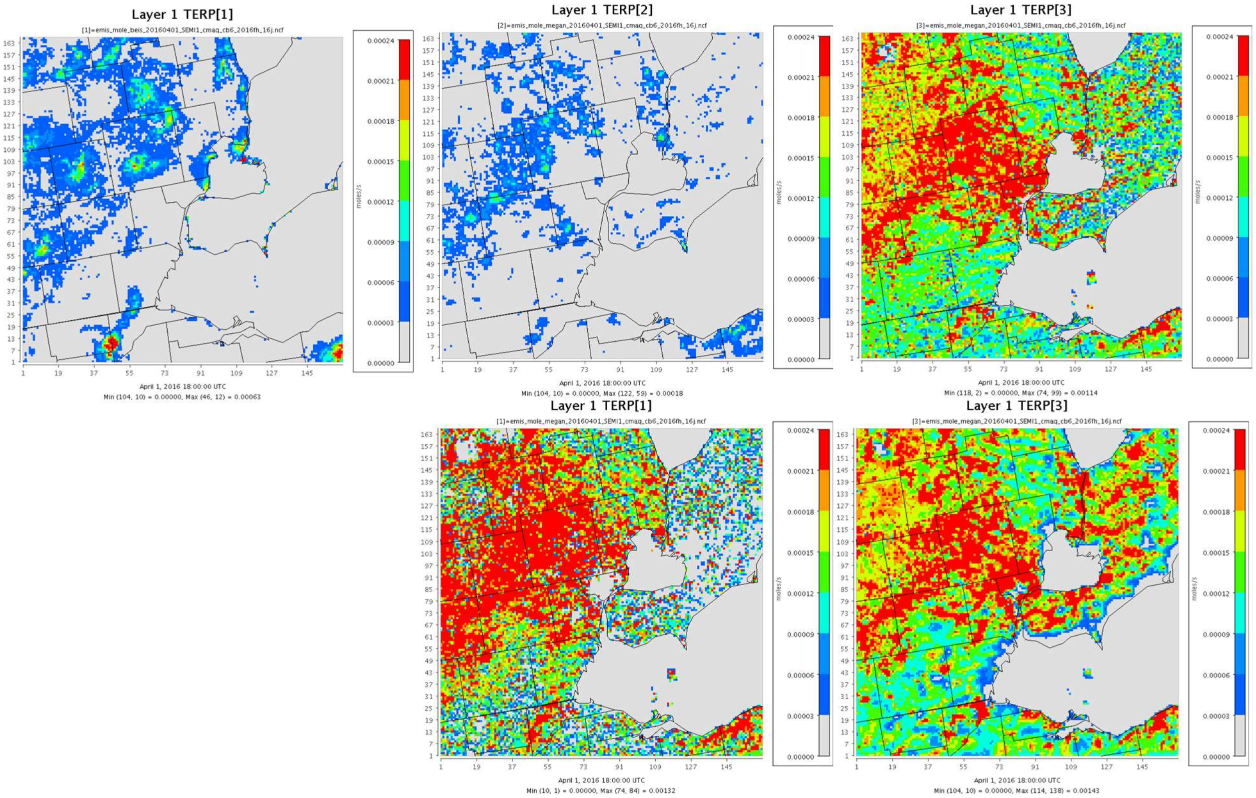


Figure 3-24. TERP emissions rates distribution on the SEMI1 grid at 18Z on April 1, 2016, generated by BEIS3 (top left), MEGAN using Default 2013 LAIv (top middle), MEGAN using GLASS 2013 500m LAIv (bottom left), MEGAN using GLASS 2016 500m LAIv (top right), and MEGAN using GLASS 2016 0.05Degree LAIv (bottom right).

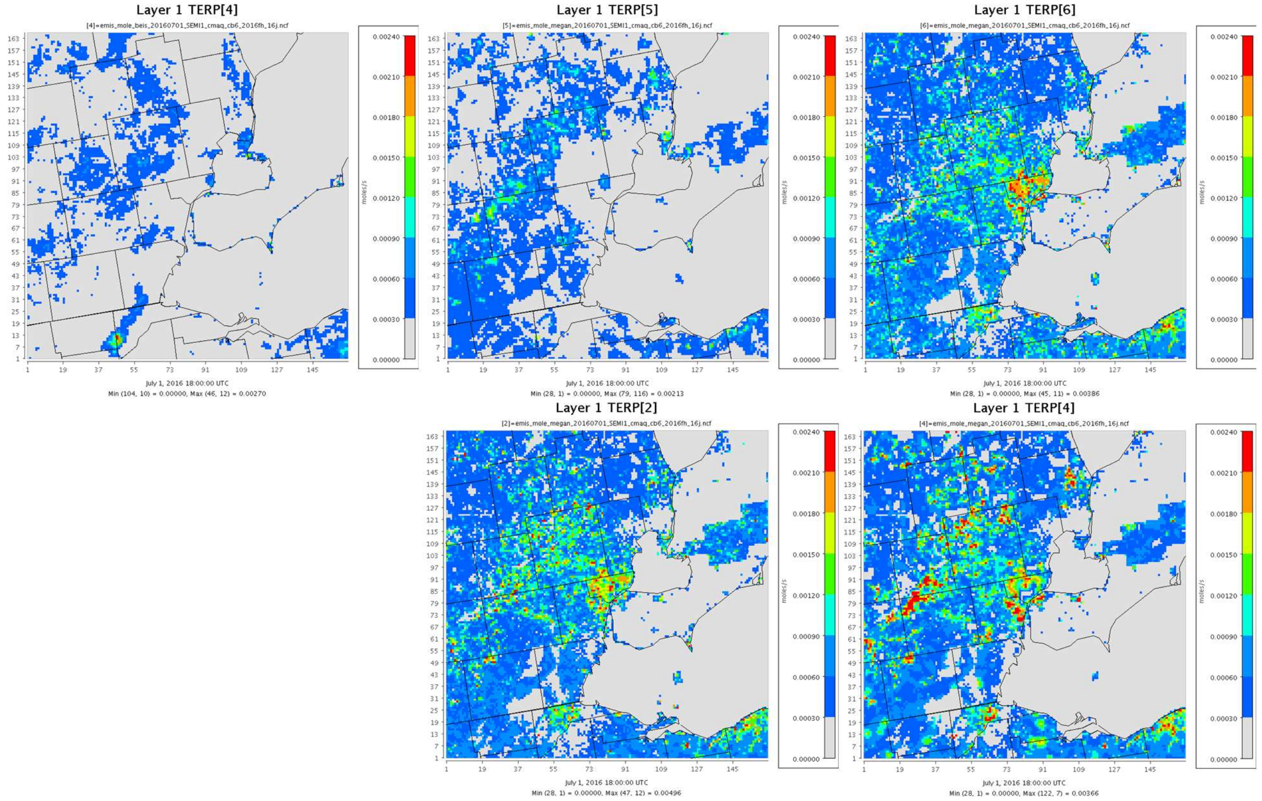


Figure 3-25. TERP emissions rates distribution on the SEMI1 grid at 18Z on July 1, 2016, generated by BEIS3 (top left), MEGAN using Default 2013 LAIv (top middle), MEGAN using GLASS 2013 500m LAIv (bottom left), MEGAN using GLASS 2016 500m LAIv (top right), and MEGAN using GLASS 2016 0.05Degree LAIv (bottom right).

Figures 3-26 and 3-27 show side by side comparisons of the hourly emissions rates of species NO from soil generated by the five methods on a spring (April 1) and a summer day (July 1). The spatial patterns of the NO emissions are significantly different between the BEIS3 and all the other four MEGAN methods in both spring and summer. BEIS3 NO emissions estimates in spring and summer are both much higher than all the MEGAN methods domain-wide, except for the Detroit Metro area, where the BEIS3 estimates are uniformly lower. In the area surrounding downtown Detroit, the estimates from the MEGAN methods are slightly higher than the BEIS3 estimates, but in downtown Detroit the MEGAN estimates are much lower, which follow more closely to the urban land cover patterns in the area. Note that all the scales are the same for summer and spring. Comparing the summer emissions to spring, the estimates from BEIS3 are 1-2 times higher, while the MEGAN methods are 2-3 times higher.

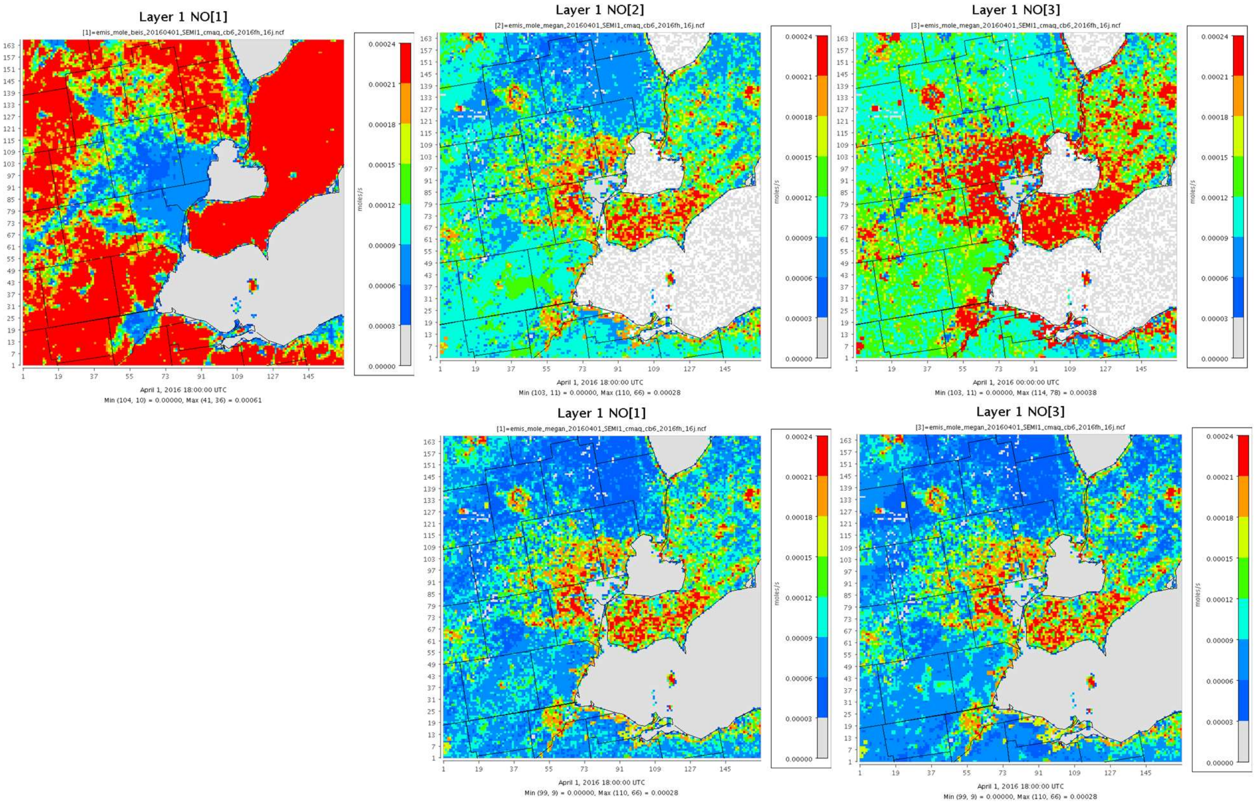


Figure 3-26. NO emissions rates distribution on the SEMI1 grid at 18Z on April 1, 2016, generated by BEIS3 (top left), MEGAN using Default 2013 LAIv (top middle), MEGAN using GLASS 2013 500m LAIv (bottom left), MEGAN using GLASS 2016 500m LAIv (top right), and MEGAN using GLASS 2016 0.05Degree LAIv (bottom right).

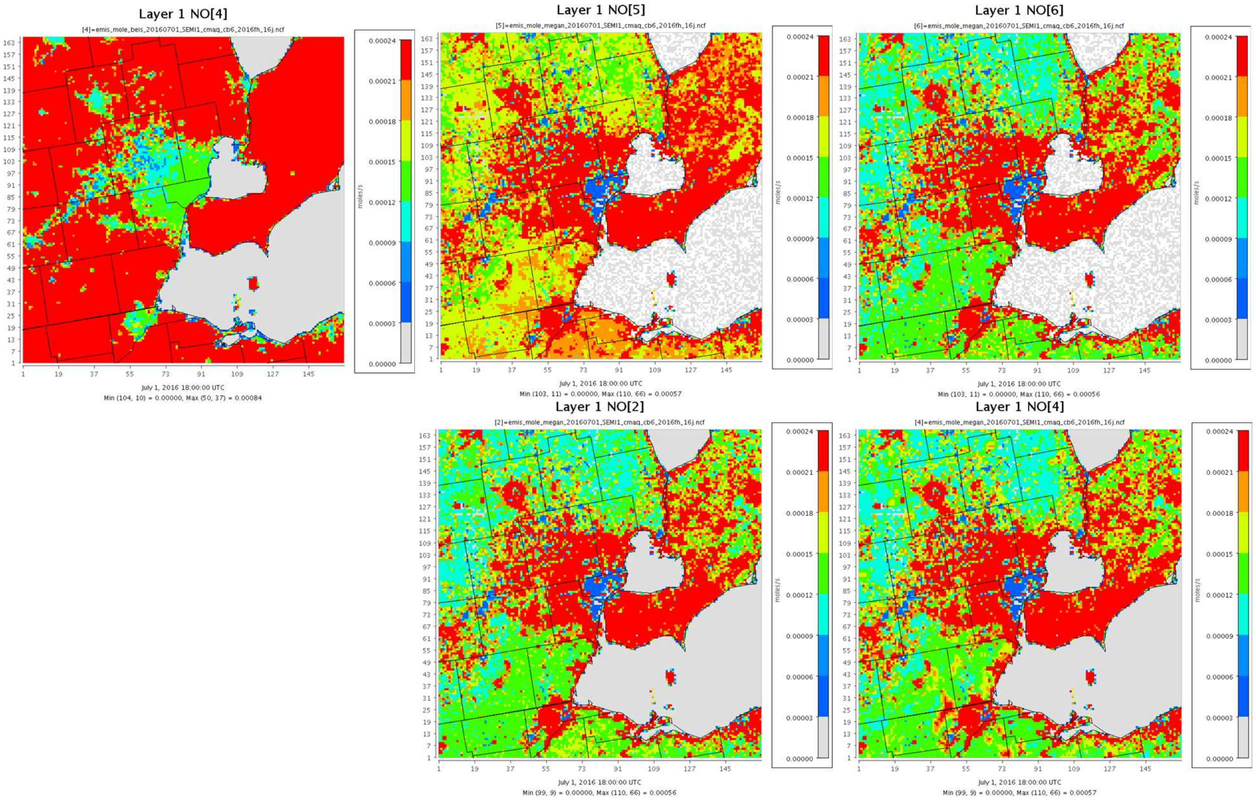


Figure 3-27. NO emissions rates distribution on the SEMI1 grid at 18Z on July 1, 2016, generated by BEIS3 (top left), MEGAN using Default 2013 LAIv (top middle), MEGAN using GLASS 2013 500m LAIv (bottom left), MEGAN using GLASS 2016 500m LAIv (top right), and MEGAN using GLASS 2016 0.05Degree LAIv (bottom right).

In summary, the biogenic emissions estimates from BEIS3 and MEGAN Default 2013 generally resemble each other much more than the three MEGAN GLASS methods, with regards to both the emission rates levels and the seasonal changes. The three MEGAN GLASS estimates are quite similar to each other, but differ significantly with the MEGAN Default 2013 method. The seasonal changes found in the BEIS3 and MEGAN Default 2013 estimates are more reasonable than the three MEGAN GLASS estimates. The distribution of NO emissions levels in downtown Detroit compared to levels in the surrounding area follow more closely to the urban land cover patterns in the MEGAN estimates than in the BEIS3 estimates.

3.4 Summary of the Updated Emissions Sectors for Sensitivity Tests

The source sectors with emissions updated for the specific sensitivity tests are summarized in Table 3-10. The sector IDs are usually named with the original sector ID plus an extension to reflect the updates. Emissions files were generated for all these sectors for the entire 2016 ozone season on the SEMI1 grid. All the sectors have gone through QA/QC procedures. These sectors were used in various combinations for individual and incremental sensitivity tests. The next chapter will describe how these updated sectors' emissions were used for each specifically designed sensitivity test for the purpose of configuration optimization of the base year simulation.

Table 3-10 List of sectors with emissions updated for sensitivity tests of base year simulation

Sector ID	Source Category
ptnonipm_semihcho	Updated US Non-IPM point sources with addition of HCHO emissions
ptegu_semihcho	Updated US EGU point sources with addition of HCHO emissions
ptnonipm_semivcp	Updated US Non-IPM point sources with addition of VCP VOC emissions
ptnonipm_semihchovcp	Updated US Non-IPM point sources with additions of HCHO and VCP VOC emissions
nonpt_semivcp	US non-point sources with addition of VCP VOC emissions
nonpt_semivcpgspro	US non-point sources with addition of VCP VOC emissions using update VOC speciation profiles
megan	Biogenic sources using MEGAN with 2016 GLASS LAIv
megan2013	Biogenic sources using MEGAN Default 2013 LAIv

Section 4: Sensitivity Tests and Base Year Simulation Configuration Optimization

This section describes the sensitivity tests we have conducted for the base year simulation. Model performance evaluation procedures and results are presented for evaluating performance of these tests. Further analysis and interpretation of the evaluation results justify the best performing model configuration to be determined as the optimized base year simulation. The objective is to select a model and data configuration that best reproduces observed 2016 high ozone conditions in the SEMI region.

4.1 Base Year Simulation Sensitivity Tests

We conducted nine ozone season base year simulations, including the basecase 2016 simulation and eight sensitivity simulations (Table 4-1). These eight sensitivity simulations are designed to assess the improvements of model performance from addition of HCHO emissions, VCP VOC emissions, and alternative biogenic emissions, separately or in various combinations.

All these base year simulations used the same CAMx model executable with the same configuration choices and the same model inputs, except for the different emissions inputs listed in Table 4-1. The different emissions inputs represent each sensitivity test's deviation from the default 2016 emissions (i.e. the 2016fh_16j emissions from the EPA 2016v1platform, see section 2.6 and Table 3-4) used in the basecase 2016 simulation. All the 9 runs were conducted on a supercomputer using 96 processors from 4 computing nodes.

Table 4-1. List of base year air quality modeling sensitivity tests

Sensitivity Test -id	Difference in Emissions Input	Anthropogenic emissions	Sensitivity emphasis
base	default sectors of ptnonipm, nonpt, beis, ptegu	Default 2016 Emissions	Basecase simulation
hcho	ptnonipm_semihcho	Default 2016 with addition of HCHO emissions for non-EGU point sources	Addition of HCHO emissions for non-EGU point sources
hchovcp	ptnonipm_semihchovcp, nonpt_semivcp	Default 2016 with addition of HCHO and VCP VOC emissions	Addition of HCHO and VCP VOC emissions
hchovcppro	ptnonipm_semihchovcp, nonpt_semivcpgspro	Default 2016 with addition of HCHO and VCP VOC emissions using updated VOC profiles	Addition of HCHO and VCP VOC emissions using updated VOC profiles
vcp	ptnonipm_semivcp, nonpt_semivcp	Default 2016 with addition of VCP VOC emissions	Addition of VCP VOC emissions
megan	megan	Default 2016 with megan as biogenic emissions	Replacing beis with megan using 2016 GLASS 500m LAIv
meg2013	megan2013	Default 2016 with megan2013 as biogenic emissions	Replacing beis with megan using default 2013 LAIv

combine	ptnonipm_semihchovcp, nonpt_semivcpspro, megan2013	Default 2016 with addition of HCHO and VCP VOC emissions using updated VOC profiles and megan2013 as biogenic emissions	Addition of HCHO and VCP VOC emissions using updated VOC profiles and megan using default 2013 LAIv
hchoext	ptnonipm_semihcho, ptegu_semihcho	Default 2016 with addition of HCHO emissions for non-EGU and EGU point sources	Addition of HCHO emissions for non-EGU and EGU point sources

All the CAMx modeling outputs were first converted to I/O API format by using the CAMx2IOAPI program and were further post-processed for extraction of the most relevant species and conversion of hourly values to more convenient form of variables including daily averages (24-hour average), MDA1 O_3 and MDA8 O_3. Tile-plots are also plotted to show changes of daily MDA8 O_3 between the basecase and sensitivity simulations and among sensitivity experiment simulations. We also used the sitecmp and sitecmp_o3 programs to match the observations of ozone and precursor variables with their corresponding simulations in time series at the monitoring sites in the Detroit, MI NAA (i.e. the SEMI NAA). All the observations are matched with the model predictions in the grid cell that contains the monitor. The post-processed datasets are in csv format and were used for calculating model performance statistics and for producing time series plots and scatter plots for evaluation analysis.

4.2 Model Performance Evaluation Method

4.2.1 Ambient Ozone and Precursors Data

We collected the available surface air quality measurement data over the SEMI region for the 2016 ozone season. In particular, we collected surface measurement data of air quality from the U.S. EPA Air Quality System (AQS). AQS compiles and provides access to datasets from multiple national observational networks/programs, including State and Local Air Monitoring Stations (SLAMS) and Photochemical Assessment Monitoring Stations (PAMS). The SLAMS network provides hourly measurements of criteria air pollutants including $PM_{2.5}$, PM_{10}, O_3, SO_2, NO_2, CO etc. The PAMS network measures photochemical smog-related species such as O_3, NO, NO_2, NOx, NOy, and VOCs. Surface measurements from the EPA AQS database are already quality-checked and well documented (https://aqs.epa.gov/aqsweb/documents/AQS_Reports_Guide.html#_qa_data_quality_indicator_report_amp256). Additionally, we collected VOC measurements from the Windsor West Monitor available from the Canadian National Air Pollution Surveillance (NAPS) program, which is the main source of ambient air quality data in Canada.

The ambient air quality measurement data that were used for evaluating model performance in this study are summarized in Table 4-.

Table 4-2. Surface Air Quality Data available for model performance evaluation in the SEMI Region

Variable	Averaging time	Database/Networks
O_3 and NO_2	Hourly	SLAMS
VOCs, NO, NO_2 and NO_y	Daily or Hourly	PAMS, SLAMS

VOC	Daily	NAPS*

*The National Air Pollution Surveillance (NAPS) program is the main source of ambient air quality data in Canada.

The collected O_3 observation data in 2016 are from 10 sites monitoring O_3 in the Detroit, MI NAA, shown on the map in Figure 4-35 and listed in Table 4-2 with the 2016-2018 ozone design values.

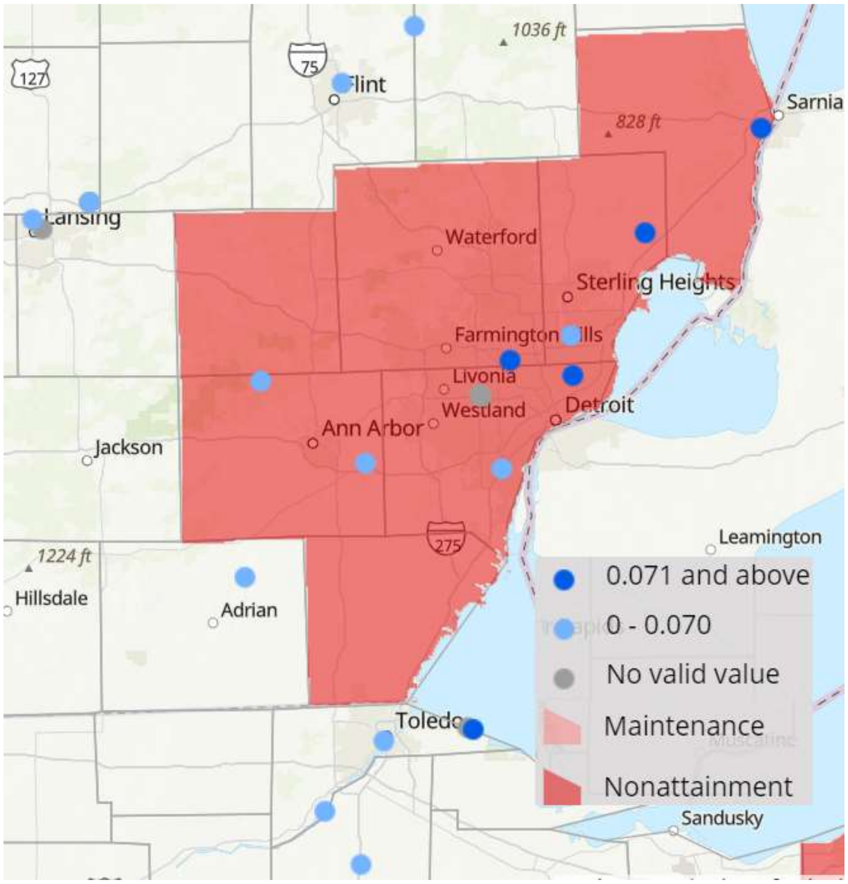


Figure 4-1. The Detroit, MI NAA ozone monitor locations labeled with ozone design value.

Table 4-3. AQS ozone sites list with 2016-2018 ozone design values in Detroit, MI NAA

AQS Site ID	Local Site Name	16-18 DV (ppm)	2016 4th (ppm)	2017 4th (ppm)	2018 4th (ppm)	Number of Exceedances		
						2016	2017	2018
260990009	New Haven	0.072	0.075	0.066	0.076	6	3	10
260991003	Warren - Fire Station 29900 Hoover at Common	0.069	0.071	0.064	0.072	4	1	4
261250001	Oak Park	0.073	0.075	0.069	0.077	6	2	9
261470005	Port Huron	0.072	0.073	0.067	0.076	4	2	7
261610008	Towner St, South; 2 Lane Residential - Hospital	0.069	0.069	0.068	0.070	3	2	3
261619991	Ann Arbor	0.071	0.074	0.069	0.072	5	1	4

261630001	Allen Park	0.068	0.070	0.067	0.069	3	0	2
261630019	East 7 Mile	0.074	0.074	0.076	0.074	8	7	7
261630093	Eliza-NR	0.049*	0.058	0.054	0.036	0	0	0
261630094	Eliza Downwind	0.057*	0.070	0.065	0.038	3	1	0

*Invalid DV

The collected ozone precursor measurements data including NO, NO2, NOx, NOy and VOC species measurements in 2016 over the SEMI region are from the monitoring sites listed in Table 4-4. Part of these monitoring sites are shown on the map in Figure 4.2.

Table 4-4. Monitoring sites list measuring NO, NO2, NOy and VOCs in Detroit, MI NAA

AQS Site ID	Local Site Name	Measurements
261630001	Allen Park	NO, NOy
261630005	Jenison	VOC (FORM)
261630015	Detroit - SWHS	VOC (FORM)
261630019	East 7 Mile	NO, NO2, NOx
261630033	Dearborn	VOC (FORM)
261630093	Eliza NR	NO, NO2, NOx
261630094	Eliza Downwind	NO, NO2, NOx
261630095	Livonia Near-road	NO, NO2, NOx
261631005	1300 S FORT ST (Northwest)	VOC
261631006	1300 S FORT ST (West corner)	VOC
261631008	1300 S FORT ST (Northeast corner)	VOC
261631009	MARK TWAIN MIDDLE SCHOOL, 12800 VISGER ST	VOC
261631010	9300 W JEFFERSON	NO, NO2, NOx
261631011	9300 W JEFFERSON	NO, NO2, NOx

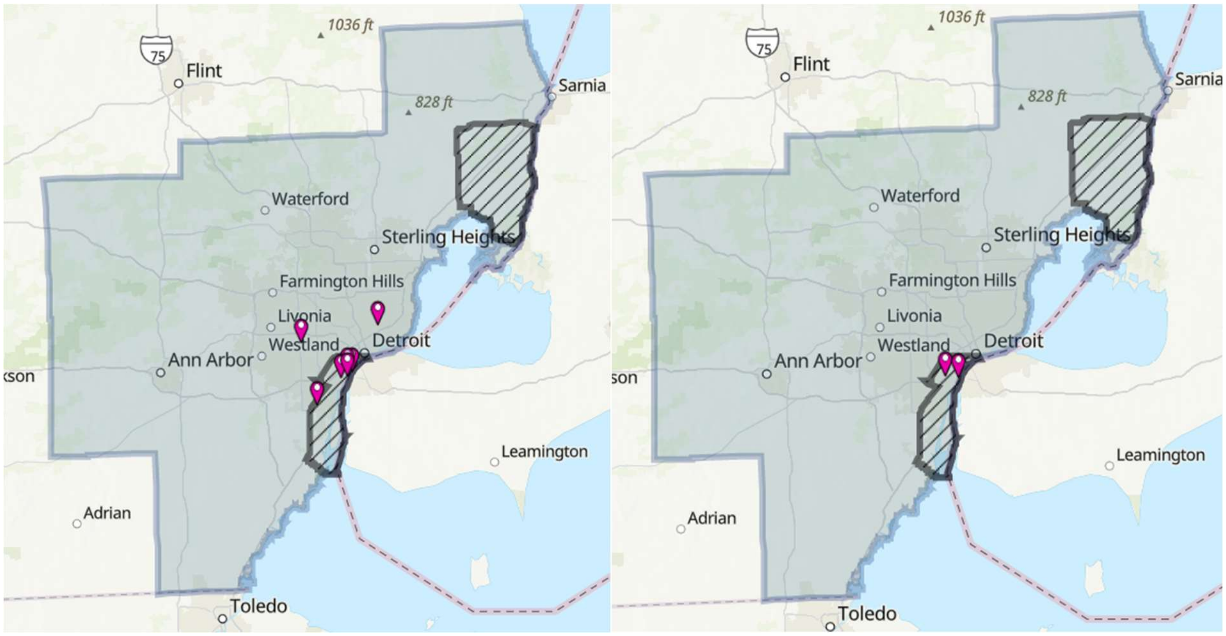


Figure 4-2. Locations of ozone precursor monitors in Detroit, MI NAA (not all the sites listed in Table 5-3 are shown): NO, NO2, NOx and NOy monitors (left), VOC monitors (right) .

Figure 4-3 shows the location of the NAPS's Windsor West monitor from which we collected daily VOC measurements.

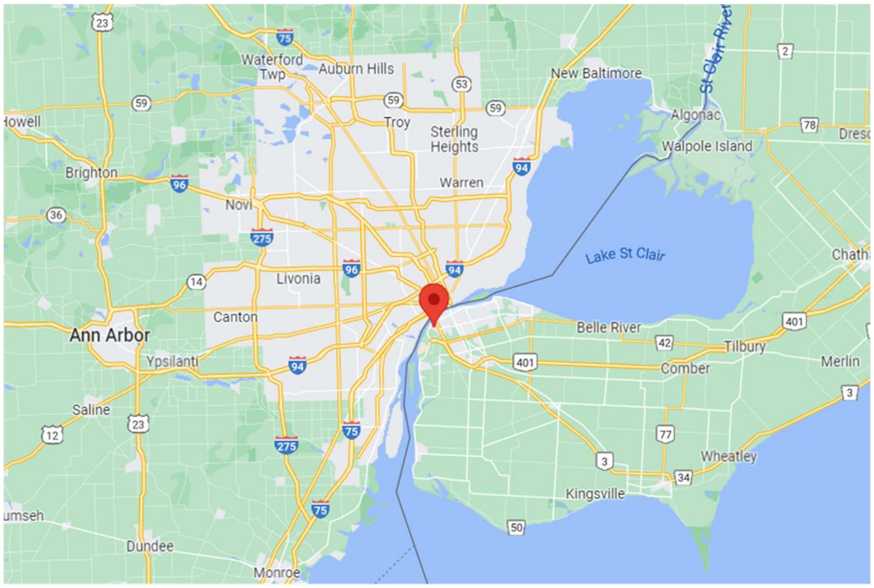


Figure 4-3. Location of the Windsor West Monitor (NAPS ID 60211) which measures VOC species.

We carried out additional checks on the collected measurement data to assure the data's reliability. During the procedure, we removed some continuous zero data of the benzene and toluene measurements from the AQS dataset.

4.2.2 Evaluation Procedures of Ozone and Precursors

The ultimate objective of the evaluation is to ensure that the 2016 base year ozone season air quality simulation is acceptable to the US EPA for ozone attainment demonstration modeling based on model performance statistics. The model performance evaluation was conducted for ozone and ozone precursors through comparison of simulation results against the collected ground-based observations.

We used the model performance statistics as described in LADCO (2019, 2020) and recommended by US EPA (2018) for the base year simulation performance evaluation. In particular, the performance statistics used to evaluate the simulations included mean observation, mean prediction, mean bias, mean error, normalized mean bias (NMB), normalized mean error (NME), and correlation coefficient (R). All statistics are calculated from the model predictions in the grid cell that contains the monitor, not from the array of grid cells near the monitor.

The equations to calculate NMB and NME are as follows:

$$NMB = \frac{\sum_{i=1}^{N}(\mathrm{P_i} - \mathrm{O_i})}{\sum_{i=1}^{N}\mathrm{O_i}} \times 100$$

$$NME = \frac{\sum_{i=1}^{N}|\mathrm{P_i} - \mathrm{O_i}|}{\sum_{i=1}^{N}\mathrm{O_i}} \times 100$$

Where N is the number of pairs of observation (O) and prediction (P) data.

For ozone, we calculated separate statistics for daily maximum 1-hr average (MDA1), and daily maximum 8-hr average (MDA8) ozone concentrations using (1) no threshold and (2) a threshold of ≥60 ppb (observed value). Using a 60-ppb observed O_3 cut-off threshold when calculating O_3 model performance statistics is recommended by EPA (2018). Evaluations were performed at the regional level by season and by month and at each monitoring site, as recommended by Emery et al., (2017). The same statistics were calculated for hourly (1-hour average) or daily (24-hour average) ozone precursors and related gas-phase oxidants (i.e., NO, NO_2, NO_x, NO_y, and VOC species), depending on observation availability.

In addition to the tables of the statistical performance metrics commonly used, time series of predicted and observed concentrations at a monitoring site and scatter plots of predicted against observed concentrations were also produced. It should be stressed that the model performance goals recommended in the literature and by EPA are not used to assign passing or failing grades to model performance, but rather to help interpret the model performance and intercompare across locations, species, time periods and model applications, specifically the sensitivity test simulations. It is also necessary to understand measurement artifacts to make meaningful interpretation of the model performance evaluation.

We compare modeled ozone statistics to commonly used evaluation criteria for ozone model performance (Emery et al., 2017). For mean normalized bias (MNB) and mean normalized error (MNE), the predicted and observed ozone pairs with the observed ozone value greater than 60 ppb are used. Recommended performance goals and criteria are useful to identify areas that can be improved upon and hence the deficiencies of the simulation.

4.3 Model Performance Evaluation Results and Analysis

Here we compare the performance among the base and sensitivity simulations to evaluate the best performing ozone model configuration for the SEMI region. We first present the performance evaluation results, and then interpret the results with a goal of selecting the optimal simulation of high ozone in 2016 for the SEMI region.

VOC species measurements were only reported for benzene (BENZ), toluene (TOL) and formaldehyde (FORM) from the AQS sites in the SEMI region during year 2016. The basecase simulation overpredicted BENZ, but unpredicted TOL and FORM, with a much larger underprediction of FORM (Table 4-5). None of the sensitivity tests changed BENZ performance significantly. The tests with the addition of VCP VOCs emissions (hchovcp, hchovcppro, vcp and combine) enhanced the TOL level but made overpredictions that slightly worsened the TOL performance. The tests with the addition of HCHO emissions (hcho, hchoext, hchovcp and hchovcppro) enhanced the FORM concentrations (Figure 4-4 and Figure 4-5) and improved the FORM performance in terms of both NMB and NME, though the correlation slightly decreased (Table 4-5).

Table 4-5. Ozone season performance of VOC species against daily measurements at AQS sites in Detroit NAA

	BENZ (122 pairs)				TOL (150 pairs)				FORM (59 pairs)			
	avg (ppb)	NMB (%)	NME (%)	R	avg (ppb)	NMB (%)	NME (%)	R	avg (ppb)	NMB (%)	NME (%)	R
obs	0.29				1.11				4.3			
base	0.47	64.7	102.8	0.38	0.95	-14.2	80.4	0.13	2.0	-52.7	53.3	0.53
hcho	0.47	64.7	102.8	0.38	0.95	-14.3	80.3	0.13	2.5	-41.8	44.6	0.46
hchoext	0.47	64.7	102.8	0.38	0.95	-14.3	80.3	0.13	2.5	-41.7	44.6	0.46
hchovcp	0.48	66.4	102.8	0.38	1.47	32.0	99.3	0.01	2.5	-40.9	43.8	0.47
hchovcppro	0.48	66.4	102.8	0.38	1.46	32.0	99.3	0.01	2.5	-40.9	43.9	0.47
vcp	0.48	66.4	102.8	0.38	1.47	32.0	99.4	0.01	2.0	-51.8	52.4	0.54
megan	0.47	64.7	102.8	0.38	0.95	-14.2	80.4	0.13	1.9	-54.3	54.9	0.49
megan2013	0.47	64.7	102.8	0.38	0.95	-14.3	80.4	0.13	1.8	-58.8	58.9	0.47
combine	0.48	66.3	102.8	0.38	1.46	31.9	99.3	0.01	2.3	-47.0	48.9	0.42

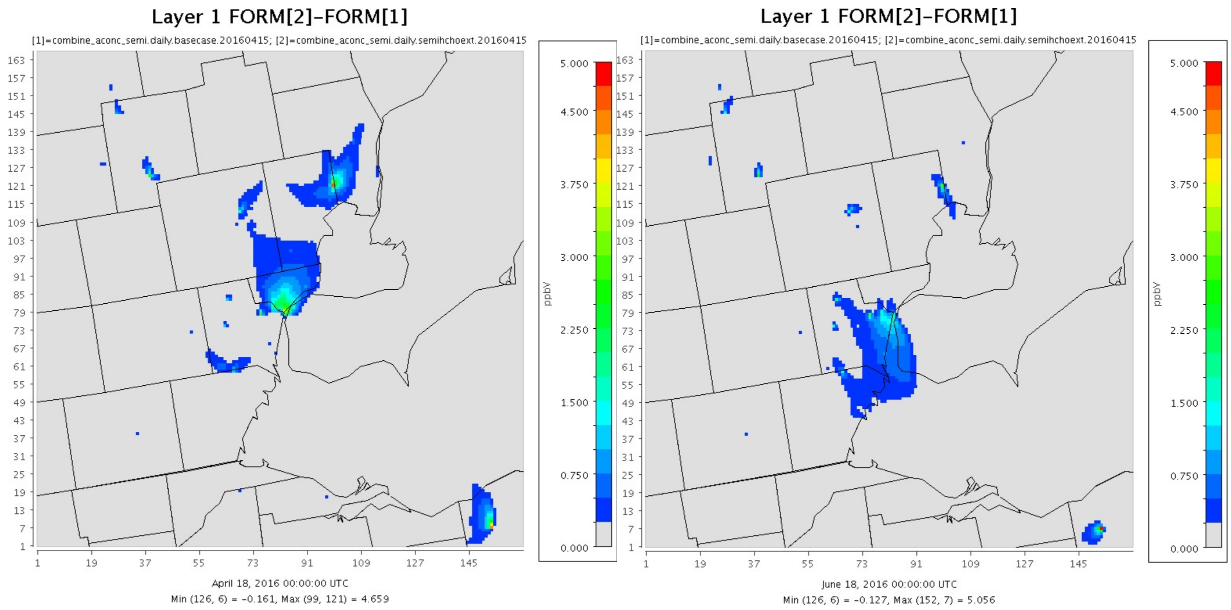


Figure 4-4. Increased FORM concentrations in the region due to the addition of HCHO emissions.

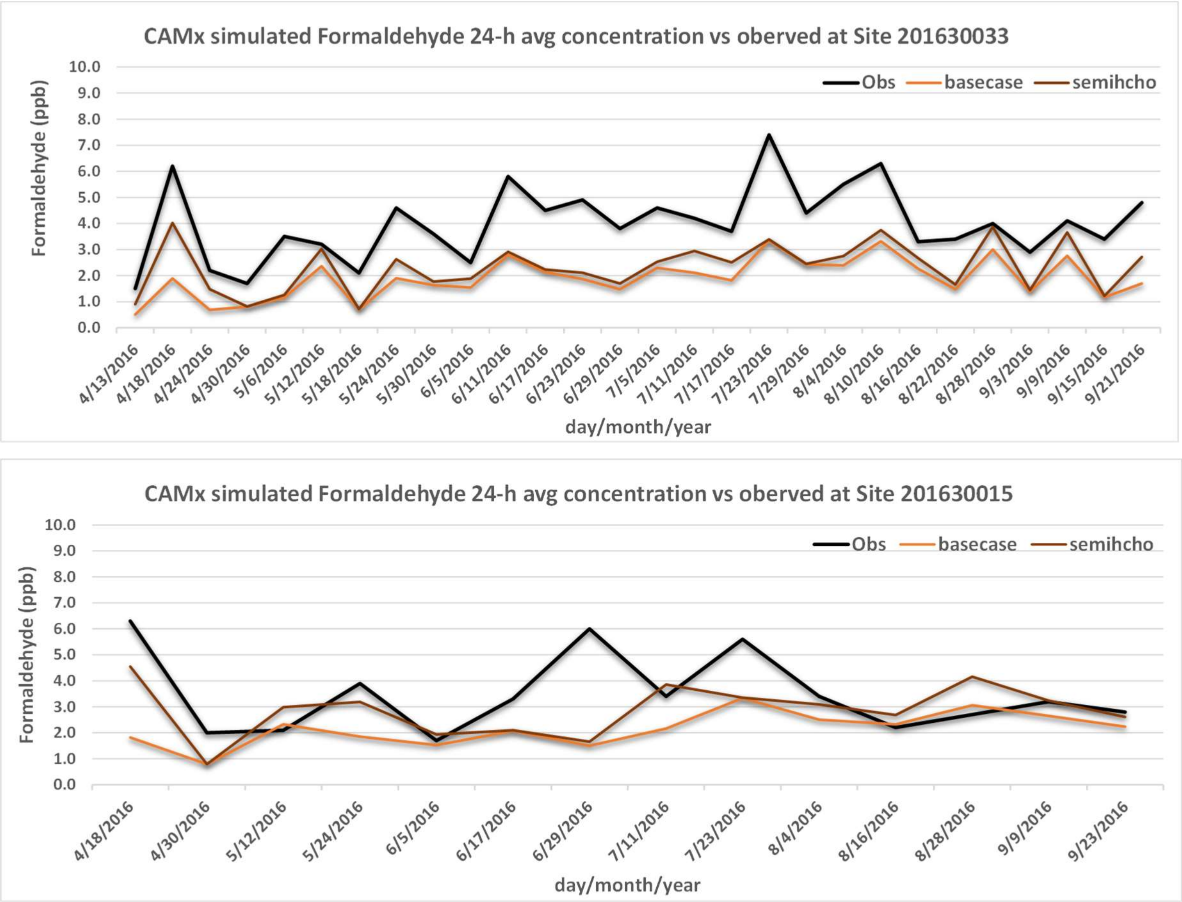


Figure 4-5. Improved FORM concentrations against measurements at monitoring sites due to the addition of HCHO emissions.

VOC measurements at the Windsor West site were reported for more species but with a small size of the data pool; only 26 pairs of data were available for evaluation. At this site, the basecase simulation slightly overpredicted BENZ and ETH, underpredicted ETHA, but overpredicted TOL and XYL (Table 4-6 and Table 4-7). The basecase simulation underpredicted isoprene (ISOP) but did a good job on predicting terpene (TERP) at this site. The addition of VCP VOCs emissions (hchovcp, hchovcppro, vcp and combine) didn’t change the performance of BENZ, ETH and ETHA, but enhanced the TOL and XYL concentrations hence worsened the overpredictions (Table 4-6 and Table 4-7). The alternative biogenic emissions from MEGAN using the GLASS 2016 LAIv increased the ISOP concentrations and improved ISOP performance but worsened the TERP performance by significant overprediction. The alternative biogenic emissions from MEGAN using the default 2013 LAIv changed the TERP performance from slight overprediction to slight underprediction, but decreased the ISOP concentrations and worsened ISOP performance (Table 4-6 and Table 4-7).

The addition of VCP VOC emissions enhanced the MDA8 O3 concentrations in the region (for example Figure 4-6).

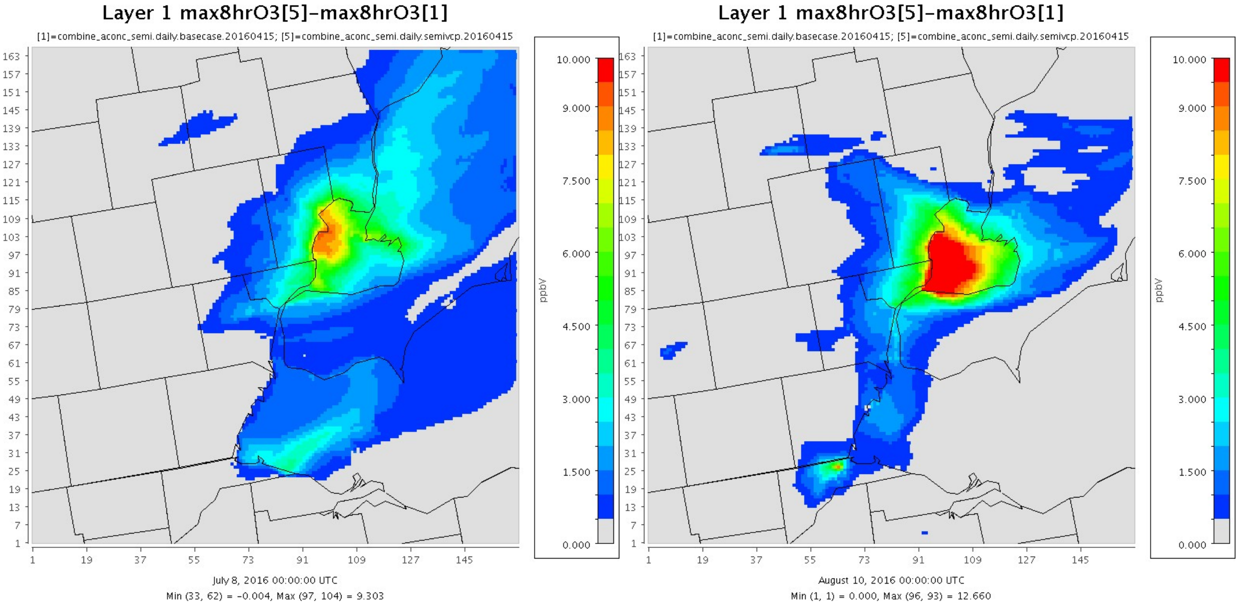


Figure 4-6. Increased MDA8 O_3 concentrations in the region due to the addition of VCP VOC emissions.

The switch of biogenic emissions from BEIS3 to MEGAN using the GLASS 2016 LAIv generally increased the MDA8 O3 concentrations in the region (for example Figure 4-7). However, the switch of biogenic emissions from BEIS3 to MEGAN using the default 2013 LAIv significantly decreased the MDA8 O3 concentrations in the region (for example Figure 4-8),

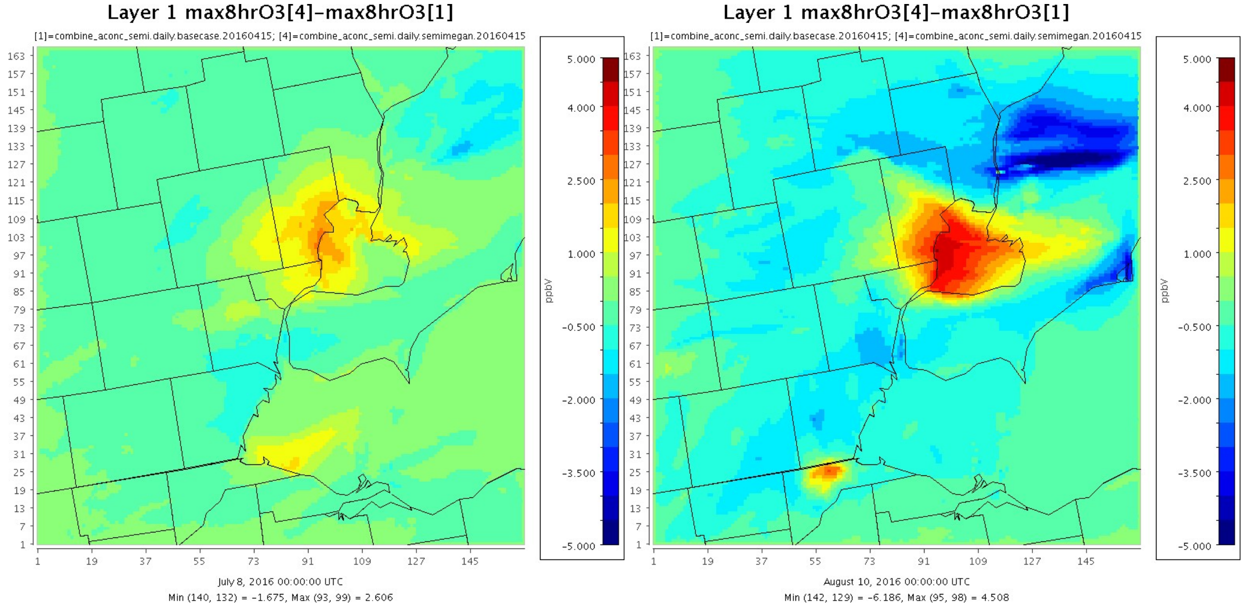


Figure 4-7. Generally increased MDA8 O_3 concentrations in the region due to the alternative biogenic emissions from MEGAN using the GLASS 2016 LAIv .

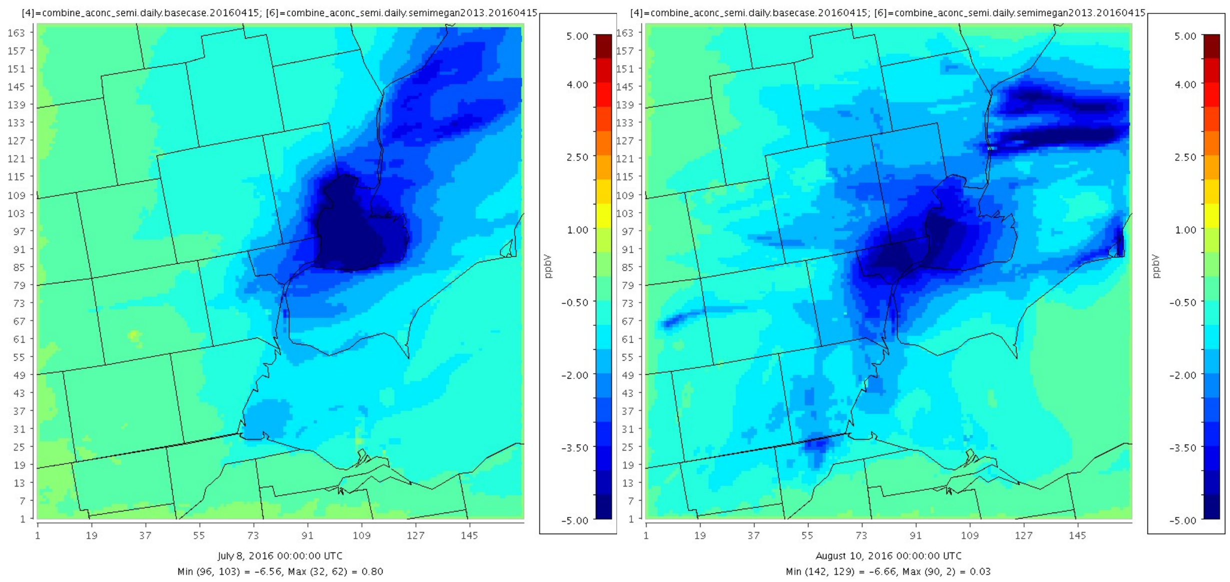


Figure 4-8. Decreased MDA8 O_3 concentrations in the region due to the alternative biogenic emissions from MEGAN using the Default 2013 LAIv .

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There are plenty of NO, NO2, NOx and NOy measurements from the AQS sites in the region for the evaluation. The basecase simulation underpredicted NO, NO2, NOx and NOy, but with a lesser degree of underprediction for NO2 and NOy (Table 4-8). The performances are all reasonable for all the four species in terms of NMB, NME and specifically the correlation of R. None of the eight sensitivity tests changed these performances significantly (Table 4-8).

Tables 4-9, 4-10, 4-11 and 4-12 present the ozone season and monthly MDA8 O_3 performance throughout the Detroit NAA including all the ten ozone sites, while Tables 4-13, 4-

14, 4-15 and 4-16 present the ozone season and monthly MDA1 O_3 performance for the entire Detroit NAA.

Table 4-6. Ozone season performance of VOC species against daily measurements (26 pairs) at the Windsor West site: mean predictions (ppb) versus mean observation (ppb)

	ISOP		BENZ		ETH		ETHA		TOL		XYL		TERP	
Test-ID	Obs	sim	obs	sim	obs	sim	obs	sim	obs	sim	obs	sim	obs	sim
base	0.22	0.08	0.13	0.17	0.78	0.93	5.39	1.91	0.39	0.71	0.23	0.45	0.04	0.05
hcho	0.22	0.08	0.13	0.17	0.78	0.93	5.39	1.91	0.39	0.71	0.23	0.45	0.04	0.05
hchoext	0.22	0.08	0.13	0.17	0.78	0.93	5.39	1.91	0.39	0.71	0.23	0.45	0.04	0.05
hchovcp	0.22	0.08	0.13	0.18	0.78	0.94	5.39	1.91	0.39	0.92	0.23	0.58	0.04	0.05
hchovcppro	0.22	0.08	0.13	0.18	0.78	0.94	5.39	1.91	0.39	0.92	0.23	0.58	0.04	0.05
vcp	0.22	0.08	0.13	0.18	0.78	0.94	5.39	1.91	0.39	0.92	0.23	0.58	0.04	0.05
megan	0.22	0.14	0.13	0.17	0.78	0.82	5.39	2.21	0.39	0.71	0.23	0.45	0.04	0.15
megan2013	0.22	0.03	0.13	0.17	0.78	0.74	5.39	1.95	0.39	0.71	0.23	0.45	0.04	0.04
combine	0.22	0.03	0.13	0.18	0.78	0.74	5.39	1.95	0.39	0.92	0.23	0.58	0.04	0.05

Table 4-7. Ozone season performance of VOC species against daily measurements at the Windsor West site: NMB (%) and NME (%)

	ISOP		BENZ		ETH		ETHA		TOL		XYL		TERP	
Test-ID	NMB	NME	NMB	NME	NMB	NME	NMB	NME	NMB	NME	NMB	NME	NMB	NME
base	-62.3	71.4	32.1	38.1	20.6	45.8	-64.6	64.7	82.7	82.7	100.7	101.8	8.5	36.6
hcho	-62.5	71.5	32.0	38.1	20.5	45.8	-64.6	64.7	82.7	82.7	100.6	101.7	8.4	36.6
hchoext	-62.5	71.5	32.0	38.1	20.5	45.8	-64.6	64.7	82.7	82.7	100.6	101.6	8.4	36.6
hchovcp	-62.5	71.2	33.9	39.8	20.6	45.9	-64.5	64.7	136.3	136.3	157.1	158.0	20.9	42.7
hchovcppro	-62.5	71.2	33.9	39.8	20.6	45.9	-64.5	64.7	136.3	136.3	157.0	158.0	20.9	42.7
vcp	-62.4	71.1	33.9	39.8	20.6	46.0	-64.5	64.7	136.4	136.4	157.3	158.2	21.0	42.7
megan	-38.2	58.3	32.1	38.1	5.4	39.0	-59.0	59.5	82.8	82.8	100.9	102.0	226.1	226.1
megan2013	-85.3	85.3	32.0	38.0	-4.8	34.4	-63.9	64.1	82.7	82.7	101.2	102.3	-8.7	34.7
combine	-85.2	85.2	33.8	39.7	-4.8	34.5	-63.8	64.0	136.2	136.2	157.6	158.5	3.4	37.8

Table 4-8. Ozone season performance of NO, NO2, NOx and NOy against hourly measurements at AQS sites in Detroit NAA

	NO (15113 pairs)				NO2 (11325 pairs)				NOx (11325 pairs)				NOy (3794 pairs)			
	avg (ppb)	NMB (%)	NME (%)	R	avg (ppb)	NMB (%)	NME (%)	R	avg (ppb)	NMB (%)	NME (%)	R	avg (ppb)	NMB (%)	NME (%)	R
obs	5.91				11.19				17.68				15.15			
base	1.35	-77.2	86.4	0.39	6.91	-38.3	51.4	0.48	8.28	-53.2	61.1	0.52	9.67	-36.2	49.1	0.62
hcho	1.34	-77.3	86.4	0.39	6.91	-38.3	51.4	0.48	8.28	-53.2	61.1	0.52	9.66	-36.2	49.1	0.62
hchoext	1.34	-77.3	86.4	0.39	6.91	-38.3	51.4	0.48	8.28	-53.2	61.1	0.52	9.66	-36.2	49.1	0.62
hchovcp	1.30	-78.1	86.5	0.40	6.87	-38.6	51.5	0.48	8.20	-53.6	61.2	0.52	9.66	-36.2	49.1	0.63
hchovcppro	1.30	-78.1	86.5	0.40	6.88	-38.6	51.5	0.48	8.20	-53.6	61.2	0.52	9.66	-36.2	49.1	0.63
vcp	1.30	-78.0	86.5	0.40	6.88	-38.5	51.5	0.48	8.20	-53.6	61.2	0.52	9.66	-36.2	49.1	0.62
megan	1.33	-77.4	86.4	0.40	6.88	-38.5	51.5	0.48	8.25	-53.4	61.1	0.52	9.65	-36.3	49.1	0.63
megan2013	1.38	-76.7	86.4	0.39	6.93	-38.1	51.3	0.48	8.34	-52.8	60.9	0.52	9.63	-36.4	49.2	0.62
combine	1.32	-77.6	86.4	0.40	6.90	-38.4	51.4	0.48	8.25	-53.3	61.0	0.52	9.63	-36.4	49.1	0.63

Table 4-9. Ozone season and monthly Detroit NAA-wide MDA8 O_3 performance: mean predictions versus mean observation

Period	**Cut**	**#Pair**	**Obs (ppb)**	**Sim (ppb)**								
				base	**hcho**	**hchoext**	**hchovcp**	**hchovcppro**	**vcp**	**megan**	**meg2013**	**combine**
Season	**0**	1619	45.51	46.66	46.68	46.68	47.51	47.51	47.49	46.67	45.85	46.76
	60	190	66.90	61.00	61.04	61.05	62.45	62.45	62.40	61.02	59.57	61.14
April	**0**	185	44.93	40.21	40.23	40.23	40.89	40.89	40.86	40.21	39.78	40.46
	60	26	68.75	60.07	60.13	60.13	62.28	62.28	62.17	59.88	58.53	60.68
May	**0**	309	47.00	43.20	43.22	43.22	44.05	44.05	44.03	43.19	42.54	43.43
	60	33	69.14	59.46	59.51	59.51	61.32	61.31	61.27	59.59	58.05	60.03
June	**0**	292	50.93	47.69	47.71	47.71	48.52	45.82	48.49	47.57	46.82	46.72
	60	74	66.66	58.80	58.83	58.83	59.78	59.78	59.74	58.70	57.65	58.75
July	**0**	309	46.97	51.61	51.63	51.63	52.30	52.30	52.28	51.62	50.70	51.47
	60	28	64.22	63.71	63.75	63.75	65.19	65.19	65.16	64.14	61.99	63.72
Aug	**0**	300	43.22	49.91	49.93	49.93	50.69	50.69	50.67	50.03	49.03	49.88
	60	22	67.17	68.34	68.36	68.37	69.65	69.65	69.62	68.33	66.47	68.01
Sept	**0**	224	37.95	44.25	44.27	44.28	45.57	45.57	45.54	44.30	43.24	44.63
	60	7	61.95	61.19	61.24	61.25	63.02	63.02	62.96	61.06	59.49	61.41

Table 4-10. Ozone season and monthly Detroit NAA-wide MDA8 O_3 performance: comparison of NMB

Period	**Cut**	**#Pair**	**Obs (ppb)**	**NMB (%)**								
				base	**hcho**	**hchoext**	**hchovcp**	**hchovcppro**	**vcp**	**megan**	**meg2013**	**combine**
Season	**0**	1619	45.51	2.5	2.6	2.6	4.4	4.4	4.3	2.5	0.7	2.7
	60	190	66.90	-8.8	-8.8	-8.8	-6.7	-6.7	-6.7	-8.8	-11	-8.6
April	**0**	185	44.93	-10.5	-10.5	-10.5	-9.0	-9.0	-9.1	-10.5	-11.5	-10.0
	60	26	68.75	-12.6	-12.5	-12.5	-9.4	-9.4	-9.6	-12.9	-14.9	-11.7
May	**0**	309	47.00	-8.1	-8.0	-8.0	-6.3	-6.3	-6.3	-8.1	-9.5	-7.6
	60	33	69.14	-14.0	-13.9	-13.9	-11.3	-11.3	-11.4	-13.8	-15.0	-13.2
June	**0**	292	50.93	-6.4	-6.3	-6.3	-4.7	-4.7	-4.8	-6.6	-8.1	-6.3
	60	74	66.66	-11.8	-11.7	-11.7	-10.3	-10.3	-10.4	-11.9	-13.5	-11.9
July	**0**	309	46.97	9.9	9.9	9.9	11.3	11.3	11.3	9.9	7.9	9.6
	60	28	64.22	-0.8	-0.7	-0.7	1.5	1.5	1.5	-0.1	-3.5	-0.8
Aug	**0**	300	43.22	15.5	15.5	15.5	17.3	17.3	17.2	15.8	13.4	15.4
	60	22	67.17	1.7	1.8	1.8	3.7	3.7	3.6	1.7	-1.0	1.2
Sept	**0**	224	37.95	16.6	16.7	16.7	20.1	20.1	20.0	16.7	13.9	17.6
	60	7	61.95	-1.2	-1.1	-1.1	1.7	1.7	1.6	-1.4	-4.0	-0.9

Table 4-11. Ozone season and monthly Detroit NAA-wide MDA8 O_3 performance: comparison of NME

Period	Cut	#Pair	Obs (ppb)	NME (%)								
				base	hcho	hchoext	hchovcp	hchovcppro	vcp	megan	meg2013	combine
Season	**0**	1619	45.51	16.1	16.1	16.1	16.7	16.7	16.7	16.3	15.8	16.3
	60	190	66.90	12.4	12.3	12.3	11.9	11.9	11.9	12.6	13.3	12.5
April	**0**	185	44.93	17.5	17.5	17.5	16.4	16.4	16.4	17.6	18.3	17.1
	60	26	68.75	12.6	12.5	12.5	9.7	9.7	9.7	12.9	14.9	11.7
May	**0**	309	47.00	16.1	16.1	16.1	15.4	15.4	15.4	16.2	16.8	15.9
	60	33	69.14	15.2	15.1	15.1	13.8	13.8	13.8	15.3	16.6	14.7
June	**0**	292	50.93	14.3	14.3	14.3	14.8	14.8	14.7	14.4	14.7	14.9
	60	74	66.66	12.9	12.9	12.9	12.5	12.5	12.6	13.0	14.1	13.4
July	**0**	309	46.97	14.4	14.4	14.4	15.4	15.4	15.4	14.5	13.4	14.3
	60	28	64.22	12.0	12.1	12.1	13.3	13.3	13.3	12.4	11.4	12.3
Aug	**0**	300	43.22	17.3	17.3	17.4	18.9	18.9	18.8	17.7	15.9	17.5
	60	22	67.17	8.3	8.3	8.3	9.2	9.2	9.2	8.9	8.2	8.9
Sept	**0**	224	37.95	18.9	18.9	18.9	21.8	21.8	21.7	19.3	17.6	20.1
	60	7	61.95	6.0	6.0	6.0	6.4	6.4	6.3	6.0	6.6	6.8

Table 4-12. Ozone season and monthly Detroit NAA-wide MDA8 O_3 performance: comparison of R

Period	Cut	#Pair	Obs (ppb)	R								
				base	hcho	hchoext	hchovcp	hchovcppro	vcp	megan	meg2013	combine
Season	**0**	1619	45.51	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69
	60	190	66.90	0.30	0.30	0.30	0.30	0.30	0.30	0.30	0.30	0.30
April	**0**	185	44.93	0.79	0.79	0.79	0.80	0.80	0.80	0.78	0.7	0.79
	60	26	68.75	0.76	0.77	0.77	0.82	0.82	0.81	0.75	0.68	0.79
May	**0**	309	47.00	0.70	0.70	0.70	0.70	0.70	0.70	0.70	0.69	0.70
	60	33	69.14	0.44	0.43	0.43	0.31	0.31	0.32	0.41	0.44	0.33
June	**0**	292	50.93	0.77	0.77	0.77	0.74	0.74	0.74	0.77	0.77	0.75
	60	74	66.66	0.44	0.44	0.44	0.42	0.42	0.42	0.46	0.45	0.44
July	**0**	309	46.97	0.68	0.68	0.68	0.68	0.68	0.68	0.68	0.68	0.68
	60	28	64.22	0.03	0.03	0.03	0.04	0.04	0.04	0.06	0.05	0.06
Aug	**0**	300	43.22	0.82	0.82	0.82	0.80	0.80	0.81	0.81	0.81	0.80
	60	22	67.17	0.60	0.60	0.60	0.56	0.56	0.56	0.57	0.57	0.53
Sept	**0**	224	37.95	0.80	0.80	0.80	0.79	0.79	0.79	0.79	0.79	0.78
	60	7	61.95	-0.76	-0.75	-0.75	-0.53	-0.53	-0.54	-0.74	-0.80	-0.60

Table 4-13. Ozone season and monthly Detroit NAA-wide MDA1 O_3 performance: mean predictions versus mean observation

Period	**Cut**	**#Pair**	**Obs (ppb)**	**Sim (ppb)**								
				base	**hcho**	**hchoext**	**hchovcp**	**hchovcppro**	**vcp**	**megan**	**meg2013**	**combine**
Season	**0**	1628	50.57	50.95	50.97	50.97	52.10	52.10	52.07	51.00	49.96	51.20
	60	347	69.23	64.89	64.93	64.93	66.98	66.98	66.92	65.04	63.13	65.43
April	**0**	186	49.42	44.11	44.13	44.13	44.85	44.85	44.83	44.09	43.64	44.37
	60	34	71.53	63.47	63.51	63.51	65.58	65.58	65.51	63.36	61.92	63.97
May	**0**	310	51.07	46.49	46.51	46.51	47.65	47.65	47.62	46.49	45.68	46.89
	60	58	69.74	61.35	61.40	61.40	63.77	63.77	63.69	61.45	59.62	62.30
June	**0**	293	56.07	52.05	52.08	52.08	53.23	53.23	53.19	51.92	50.94	52.22
	60	112	69.72	63.16	63.20	63.21	64.65	64.65	64.59	63.07	61.65	63.30
July	**0**	310	52.50	56.33	56.35	56.35	57.29	57.29	57.28	56.43	55.24	56.34
	60	66	69.08	65.92	65.94	65.94	67.38	67.38	67.36	66.22	64.15	65.86
Aug	**0**	306	48.69	54.90	54.92	54.93	55.98	55.98	55.95	55.12	53.81	54.99
	60	53	68.55	72.14	72.20	72.20	74.68	74.68	74.61	72.68	70.03	72.89
Sept	**0**	223	43.48	48.48	48.51	48.51	50.28	50.28	50.24	48.60	47.29	49.22
	60	24	67.17	64.67	64.72	64.73	69.58	69.57	69.48	65.16	62.17	67.29

Table 4-14. Ozone season and monthly Detroit NAA-wide MDA1 O_3 performance: comparison of NMB

Period	Cut	#Pair	Obs (ppb)	NMB (%)								
				base	hcho	hchoext	hchovcp	hchovcppro	vcp	megan	meg2013	combine
Season	**0**	1628	50.57	0.7	0.8	0.8	3.0	3.0	3.0	0.8	-1.2	1.3
	60	347	69.23	-6.3	-6.2	-6.2	-3.2	-3.3	-3.3	-6.1	-8.8	-5.5
April	**0**	186	49.42	-10.7	-10.7	-10.7	-9.3	-9.3	-9.3	-10.8	-11.7	-10.2
	60	34	71.53	-11.3	-11.2	-11.2	-8.3	-8.3	-8.4	-11.4	-13.4	-10.6
May	**0**	310	51.07	-9.0	-8.9	-8.9	-6.7	-6.7	-6.8	-9.0	-10.6	-8.2
	60	58	69.74	-12.0	-12.0	-12.0	-8.6	-8.6	-8.7	-11.9	-14.5	-10.7
June	**0**	293	56.07	-7.2	-7.1	-7.1	-5.1	-5.1	-5.1	-7.4	-9.1	-6.9
	60	112	69.72	-9.4	-9.4	-9.3	-7.3	-7.3	-7.4	-9.5	-11.6	-9.2
July	**0**	310	52.50	7.3	7.3	7.3	9.1	9.1	9.1	7.5	5.2	7.3
	60	66	69.08	-3.2	-3.1	-3.1	-1.0	-1.0	-1.1	-2.7	-5.8	-3.3
Aug	**0**	306	48.69	12.8	12.8	12.8	15.0	15.0	14.9	13.2	10.5	12.9
	60	53	68.55	5.2	5.3	5.3	8.9	8.9	8.8	6.0	2.2	6.3
Sept	**0**	223	43.48	11.5	11.6	11.6	15.6	15.6	15.5	11.8	8.8	13.2
	60	24	67.17	-3.7	-3.6	-3.6	3.6	3.6	3.4	-3.0	-7.4	0.2

Table 4-15. Ozone season and monthly Detroit NAA-wide MDA1 O_3 performance: comparison of NME

Period	Cut	#Pair	Obs (ppb)	NME (%)								
				base	hcho	hchoext	hchovcp	hchovcppro	vcp	megan	meg2013	combine
Season	**0**	1628	50.57	15.3	15.3	15.3	16.1	16.1	16.1	15.5	15.1	15.7
	60	347	69.23	12.0	12.0	12.0	12.4	12.4	12.4	12.3	12.7	12.6
April	**0**	186	49.42	17.2	17.2	17.2	16.3	16.3	16.3	17.2	18.0	16.8
	60	34	71.53	11.3	11.3	11.3	9.6	9.6	9.6	11.5	13.4	10.9
May	**0**	310	51.07	16.5	16.5	16.5	15.9	15.9	15.8	16.6	17.3	16.4
	60	58	69.74	14.9	14.9	14.9	13.8	13.8	13.8	15.2	16.4	14.6
June	**0**	293	56.07	14.3	14.3	14.3	15.0	15.0	15.0	14.3	14.5	15.0
	60	112	69.72	12.7	12.7	12.7	13.0	13.0	12.9	12.9	13.7	13.4
July	**0**	310	52.50	13.1	13.1	13.1	14.2	14.1	14.1	13.3	12.3	13.2
	60	66	69.08	10.4	10.4	10.4	11.2	11.2	11.2	10.9	10.5	10.9
Aug	**0**	306	48.69	16.1	16.1	16.1	17.9	17.9	17.8	16.5	14.6	16.4
	60	53	68.55	11.3	11.3	11.3	14.1	14.1	14.0	12.0	9.8	12.6
Sept	**0**	223	43.48	15.8	15.8	15.8	18.6	18.6	18.5	16.2	15.0	17.4
	60	24	67.17	8.2	8.2	8.2	10.4	10.4	10.4	8.4	9.8	11.2

Table 4-16. Ozone season and monthly Detroit NAA-wide MDA1 O_3 performance: comparison of R

Period	Cut	#Pair	Obs (ppb)	R								
				base	**hcho**	**hchoext**	**hchovcp**	**hchovcppro**	**vcp**	**megan**	**meg2013**	**combine**
Season	**0**	1628	50.57	0.72	0.72	0.72	0.71	0.71	0.71	0.71	0.72	0.71
	60	347	69.23	0.44	0.44	0.44	0.43	0.43	0.43	0.43	0.42	0.42
April	**0**	186	49.42	0.79	0.79	0.79	0.81	0.81	0.81	0.79	0.78	0.80
	60	34	71.53	0.85	0.86	0.86	0.87	0.87	0.87	0.84	0.78	0.85
May	**0**	310	51.07	0.71	0.71	0.71	0.71	0.71	0.71	0.71	0.70	0.70
	60	58	69.74	0.46	0.46	0.46	0.42	0.42	0.42	0.45	0.46	0.43
June	**0**	293	56.07	0.78	0.78	0.78	0.74	0.74	0.74	0.78	0.79	0.75
	60	112	69.72	0.44	0.44	0.44	0.43	0.43	0.44	0.44	0.43	0.44
July	**0**	310	52.50	0.71	0.71	0.71	0.71	0.71	0.71	0.71	0.71	0.71
	60	66	69.08	0.56	0.56	0.56	0.56	0.56	0.56	0.55	0.55	0.56
Aug	**0**	306	48.69	0.81	0.81	0.81	0.80	0.80	0.80	0.80	0.81	0.80
	60	53	68.55	0.54	0.53	0.53	0.48	0.48	0.48	0.51	0.52	0.46
Sept	**0**	223	43.48	0.81	0.81	0.81	0.79	0.79	0.79	0.80	0.80	0.78
	60	24	67.17	0.20	0.20	0.20	0.16	0.16	0.16	0.25	0.16	0.15

Both the MDA1 O_3 and MDA8 O_3 performances indicated that the basecase simulation slightly underpredicted ozone in the region, especially in months of April through July, with much larger underprediction for high ozone (higher than 60ppb). The addition of HCHO emissions alone (hcho and hchoext) changed the ozone performances only slightly. The alternative biogenic emissions from MEGAN using the 2016 GLASS LAIv didn't change the ozone performance significantly, however the alternative biogenic emissions derived from MEGAN using the Default 2013 LAIv increased the underprediction of high ozone in the region. The tests with the addition of VCP VOC emissions (hchovcp, hchovcppro and vcp) all enhanced the ozone concentrations in a similar way and improved the ozone performance by reducing underpredictions in general, more significantly for high ozone in the region. Little differences are found among tests with additional VCP VOC emissions. The updated VCP VOC speciation profiles did not much change simulated ozone concentrations in the region. The test with both the addition of VCP VOC emissions and the alternative biogenic emissions MEGAN using the Default 2013 LAIv (with the addition of HCHO emissions as well) produced no significant changes to the ozone performance probably due to decreased ozone concentrations resulting from MEGAN biogenic emissions canceling increased ozone concentrations resulting from additional VCP VOC emissions.

4.4 Recommendation for the Optimal Base Year Simulation

Supported by the above analysis comparing the ozone and precursor performances among the sensitivity tests, and considering all the information with the cons and pros together, we worked with LADCO and Michigan EGLE to recommend the configuration with additional HCHO and VCP VOCs emissions as the optimal choice for the base year air quality modeling.

The performance evaluation strongly supports the idea that we should include additional HCHO emissions. We included the addition of VCP VOCs mainly due to better performance for MAD8 O_3 larger than 60 ppb, keeping in mind that the addition of VCP VOC emissions worsened the performance of VCP-related VOC species such as TOL and XYL at monitoring locations. The performance evaluation doesn't support switching to MEGAN biogenic emissions for the region, mainly due to the simulated lower O_3 levels and worsened performance of isoprene (using the default 2013 LAIv), as well as excessive terpene emissions (using the GLASS 2016 LAIv).

We compared the optimal simulation results to the modeled MDA8 O_3 statistics for each of the ten sites in Detroit NAA (Table 4-17) based on commonly used evaluation criteria for ozone model performance: NMB <±15%, NME <25%, and R >0.50 (Emery et al., 2017). Note that Emery et al., 2017 recommend no cutoff for R. The optimal MDA8 O_3 performance against the AQS observations at all ten sites during the entire ozone season achieved the performance criteria for modeled ozone statistics recommended by Emery et al., 2017, except that the R with no cutoff is 0.44 at the Eliza Near Road site with ID of 261630093. Note that at this site, the NMB and NME without the cutoff are quite large (as 29.6% and 34.4% respectively) and there are only two higher than 60 ppb MDA8 O_3 concentrations that were observed during 2016 ozone season. Though not exceeding the recommended levels of performance for MDA8 ozone with 60 ppb cutoff, the optimal simulation still generally underpredicts larger than 60 ppb ozone in April through June, but overpredicts larger than 60 ppb ozone in July through September. The MDA1 O_3 performances (not shown here) are like MDA8 O_3 at the site level.

Table 4-17. Ozone season MDA8 O_3 performance of optimal simulation at each site in Detroit NAA

Site-Id	*sitename*	*cut*	*#pair*	*Obs (ppb)*	*Sim (ppb)*	*NMB (%)*	*NME(%)*	*R*
260990009	New Haven	0	156	46.04	48.06	4.4	15.8	0.71
		60	17	65.47	61.48	-6.1	9.1	0.65
260991003	Warren - Fire Station	0	166	46.70	48.67	4.2	14.6	0.77
		60	23	66.11	62.85	-4.9	11.2	0.42
261250001	Oak Park	0	166	47.34	48.93	3.3	16.3	0.72
		60	25	67.64	63.09	-6.7	11.6	0.35
261470005	Port Huron	0	164	43.69	43.64	-0.1	14.3	0.83
		60	16	66.87	65.08	-2.7	8.9	0.58
261610008	Towner St	0	162	45.32	47.48	4.8	14.3	0.75
		60	17	65.73	62.32	-5.2	11.4	0.22
261619991	Ann Arbor	0	155	46.32	46.72	9.0	16.7	0.66
		60	17	68.41	59.38	-13.2	15.1	0.27
261630001	Allen Park	0	165	45.73	48.32	5.7	16.8	0.69
		60	19	67.01	60.96	-9.0	13.7	0.09
261630019	East 7 Mile	0	159	49.37	48.25	-2.3	13.3	0.75
		60	30	66.82	61.97	-7.3	11.9	0.07
261630093	Eliza-NR	0	160	36.83	47.74	29.6	34.4	0.44
		60	2	63.94	65.68	2.7	18.0	-1.0
261630094	Eliza Downwind	0	156	46.04	48.06	4.4	15,8	0.71
		60	17	65.47	61.48	-6.1	9.1	0.65

Figures 4-9 through 4-18 show timeseries of simulated MDA8 O_3 concentrations from the optimal simulation versus the basecase simulation compared against the observations at each of the ten sites in Detroit NAA. Significant increases in MDA8 O_3 concentrations from the basecase simulation to the optimal simulation can be found on many of the days at each site, especially during the peaks. We produced timeseries plots for other species, and other types of plots too, such as scatter plots and tile plots, to fulfill the whole evaluation of the model performance, but these are not shown here.

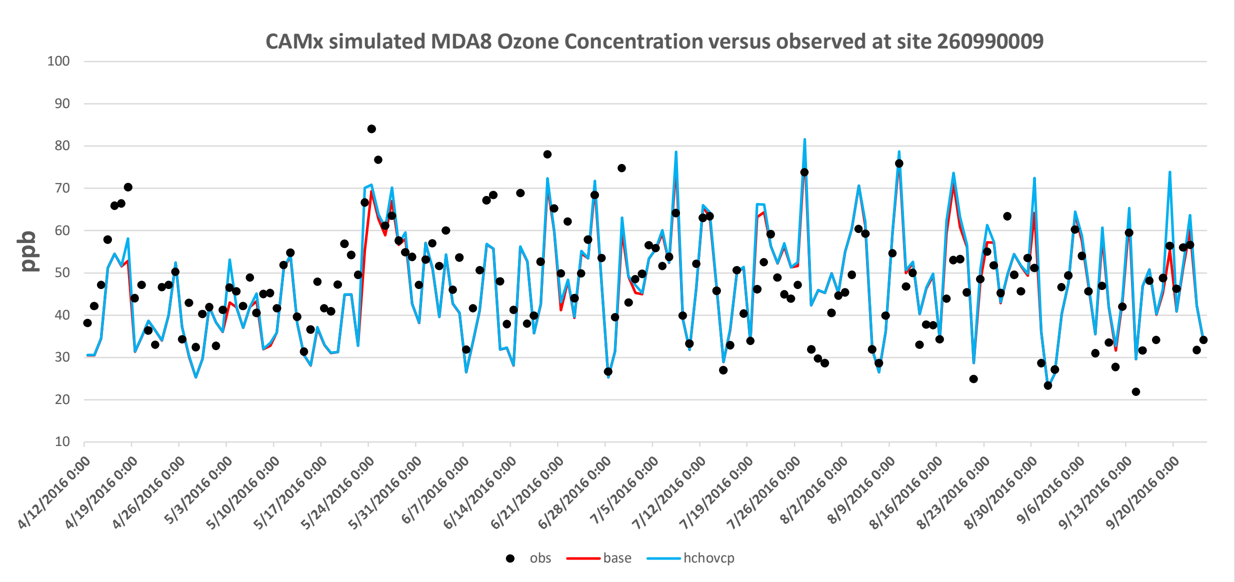

Figure 4-9. Timeseries of CAMx simulated MDA8 O_3 concentrations from the optimal simulation (hchovcp) versus the basecase simulation against the observations at the New Haven site (ID 260990009).

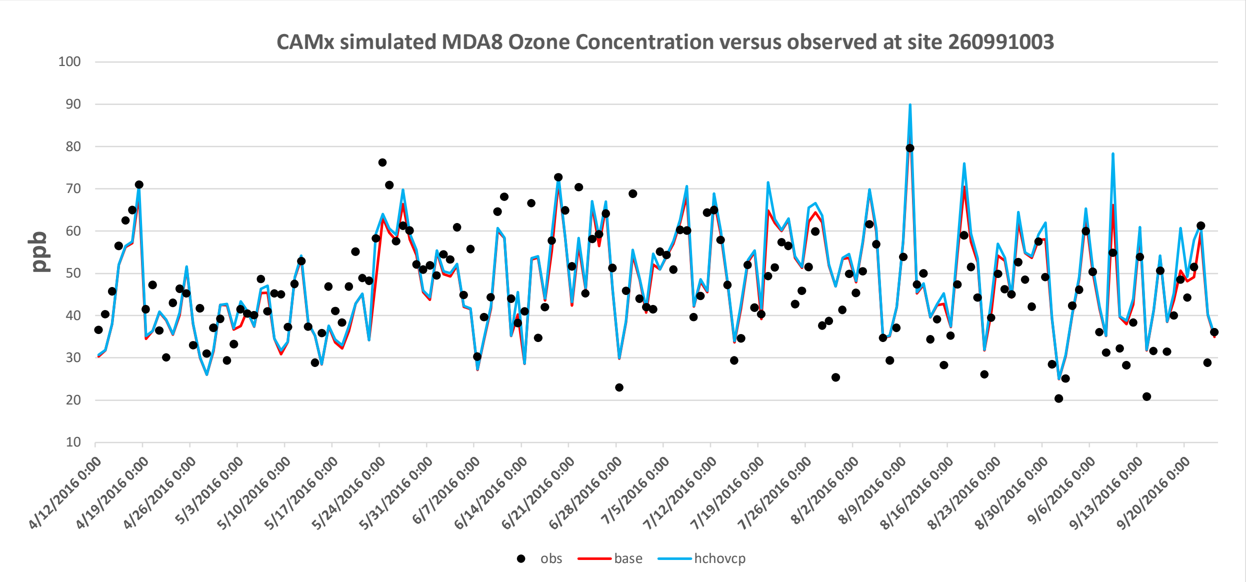

Figure 4-10. Timeseries of CAMx simulated MDA8 O_3 concentrations from the optimal simulation (hchovcp) versus the basecase simulation against the observations at the Warren Fire Station site (ID 260991003).

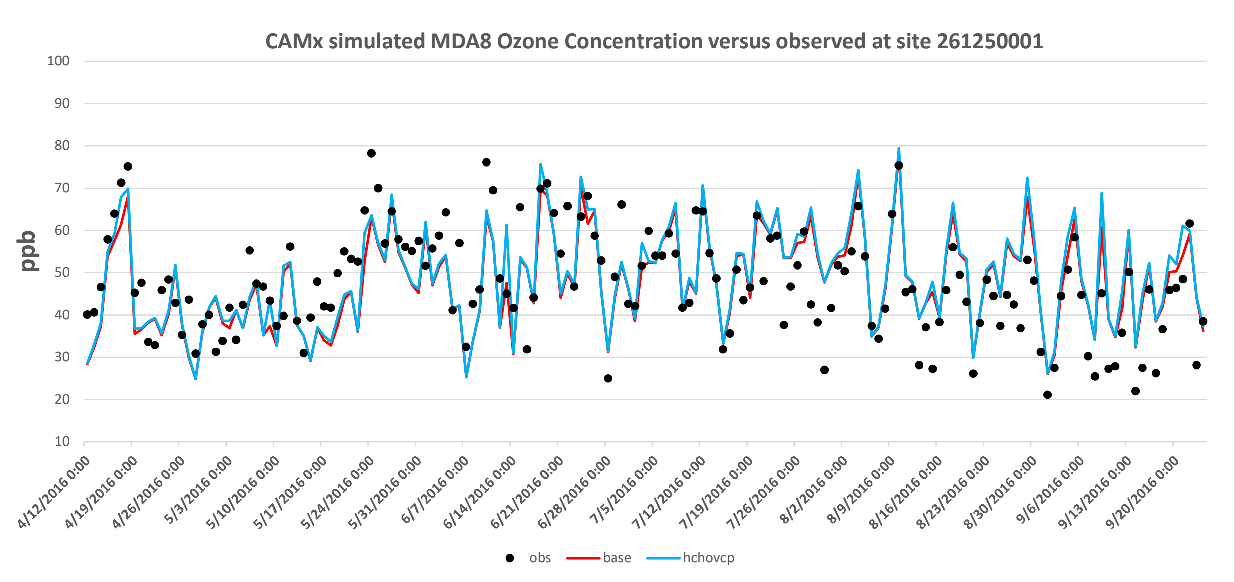

Figure 4-11. Timeseries of CAMx simulated MDA8 O_3 concentrations from the optimal simulation (hchovcp) versus the basecase simulation against the observations at the Oak Park site (ID 261250001).

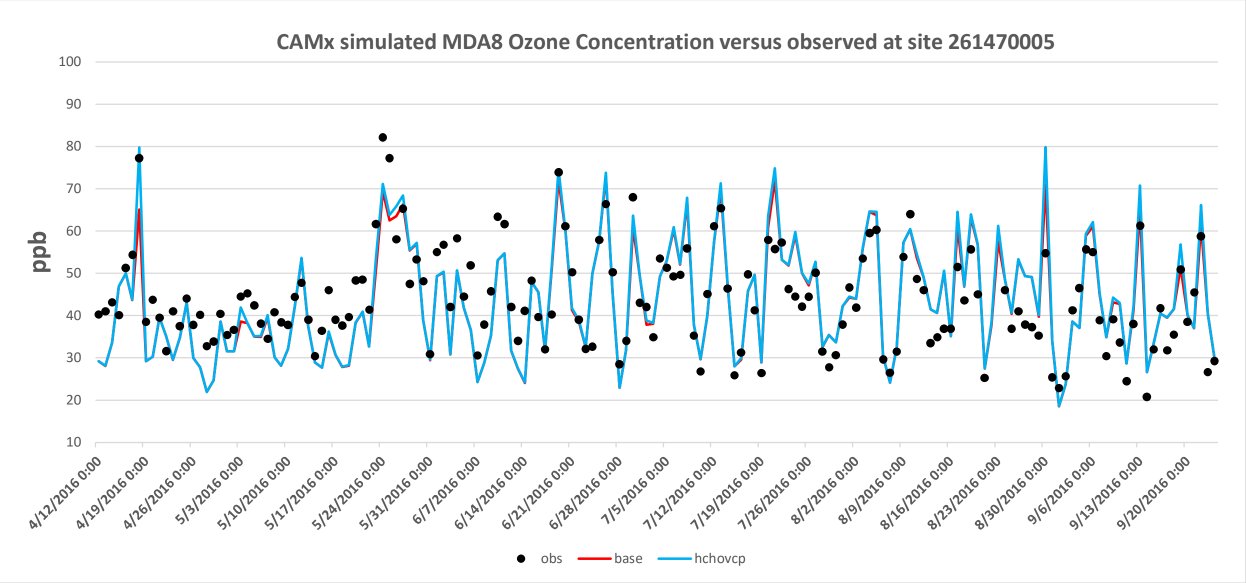

Figure 4-12. Timeseries of CAMx simulated MDA8 O_3 concentrations from the optimal simulation (hchovcp) versus the basecase simulation against the observations at the Port Huron site (ID 261470005).

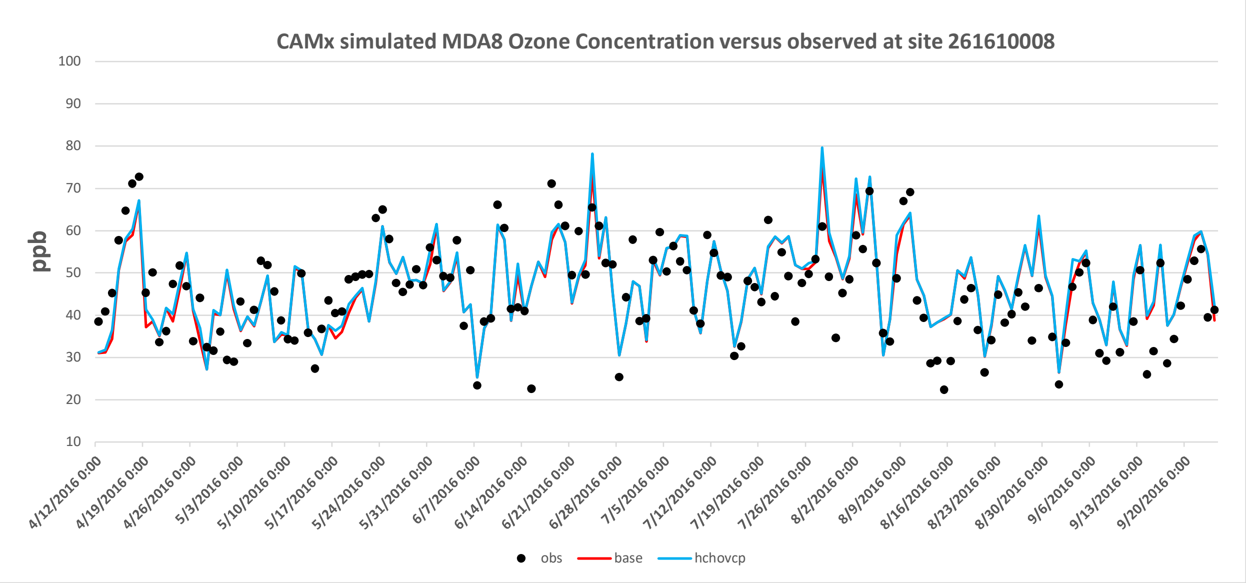

Figure 4-13. Timeseries of CAMx simulated MDA8 O_3 concentrations from the optimal simulation (hchovcp) versus the basecase simulation against the observations at the Towner St site (ID 261610008).

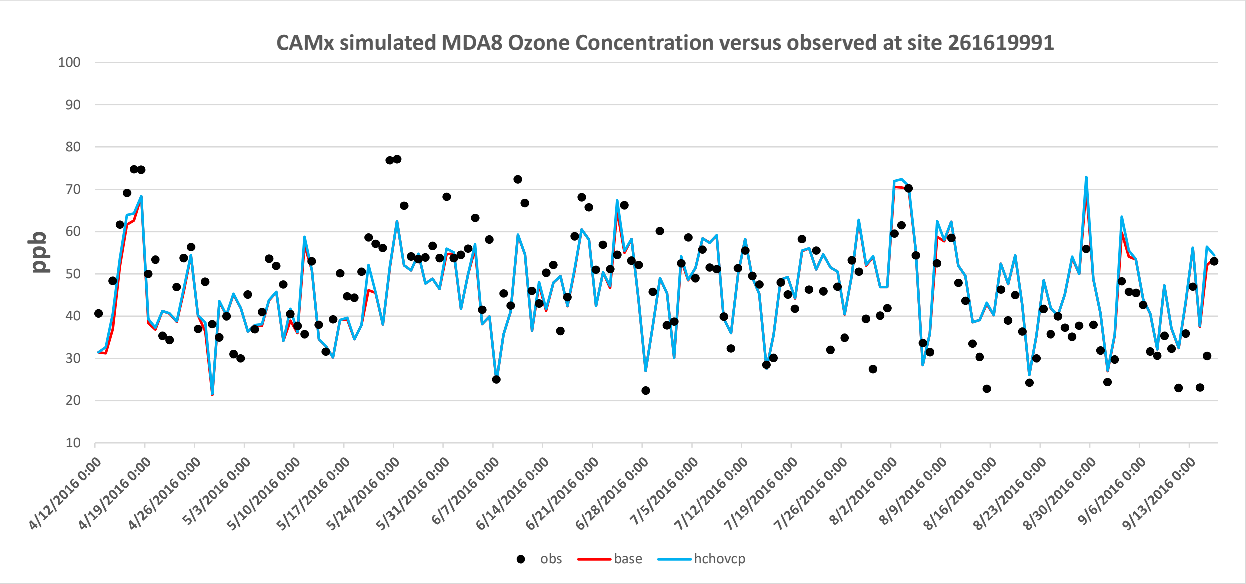

Figure 4-14. Timeseries of CAMx simulated MDA8 O_3 concentrations from the optimal simulation (hchovcp) versus the basecase simulation against the observations at the Ann Arbor site (ID 261619991).

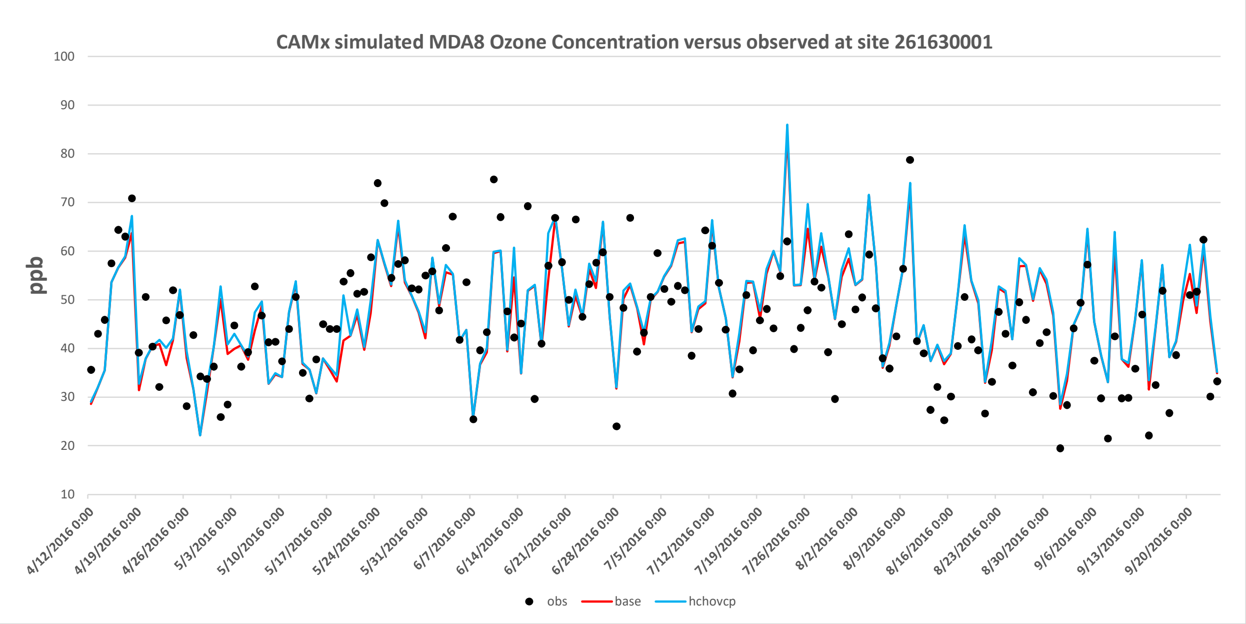

Figure 4-15. Timeseries of CAMx simulated MDA8 O_3 concentrations from the optimal simulation (hchovcp) versus the basecase simulation against the observations at the Allen Park site (ID 261630001).

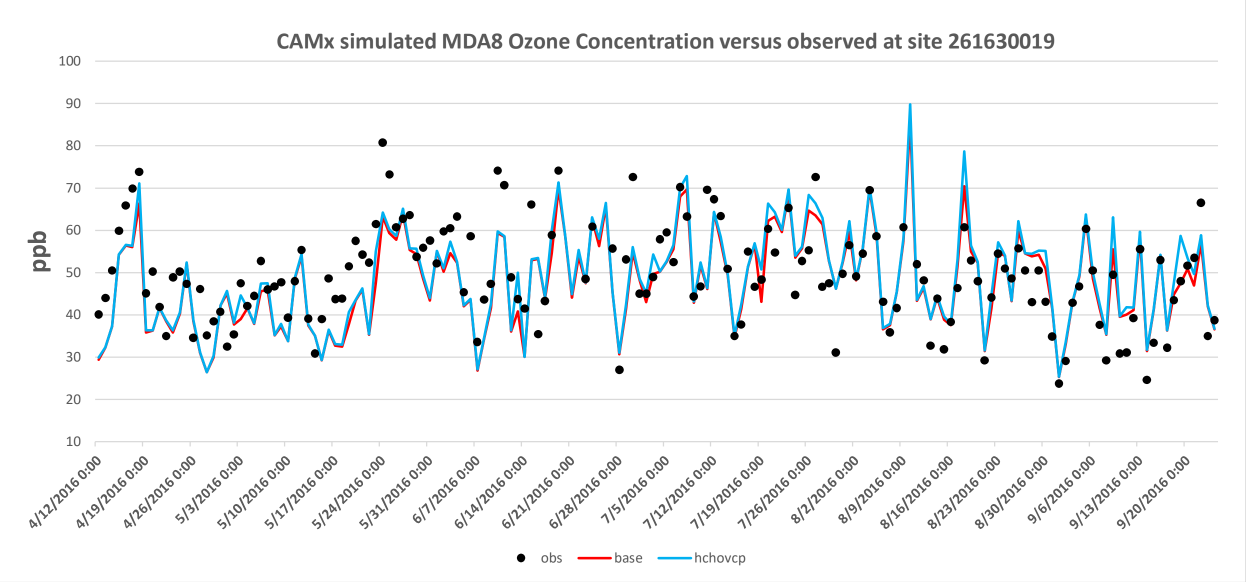

Figure 4-16. Timeseries of CAMx simulated MDA8 O_3 concentrations from the optimal simulation (hchovcp) versus the basecase simulation against the observations at the East 7 Mile site (ID 261630019).

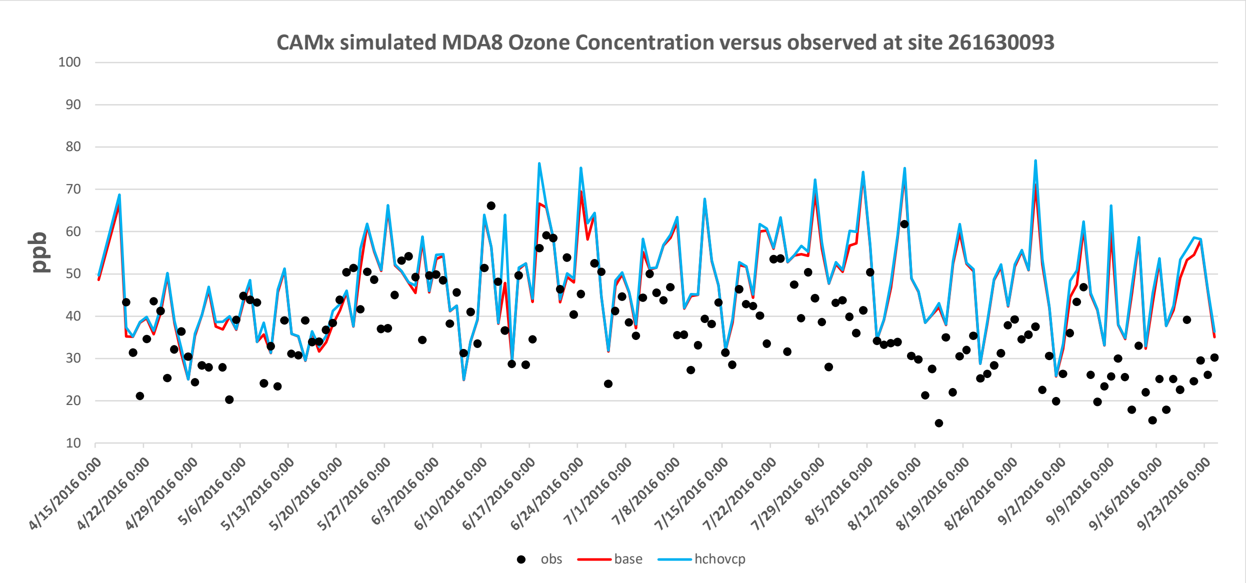

Figure 4-17. Timeseries of CAMx simulated MDA8 O_3 concentrations from the optimal simulation (hchovcp) versus the basecase simulation against the observations at the Eliza-NR site (ID 261630093).

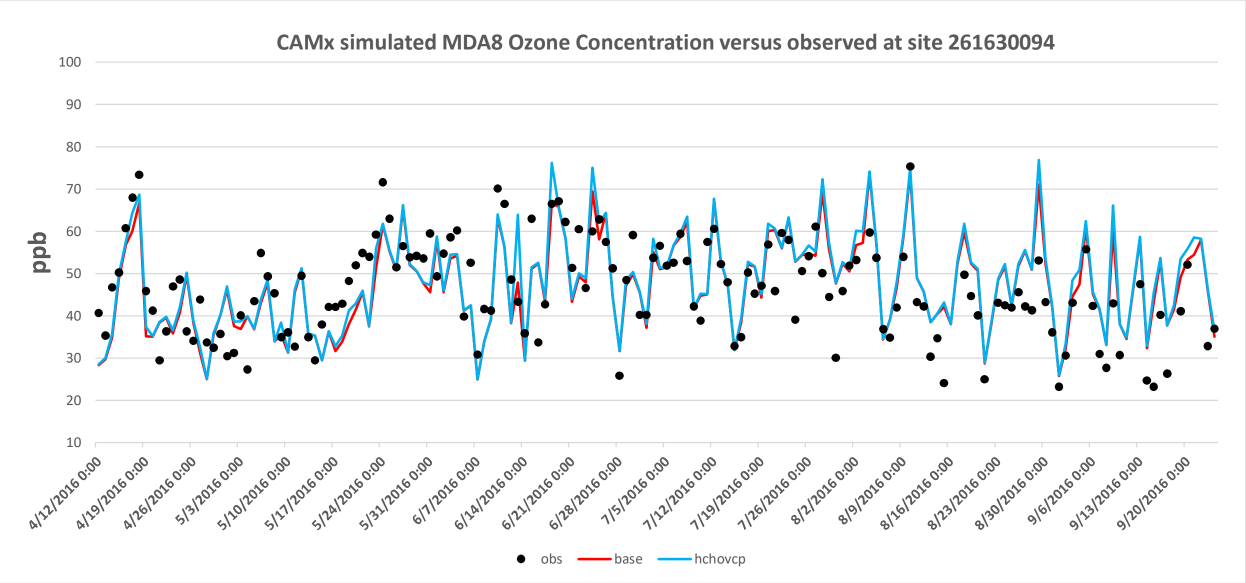

Figure 4-18. Timeseries of CAMx simulated MDA8 O_3 concentrations from the optimal simulation (hchovcp) versus the basecase simulation against the observations at the Eliza Downwind site (ID 261630094).

Section 5: Emission Inputs Preparation for Future Year Control Scenarios

This section describes how we prepared the base 2023 emissions and the controlled emissions for the future year emissions control experiments. We worked with LADCO and Michigan EGLE to determine the following four separate emissions control scenarios for experiments: 1) VOCs control scenario for the Reasonably Available Control Technologies (RACT), especially those that reduce VCP VOC emissions from non-EGU point sources, and the Ozone Transport Commission (OTC)-derived rules for Architectural and Industrial Maintenance (AIM) coatings and Consumer and Commercial Products to reduce VOC emissions from non-point VCPs, 2) NOx control scenario for Good Neighbor-like NOx RACT on non-EGU point sources, 3) HCHO control scenario for eliminating HCHO emissions from all stationary engines due to the adoption of oxycat or other controls in addition to any NOx emissions reductions obtained from the NOx RACT on the same engines at non-EGU point sources, 4) the above NOx and VOC control strategies combined together.

5.1 Base 2023 Emissions

The base 2023 emissions were prepared for conducting the “on-the-books” (OTB) simulation for the future year 2023. We used the 2023fh_16j inventories that were projected from the 2016fh_16j inventories as the starting point for preparing the base 2023 emissions. Supported by the optimization tests on the 2016 base year inventories, we updated the ptnonipm and nonpt sectors with augmented HCHO and VCP emissions and included them in the base 2023 emissions.

We implemented the same methods described in sections 3.1 and 3.2, respectively, for the HCHO emissions improvement and the VCP VOC emissions improvements, this time to the relevant 2023fh_16j inventories. We conducted SMOKE modeling to prepare the base 2023 emissions on the SEMI1 grid for inputs to CAMx for the entire 2016 ozone season. The results of the ozone season 2023 OTB simulation will be compared to the optimized 2016 simulation results for evaluation of the changes due to OTB controls in future year base case ozone concentrations relative to the base year.

5.2 VOCs control scenario

We worked with Michigan EGLE to develop 2023 emissions inventories for a VOC control scenario that reflects the impact of new ozone SIP rules being contemplated or implemented in the Detroit, MI ozone NAA by Michigan EGLE. Table 5-1 lists all the 7 counties in the Detroit MI ozone NAA.

Table 5-1. List of Counties in the Detroit, MI NAA

County Name	FIPS (County ID)
Livingston	26093
Marcomb	26099
Monroe	26115

Oakland	26125
St Clair	26147
Washtenwa	26161
Wayn	26163

EGLE provided datasheets “Copy of SCCs for Part 6.xlxs” that include the SCC lists for the categories of sources that EGLE draft rules apply to. These SCC lists are separated by individual rules or groups of rules. The control factors for the rule categories are listed in Table 5-2, along with their matching SCCs. The last two rule categories in the Table, i.e. consumer and commercial products (Consumer Prod) and Architectural and Industrial Maintenance (AIM) coatings, are mainly area source categories. While the other three rule categories are mostly non-EGU sources.

Table 5-2 VCP VOC emissions reduction factors by rule categories with the matching SCC (with leading digits) lists.

Rule Category	SCC for nonpt	SCC for ptnonipm	VOCs Emission Reductions
Gas marketing; 606-609 (expand geo)		40400154, 40399999, 30699999, 404002	5%
Coating; 610a, 620a, 621a, 624a, 632 (exempt levels, etc)	2415300, 2461021, 2301040000	402015, 402016, 402011, 402013, 402014, 402017, 402018, 402020, 30700407, 402044, 402042, 402047, 402046, 402041, 402043, 402045, 4010025, 4010029, 402021, 402025, 403888, 306008, 306888, 403011, 405003, 40500515, 40500516, 301060, 30181001, 31000220, 40400251, 301014, 301080, 301065, 402022, 308010	10%
Misc new RACT rules; 633-644	2440020000, 2401020	305012, 308007, 301009, 401003, 405002, 405004, 30105001, 402007, 305012, 308007, 402019, 40200101, 40200201, 40200301, 40200401, 40200501, 40200601, 402024, 310001, 310888, 310003, 404003	20%
Consumer prod; 660 (tighten for RFP)	24601, 24602, 24604, 24651, 24652, 24654		10%
AIM; 662 (new, for RFP)	2401001, 2401002,		20%

	2401003, 240110		

We directly updated the nonpt and ptnonipm inventories of 2023 base emissions by reducing the VCP VOC emissions from the original amount using the appropriate reduction factors for the sources with the identified SCCs listed in Table 5-2. The reductions are only applied to the matched sources in the 7 counties in the Detroit, MI NAA, by searching through the inventory records for SCC codes that matched with the specific leading digits and for the county IDs that matched with the list in Table 5-1.

We then conducted the SMOKE modeling using the VCP VOC emissions-controlled inventories of the nonpt and ptnonipm sectors to prepare the CAMx-ready emissions inputs. The model-ready emissions files of the 2023 base VOC emissions and the controlled VOC emissions from the two sectors were compared for QA/QC. For easier comparison, the SMOKE inlineto2d program was used to convert the inline format of elevated non-EGU point source emissions file to the 2-d column total emissions.

By controlling the VCP VOC emissions in the seven counties in Detroit, MI NAA, the ptnonipm total VOC emissions in SE Michigan in the SEMI1 grid were reduced from the 2023 base's 21,600 tpy to 19,500 tpy, a reduction of 2,100 tpy (Table 5-3). The nonpt total VOC emissions in SE Michigan in the SEMI1 grid were reduced from the 2023 base's 182,000 tpy to 171,000 tpy, a reduction of 11,000 tpy. The total reduction from the VCP VOC emissions controls in the Detroit NAA is 13,100 tpy.

Table 5-3 The 2023 base versus the controlled VOC emissions in short tons per year (tpy) in SE Michigan inside the SEMI1 modeling domain.

Emissions	**Ptnonipm sector original in base 2023**	**VOC Controlled ptnonipm**	**ptnonipm reduction**
VOC (tpy)	21,600	19,500	2,100
	nonpt sector original in base 2023	**VOC Controlled nonpt**	**nonpt reduction**
VOC (tpy)	182,000	171,000	11,000
	total original in base 2023	**VOC Controlled total**	**total Reduction**
VOC (tpy)	203,600	190,500	13,100

5.3 NOx control scenario

We worked with LADCO and Michigan EGLE to develop 2023 emissions inventories for a NOx control scenario. LADCO provided datasheets in "MI_nonEGU_Controls_2022.xlxs" from a LADCO project in which Ramboll analyzed non-EGU NOx emissions controls in the LADCO region for year 2026. This analysis provided sufficient information for how to remedy transport by using RACT or better NOx controls on non-EGU point sources in the region. We followed this analysis to build a NOx-controlled non-EGU point inventory from the base 2023 emissions.

In the provided datasheet, the Ramboll analysis presents the 2026 base and controlled emissions for non-EGU sources in the Detroit, MI NAA grouped by different thresholds of 25, 50, 100 TPY potential to emit (PTE) each using three levels of control stringencies, i.e., high, medium and low, representing different types of control technologies, with high referring to lower emissions and generally more expensive controls. Michigan EGLE agreed to use a 50 TPY PTE threshold with the high stringency control technology to build the NOx control scenario. Table 5-4 presents the summary information for the non-EGU NOx emissions control analysis done by Ramboll for year 2026 using a 50 TPY PTE threshold with high stringency control technology. There are 53 non-EGU source records being picked up by the 50 TPY PTE threshold in the Detroit, MI NAA. These 53 sources contributed 5,646 tpy NOx emissions in year 2026, and the total contribution can be reduced to 2,136 tpy using the high stringency control technologies.

Table 5-4 Total emissions (in tpy) summary of the Ramboll NOx emissions control analysis on 2026 non-egu point sources in the Detroit, MI NAA using a 50TPY PTE threshold with the high stringency.

Sub Category	High	Medium	Low
Coke			
Base 2026	521	521	521
Controlled 2026	208	208	208
EXCOMB Gas			
Base 2026	381	381	381
Controlled 2026	37	124	226
Glass			
Base 2026	1005	1005	1005
Controlled 2026	335	586	1005
ICE Diesel			
Base 2026	757	757	757
Controlled 2026	36	576	576
ICE GAS			
Base 2026	199	199	199
Controlled 2026	2	32	56
Iron&Steel			
Base 2026	98	98	98
Controlled 2026	39	39	39
Lime Kiln			
Base 2026	565	565	565
Controlled 2026	396	396	396
Other			
Base 2026	1108	1108	1108
Controlled 2026	931	976	983
ProcessHeat			
Base 2026	1012	1012	1012
Controlled 2026	151	452	664
Total Base 2026	**5,646**	**5,646**	**5,646**
Total Controlled 2026	**2,136**	**3,389**	**4,153**

Table 5-5 lists each of the 53 non-EGU source records in the Detroit, MI NAA that were picked up by the 50TPY PTE threshold. Also listed are the base and the controlled NOx emissions for each source for year 2026 (from the Ramboll analysis) and the year 2023. The base 2023 NOx emissions are from the ptnonipm sector's 2023 base inventory (i.e. directly from the 2023fh_16j inventory), while the controlled 2023 NOx emissions were derived by ratioing the 2026 controlled emissions to the base emissions to scale down the 2023 base emissions. Note that the 4 records in red are new sources which are not in the 2023fh_16j inventory. For most of the sources, the 2023 base emissions and their corresponding 2026 base emissions are either the same or have a small difference, with only a couple of exceptions. The 49 sources contributed 4,583 tpy NOx emissions in base year 2023, and total contribution can be reduced to 1,888 tpy using the high stringency control technologies.

Table 5-5 List of the Detroit, MI NAA non-egu point sources with base and controlled NOx emissions (in tpy) using a 50TPY PTE threshold with the high stringency for both 2026 and 2023

region_cd	facility_id	unit_id	rel_point_id	process_id	scc	2026 base	2026 controlled	2023 base	2023 controlled
26125	6650811	125782013	127558412	180857314	20300203	42.06	0.42	40.41	0.40
26163	16662611	107254913	110789212	180878614	30300317	171.93	68.77	171.93	68.77
26163	16662611	107254913	110789512	180878614	30300317	177.14	70.86	177.14	70.86
26163	16662611	107254913	110789612	180878614	30300317	171.93	68.77	171.93	68.77
26163	8483711	1071613	968012	180787414	30301526	48.80	19.52	48.80	19.52
26163	8483711	1071613	73944212	180787414	30301526	48.80	19.52	48.80	19.52
26147	7011211	14898813	14570612	177289114	10200601	88.05	7.92	92.48	8.32
26163	8245611	6518513	6486712	159042314	30600106	31.85	3.18	27.34	2.73
26163	8245611	6516113	6480812	159043014	31000414	45.38	45.38	39.77	39.77
26163	8245611	82905913	73947612	159043414	31000415	34.95	17.47	30.63	15.31
26163	8245611	107277813	110797512	159044114	30600106	30.92	3.09	26.54	2.65
26161	8146111	112738513	115639112	159074614	20200203	31.15	0.31	27.75	0.28
26161	8146111	112738513	115639512	159074614	20200203	31.15	0.31	27.75	0.28
26163	7778911	3630513	109174512	26676414	30501618	282.50	197.75	282.50	197.75
26163	7778911	3630513	109174412	26676414	30501618	282.50	197.75	282.50	197.75
26163	8483611	1080713	978212	26420914	30390003	148.90	22.34	148.90	22.34
26163	8483611	1080713	73982712	26420914	30390003	148.90	22.34	148.90	22.34
26163	8483611	1080713	73981812	26420914	30390003	148.90	22.34	148.90	22.34
26163	8483611	1080713	73982112	26420914	30390003	148.90	22.34	148.90	22.34
26163	8483611	1080713	73982612	26420914	30390003	148.90	22.34	148.90	22.34
26163	8245611	6510613	6483912	28807014	30600106	30.12	3.01	25.85	2.59
26163	8483711	1065113	970312	26822314	10200704	29.86	2.69	31.62	2.85
26163	8483711	1065413	967412	26821714	30390003	28.05	4.21	28.05	4.21
26163	8483711	1065413	73945012	26821714	30390003	28.05	4.21	28.05	4.21
26163	8483611	1086513	977512	26511614	10200602	28.01	2.52	30.12	2.71
26163	8245611	6507913	73947312	28683314	30600201	51.15	5.12	51.15	5.11
26163	8483611	1087413	977512	26510314	30390003	46.89	7.03	46.89	7.03
26099	8227711	6611213	6578112	28289314	10200601	26.87	2.42	27.15	2.44
26125	8194811	6671913	109174612	28817914	20200203	95.05	0.95	88.74	0.89
26115	7888111	3289013	126178212	29018114	30501403	43.80	14.60	43.80	14.60
26115	7888111	3289013	126178112	29018114	30501403	43.80	14.60	43.80	14.60
26115	7888111	3289313	3182612	29017814	30501403	917.00	305.67	917.00	305.67
26115	7888111	3289313	3182612	29017714	30590003	72.05	14.41	69.92	13.98
26163	6267811	16422513	16003512	26735614	10200601	55.30	4.98	56.43	5.08
26163	6266411	16426613	109240912	26834814	20100801	25.53	1.38	25.52	1.38
26163	6266411	16426613	109240812	26834814	20100801	25.53	1.38	25.52	1.38
26163	4211011	82880813	33174712	106557614	10300601	63.20	5.69	64.49	5.80
26147	13657811	82739013	73722612	106320414	10200601	36.44	3.28	35.05	3.15
26163	7347511	94615613	10545312	129514314	10500106	53.10	7.97	53.67	8.05
26125	6545311	94625913	16950512	129530414	20400402	36.12	14.45	37.81	15.12

26163	6442811	90042213	16277012	121491114	20100802	48.39	33.87	48.38	33.87
26163	6442811	90042313	16277012	121491214	20100802	50.65	35.46	50.65	35.45
26125	6664511	99482513	73767112	139219414	20100802	38.38	26.87	38.38	26.87
26099	3998311	107269313	31097612	151915214	20100802	79.50	55.65	79.50	55.65
26147	7239111	107290013	7459512	151946314	20200401	720.50	21.62	179.43	5.38
26163	14437611	CN	STK01	28500201	28500201	62.63	62.63	-	-
26163	14437911	NS	STK01	28500201	28500201	49.14	49.14	-	-
26147	New_V1	CSXT	STK01	28500201	28500201	55.73	55.73	-	-
26163	New_V1	CSXT	STK01	28500201	28500201	55.73	55.73	-	-
26163	8172211	125759913	4376012	180799814	30599999	32.64	32.64	32.64	32.64
26125	6664511	17112513	16651412	29127214	50300601	155.55	155.55	155.55	155.55
26163	7778711	3631513	3498112	26915014	30190099	100.75	100.75	100.75	100.75
26163	16662611	107254813	110789412	151891814	30390024	196.70	196.70	196.70	196.70
Total						5646	2136	4853	1888

We developed the NOx emissions-controlled ptnonipm inventory from the 2023 base emissions by updating the 49 sources listed in Table 5-5. We then conducted the SMOKE modeling using the NOx emissions-controlled ptnonipm inventory to prepare the CAMx-ready emissions inputs. The model-ready emissions files of the 2023 base NOx emissions and the controlled NOx emissions were compared for QA/QC. The total NOx reduction from the 49 sources is 2,965 tpy, which is a 33% reduction from the total ptnonipm NOx emissions in SE Michigan in the SEMI1 modeling domain (Table 5-6).

Table 5-6 The 2023 base versus the controlled NOx emissions in short tons per year (tpy) in SE Michigan inside the SEMI1 modeling domain.

	ptnonipm sector base 2023 total	**NOx Controlled ptnonipm**	**NOx controlled Portion in base 2023**	**ptnonipm reduction**
NOx (tpy)	8,870	5,905	4,853	2,965

5.4 HCHO control scenario

We worked with Michigan EGLE to develop a 2023 emissions inventory for a HCHO control scenario by eliminating the HCHO emissions from the 49 non-EGU sources that were used to develop the NOx control scenario.

We first separated all the pollutant records of the 49 sources from other source records in the ptnonipm inventory, then conducted SMOKE modeling individually for each of the sub-sectors of ptnonipm to prepare a set of the CAMx-ready emissions inputs for the ptnonipm sector. When conducting the SMOKE modeling for the 49 sources, we used a further revised GSPRO file in which the FORM entries were removed from the new CO profiles that updated for the HCHO emissions improvement (Table 5-7, compare with the CO profiles listed in Table 3-4). By doing so, the HCHO emissions would be set to zero for these 49 sources, hence a reduction. The model-ready emissions files of the 2023 base HCHO emissions and the controlled HCHO emissions from the whole ptnonipm sector were compared for QA/QC. The total HCHO reduction from the 49 sources is 433 tpy, which is a 42% reduction from the total ptnonipm HCHO emissions in SE Michigan in the SEMI1 modeling domain (Table 5-8).

Table 5-7 Revised new CO profiles with no scaling CO emissions to HCHO

Profile ID	Profile for CO
S002	S002;"CO";"CO";1.0;28.0;1.0
S005	S005;"CO";"CO";1.0;28.0;1.0
S010	S010;"CO";"CO";1.0;28.0;1.0
S015	S015;"CO";"CO";1.0;28.0;1.0

Table 5-8 The 2023 base versus the controlled HCHO emissions in short tons per year (tpy) in SE Michigan inside the SEMI1 modeling domain.

	ptnonipm sector base 2023 total	HCHO Controlled ptnonipm	HCHO controlled Portion in base 2023	ptnonipm reduction
HCHO (tpy)	1,030	597	433	433

5.5 NOx and VOCs control combined scenario

Refer to section 5.3 and 5.3 for descriptions on building emissions-controlled inventories for the VOC and NOx control scenarios respectively. The CAMx-ready emissions inputs produced by using the VCP VOC emissions-controlled nonpt inventory are directly utilized for this combined NOx and VOC control scenario. We then conducted the SMOKE modeling using the ptnonipm inventory that includes both VCP VOC emissions-controlled and NOx emissions-controlled sources to prepare the CAMx-ready emissions inputs for the ptnonipm sector. The model-ready emissions files of the 2023 base VOC and NOx emissions and the controlled VOC and NOx emissions from the ptnonipm sector were compared for QA/QC.

5.6 Summary of the Emissions-Controlled Sectors for Future Year Simulation Experiments

The source sectors with emissions-controlled for specific scenarios are summarized in Table 5-9. The sector IDs are usually named with the 2023 base emissions sector ID plus an extension to reflect the control scenario. CAMx-ready emissions input files were generated for all these sectors for the entire 2016 ozone season on the SEMI1 grid. The next chapter will describe how these emissions-controlled sectors' emissions were treated for each specifically designed future year emissions control experiments.

Table 5-10 List of sectors with emissions updated for control scenarios for future year simulation

Sector ID	Source Category
ptnonipm_semihchovcp	Non-IPM point sources 2023 base emission that with additions of HCHO and VCP VOC emissions on top of 2023fh_16j inventory
nonpt_semivcp	US non-point sources 2023 base emissions with addition of VCP VOC emissions on top of 2023fh_16j inventory

ptnonipm_voccontrol	Non-IPM point sources with VCP VOC emissions controlled on top of 2023 base that with additions of HCHO and VCP VOC emissions
nonpt_voccontrol	US non-point sources with VCP VOC emissions controlled on top of 2023 base with addition of VCP VOC emissions
ptnonipm_noxcontrol	Non-IPM point sources with NOx emissions controlled on top of the 2023 base that with additions of HCHO and VCP VOC emissions
ptnonipm_hchocontrol	The 49 Non-IPM point sources with HCHO emissions controlled on top of the 2023 base that with additions of VCP VOC emissions
ptnonipm_nohchocontrol	The rest of Non-IPM point sources 2023 base that with additions of HCHO and VCP VOC emissions
ptnonipm_noxvoccontrol	Non-IPM point sources with both NOx and VOC emissions controlled on top of the 2023 base that with additions of HCHO and VCP VOC emissions

Section 6: Future Year Emissions Control Impacts on RRF and DVF

The emissions control scenario experiments are designed to support the overall goal of future year ozone attainment demonstration. The results of experiments here in combination with the base year simulation and the future year OTB simulation are used to investigate the proposed control scenarios' impacts on projected future year design value (FDV), which can assist demonstration of modeled attainment of the ozone NAAQS.

6.1 Future Year Emissions Control Scenario Simulations

After finishing the 2023 OTB simulation, we further conducted ozone season future year simulations for the four different emissions control scenarios (Table 6-1). These four modeling experiments assess impacts on control efficiency for achieving ozone attainment, respectively from 1) the VOC emissions reduction by implementing Reasonably Available Control Technologies (RACT), especially those that reduce VCP VOC emissions from non-EGU point sources and Ozone Transport Commission (OTC)-derived rules for Architectural and Industrial Maintenance (AIM) coatings and Consumer and Commercial Products to reduce VOC emissions from non-point VCPs, 2) NOx emissions reduction by Good Neighbor-like NOx RACT on non-EGU point sources, 3) the elimination of HCHO emissions from all stationary engines due to the adoption of oxycat or other controls in addition to any NOx emissions reductions obtained from NOx RACT on the same engines at non-EGU point sources, 4) NOx and VOC emissions reductions from the above NOx and VOC control strategies combined together.

All the modeling experiments used the same CAMx model executable with the same configuration choices and the same model inputs except the different emissions inputs listed in Table 6-1. These different emissions inputs represent each control scenario's different emissions reductions from the base 2023 emissions of the 2023 OTB simulation. All the 5 runs were conducted on a supercomputer using 96 processors from 4 computing nodes.

Table 6-1. List of future year air quality modeling experiments

Experiment - id	Difference in Emissions Input	Anthropogenic emissions	Experiment emphasis
2023base	ptnonipm_semihchovcp & nonpt_semivcp	Base 2023 Emissions	2023 OTB simulation
voccontrol	ptnonipm_voccontrol & nonpt_voccontrol	Base 2023 with VCP VOC emissions reduced	Reduction of VCP VOC emissions
noxcontrol	ptnonipm_noxcontrol & nonpt_semivcp	Base 2023 with NOx emissions for non-EGU 50TPY APTE-High sources reduced	Reduction of NOx emissions
hchocontrol	ptnonipm_hchocontrol, ptnonipm_nohchocontrol & nonpt_semivcp	Base 2023 with HCHO emissions for non-EGU 50TPY APTE-High sources eliminated	Reduction of HCHO emissions
noxvoccontrol	ptnonipm_noxvoccontrol & nonpt_voccontrol	Base 2023 with non-EGU NOx emissions for 50TPY APTE-High	Reduction of NOx emissions and VCP VOC emissions

		sources & VCP VOC emissions reduced	

All the CAMx modeling outputs were first converted to I/O API format by using the CAMx2IOAPI program and were further post-processed for extraction of the most relevant species and conversion of hourly values to more convenient forms of variables, including MDA1 O_3 and MDA8 O_3. Tile-plots were also plotted to show changes of daily MDA8 O_3 between the base year and future year simulations and among the future year experiment simulations. We also extracted the values of these variables in time series at the ten ozone monitoring sites in the Detroit, MI NAA from the simulated fields to compare with the observations during the entire ozone season period. The postprocessed datasets were then used for further future year design value prediction and analysis.

6.2 Future Year Design Value Projection Method

The ultimate objective of this project is to quantify the impacts of emissions control strategies on RRFs and future year design values (FDV) in the SEMI region. We rely on guidance provided by the U.S. EPA (U.S. EPA, 2018) for demonstrating modeled attainment of air quality goals for O_3 to analyze the CAMx outputs from the future year simulations, where the emphasis is on using model outputs in a relative sense. In the guidance, the ozone attainment test methodology uses model outputs and ambient data to estimate future year concentrations, i.e., the future year design value. Specifically, the method uses the following two equations :

Relative Reduction Factor (RRF) = Model predicted change as a ratio from base year to future year (eq. 1)
Future Year Design Value (DVF) = Base Year Design Value (DVC) × RRF (eq. 2)

In this study, we use the optimized base year simulation, i.e., the results from the “hchovcp” simulation (Table 4-1), as the base year model outputs (referred as 2016base hereafter) and use the 2016-2018 DV as the base year design value (Table 4-3). Together with the future year experiment simulation results, we estimate ozone relative reduction factors (RRFs) and further apply these RRFs to estimate future year design values for the ozone monitors in the Detroit, MI NAA (Table 4-3). Specifically, by following the guidance, we first calculate RRF for each experiment with eq. 1 using the ozone season top-10 averages of the simulated MDA8 O_3 from the 2016base results and the experiment results. We then further calculate the projected DVF for each experiment with eq. 2 by using the 2016-2018 DV and the RRF.

6.3 Emissions Control Scenario impact on RRF and DVF

This section analyzes the impacts of the emissions control scenarios on RRFs and future year ozone conditions at the ozone monitoring sites in the SEMI region. Tables of RRFs and projected 2023 DVFs for MDA8 O_3 along with the observed and simulated top-10 and top-10 average MDA8 O_3 at each of the ten sites in the Detroit, MI NAA are presented below (see Tables 6-2 through 6-11).

Table 6-2. Top10 and Top10-avg MDA8 O_3, RRFs and Projected 2023 DVs at Allen Park site (261630001)

MDA8 O_3 (ppb)	OBS	2016base	2023base	voccontrol	noxcontrol	hchocontrol	noxvoccontrol
1st	78.750	85.986	77.108	77.029	76.356	77.105	76.282
2nd	74.750	74.023	71.844	71.740	71.190	71.839	71.09
3rd	74.000	71.585	70.250	70.246	70.222	70.250	70.219
4th	70.875	69.649	69.355	69.262	70.114	69.352	70.008
5th	69.875	67.248	67.454	66.540	67.510	66.757	67.165
6th	69.250	67.119	66.774	66.410	67.152	66.574	66.446
7th	67.125	66.406	66.312	66.289	66.280	66.312	66.257
8th	67.000	66.250	65.946	65.935	65.600	65.935	65.571
9th	66.875	66.021	65.941	65.677	65.576	65.871	65.271
10th	66.875	65.323	65.678	65.670	65.218	65.677	65.212
Top10-avg	70.538	69.961	68.666	68.480	68.522	68.567	68.352
RRF			0.9815	0.9788	0.9794	0.9801	0.9770
Projected 2023 DV	68*		66.741	66.560	66.601	66.645	66.436

*2016-2018 DV

Table 6-3. Top10 and Top10-avg MDA8 O_3, RRFs and Projected 2023 DVs at New Haven site (260990009)

MDA8 O_3 (ppb)	OBS	2016base	2023base	voccontrol	noxcontrol	hchocontrol	noxvoccontrol
1st	84	81.604	74.118	73.404	74.103	74.059	73.417
2nd	78	78.723	73.245	73.112	72.868	73.225	72.742
3rd	76.75	78.643	72.946	72.825	72.575	72.924	72.462
4th	75.875	73.879	72.612	72.541	72.431	72.61	72.361
5th	74.75	73.665	72.152	71.587	72.353	71.99	71.837
6th	73.75	72.438	70.548	70.435	70.46	70.509	70.359
7th	70.25	72.37	69.523	69.456	69.377	69.521	69.376
8th	68.875	71.772	69.378	69.378	69.376	69.378	69.311
9th	68.375	70.896	69.375	69.293	69.252	69.368	69.173
10th	68.375	70.671	69.123	68.929	68.953	69.102	68.77
Top10-avg	73.900	74.466	71.302	71.096	71.175	71.269	70.981
RRF			0.9575	0.9547	0.9558	0.9571	0.9532
Projected 2023 DV	72*		68.941	68.742	68.818	68.908	68.630

*2016-2018 DV

Table 6-4. Top10 and Top10-avg MDA8 O_3, RRFs and Projected 2023 DVs at Warren-Fire Station site (260991003)

MDA8 O_3 (ppb)	OBS	2016base	2023base	voccontrol	noxcontrol	hchocontrol	noxvoccontrol
1st	79.625	89.946	82.137	81.988	81.77	82.128	81.627
2nd	76.25	78.374	73.078	72.689	73.027	73.064	72.644
3rd	72.75	76.02	72.048	71.87	72.095	72.037	71.918
4th	71	73.037	70.406	70.359	70.032	70.401	69.989
5th	70.875	71.491	70.039	69.844	69.597	70.019	69.399
6th	70.375	71.001	69.838	69.624	69.406	69.788	69.213
7th	68.857	70.578	69.15	69.042	69.312	69.126	69.166
8th	68.125	69.818	68.84	68.831	68.837	68.84	68.828
9th	66.625	69.775	68.642	68.495	68.5	68.624	68.356
10th	65	68.894	67.002	66.797	66.866	66.963	66.784
Top10-avg	70.948	73.893	71.118	70.954	70.944	71.099	70.792
RRF			0.9624	0.9602	0.9601	0.9622	0.9580
Projected 2023 DV	69*		66.408	66.255	66.246	66.391	66.104

*2016-2018 DV

Table 6-5. Top10 and Top10-avg MDA8 O_3, RRFs and Projected 2023 DVs at Oak Park site (261250001)

MDA8 O_3 (ppb)	OBS	2016base	2023base	voccontrol	noxcontrol	hchocontrol	noxvoccontrol
1st	78.25	79.408	74.083	73.985	73.886	74.056	73.83
2nd	76.125	75.735	74.042	73.975	73.667	74.041	73.569
3rd	75.375	74.289	71.482	71.286	71.471	71.479	71.276
4th	75.125	72.66	70.695	70.518	70.647	70.687	70.472
5th	71.25	72.475	69.306	69.28	69.033	69.299	69.008
6th	71.125	70.612	67.752	67.407	67.739	67.729	67.403
7th	70	69.852	67.037	66.921	66.854	67.031	66.738
8th	69.875	68.935	66.939	66.721	66.819	66.938	66.574
9th	69.5	68.807	66.853	66.694	66.756	66.853	66.509
10th	68.125	68.44	66.758	66.573	66.52	66.751	66.344
Top10-avg	72.475	72.121	69.495	69.336	69.339	69.486	69.172
RRF			0.9636	0.9614	0.9614	0.9635	0.9591
Projected 2023 DV	73*		70.341	70.181	70.184	70.333	70.015

*2016-2018 DV

Table 6-6. Top10 and Top10-avg MDA8 O_3, RRFs and Projected 2023 DVs at Port Huron site (261470005)

MDA8 O_3 (ppb)	OBS	2016base	2023base	voccontrol	noxcontrol	hchocontrol	noxvoccontrol
1st	82.125	79.826	85.957	84.795	86.72	85.637	85.669
2nd	77.25	79.768	76.182	75.777	75.901	76.014	75.529
3rd	77.25	74.85	71.954	71.905	71.643	71.948	71.597
4th	73.875	74.584	71.644	71.528	71.279	71.626	71.114
5th	68	73.788	71.364	71.186	71.221	71.327	71.111
6th	66.375	71.224	70.632	70.208	70.716	70.534	70.318
7th	65.375	71.149	69.886	69.79	69.781	69.878	69.688
8th	65.25	70.703	67.358	67.195	67.252	67.349	67.241
9th	64	68.412	67.193	67.182	67.129	67.193	66.969
10th	63.375	67.871	66.951	66.683	66.965	66.911	66.715
Top10-avg	70.288	73.218	71.912	71.625	71.861	71.842	71.595
RRF			0.9822	0.9782	0.9815	0.9812	0.9778
Projected 2023 DV	72*		70.716	70.434	70.666	70.647	70.405

*2016-2018 DV

Table 6-7. Top10 and Top10-avg MDA8 O_3, RRFs and Projected 2023 DVs at Towner St site (261610008)

MDA8 O_3 (ppb)	OBS	2016base	2023base	voccontrol	noxcontrol	hchocontrol	noxvoccontrol
1st	72.75	79.618	71.813	71.806	71.791	71.81	71.784
2nd	71.125	78.218	71.142	70.998	71.055	71.135	70.897
3rd	71.125	72.751	70.515	70.355	69.961	70.501	69.791
4th	69.375	72.316	69.504	69.311	68.981	69.43	68.802
5th	69.125	67.133	67.527	67.518	67.531	67.527	67.522
6th	67	64.201	63.026	62.779	62.78	62.929	62.779
7th	66.125	63.512	62.781	62.779	62.729	62.781	62.701
8th	66.125	63.153	62.763	62.735	62.571	62.762	62.35
9th	65.5	61.78	61.134	61.132	61.246	61.134	61.239
10th	65	61.524	61.075	61.067	61.134	61.072	61.132
Top10-avg	68.325	68.421	66.128	66.048	65.978	66.108	65.900
RRF			0.9665	0.9653	0.9643	0.9662	0.9632
Projected 2023 DV	69*		66.688	66.607	66.537	66.668	66.458

*2016-2018 DV

Table 6-8. Top10 and Top10-avg MDA8 O_3, RRFs and Projected 2023 DVs at Ann Arbor site (261619991)

MDA8 O_3 (ppb)	OBS	2016base	2023base	voccontrol	noxcontrol	hchocontrol	noxvoccontrol
1st	77.125	72.89	69.275	69.237	69.17	69.272	69.135
2nd	76.875	72.343	68.099	68.098	68.099	68.099	68.098
3rd	74.75	71.916	66.982	66.833	66.94	66.978	66.791
4th	74.625	70.769	66.192	66.116	65.531	66.177	65.46
5th	72.375	68.336	65.009	64.948	64.781	65.002	64.722
6th	70.25	67.38	63.644	63.498	63.583	63.608	63.449
7th	69.125	64.243	63.301	63.207	63.131	63.264	63.046
8th	68.25	63.916	62.071	62.071	62.071	62.071	62.071
9th	68.125	63.564	61.942	61.941	61.942	61.942	61.941
10th	66.75	62.788	60.418	60.317	60.186	60.41	60.087
Top10-avg	71.825	67.815	64.693	64.627	64.543	64.682	64.480
RRF			0.9540	0.9530	0.9518	0.9538	0.9508
Projected 2023 DV	71*		67.732	67.662	67.575	67.721	67.509

*2016-2018 DV

Table 6-9. Top10 and Top10-avg MDA8 O_3, RRFs and Projected 2023 DVs at East 7 Mile site (261630019)

MDA8 O_3 (ppb)	OBS	2016base	2023base	voccontrol	noxcontrol	hchocontrol	noxvoccontrol
1st	80.75	89.773	82.01	81.853	81.526	81.998	81.346
2nd	74.125	78.673	73.904	73.539	74.402	73.82	74.029
3rd	74.125	72.856	73.853	73.429	73.293	73.673	72.894
4th	73.875	71.312	71.06	70.887	70.835	71.019	70.669
5th	73.25	71.112	69.579	69.545	69.883	69.579	69.544
6th	72.625	70.213	69.535	69.214	69.578	69.461	69.092
7th	72.625	70.038	69.314	68.709	68.976	69.294	68.878
8th	70.714	69.617	66.824	66.772	66.642	66.796	66.596
9th	70.25	68.391	65.558	65.036	65.738	65.327	64.886
10th	69.875	66.49	65.075	64.775	64.924	65.072	64.84
Top10-avg	73.221	72.848	70.671	70.376	70.580	70.604	70.277
RRF			0.9701	0.9661	0.9689	0.9692	0.9647
Projected 2023 DV	74*		71.789	71.489	71.696	71.721	71.389

*2016-2018 DV

Table 6-10. Top10 and Top10-avg MDA8 O_3, RRFs and Projected 2023 DVs at Eliza-Nr site (261630093)

MDA8 O_3 (ppb)	OBS	2016base	2023base	voccontrol	noxcontrol	hchocontrol	noxvoccontrol
1st	66.125	76.853	71.624	71.609	71.679	71.622	71.551
2nd	61.75	76.206	71.542	71.473	71.261	71.54	71.194
3rd	59.125	75.068	70.998	70.774	70.833	70.936	70.616
4th	58.5	74.979	70.879	70.66	70.724	70.874	70.516
5th	56.125	74.112	70.473	70.361	70.459	70.472	70.347
6th	54.125	72.307	69.463	69.077	68.5	69.388	68.163
7th	53.875	68.689	67.933	67.77	67.831	67.911	67.671
8th	53.625	67.754	66.622	66.607	66.376	66.611	66.361
9th	53.5	66.207	66.382	65.816	66.102	66.325	65.555
10th	53.125	66.133	65.104	65.093	64.994	65.103	64.983
Top10-avg	56.988	71.831	69.102	68.924	68.876	69.078	68.696
RRF			0.9620	0.9595	0.9589	0.9617	0.9564
Projected 2023 DV	49*		47.139	47.017	46.984	47.122	46.861

*Invalid 2016-2018 DV

Table 6-11. Top10 and Top10-avg MDA8 O_3, RRFs and Projected 2023 DVs at Eliza Downwind site (261630094)

MDA8 O_3 (ppb)	OBS	2016base	2023base	voccontrol	noxcontrol	hchocontrol	noxvoccontrol
1st	75.375	76.853	71.624	71.609	71.679	71.622	71.551
2nd	73.375	76.206	71.542	71.473	71.261	71.54	71.194
3rd	71.625	75.068	70.998	70.774	70.833	70.936	70.616
4th	70.125	74.979	70.879	70.66	70.724	70.874	70.516
5th	68	74.112	70.473	70.361	70.459	70.472	70.347
6th	67.125	72.307	69.463	69.077	68.5	69.388	68.163
7th	66.5	68.689	68.008	67.77	68.333	67.963	67.767
8th	66.5	67.754	67.933	67.441	67.831	67.911	67.671
9th	63	66.207	66.622	66.607	66.376	66.611	66.361
10th	63	66.133	66.382	65.816	66.102	66.325	65.555
Top10-avg	68.463	71.831	69.392	69.159	69.210	69.364	68.974
RRF			0.9661	0.9628	0.9635	0.9657	0.9602
Projected 2023 DV	57*		55.065	54.880	54.920	55.043	54.733

*Invalid 2016-2018 DV

Among the ten sites, the 2016-2018 DVs at four sites are in nonattainment of the 2015 ozone NAAQS. The East 7 Mile site has the highest DVC at 74 ppb, next are Oak Park site, 73 ppb, New

Haven site, 72 ppb, and Port Huron site, 72 ppb. With on-the-book controls, the projected DVFs for these sites are all in attainment of NAAQS at under 71 ppb, except the East 7 Mile site which is still at 71.8 ppb.

At the East 7 Mile site, the VOC controls would further bring the 2023 DVF down by 0.3 ppb, while the NOx controls have less impact on DVF than the VOC controls, which would only bring the DVF down by 0.093 ppb. At this site, the HCHO controls are more effective than the NOx controls based on ppb ozone per ton of emissions reduction. Also, the impact of the NOx and VOC combined controls on DVF is slightly larger than the simple sum of the individual impacts.

The other three sites with the DVC in nonattainment of the NAAQS all have larger VOC controls impacts on DVF than the NOx control impacts. All these three sites also have larger impacts of the NOx and VOC combined controls on DVF than the simple sum of the individual impacts. At the Oak Park site, the HCHO controls have little impact on DVF, much less than the other controls. At the Port Huron site, the HCHO controls have an even larger absolute impact on DVF than the NOx controls.

Table 6-12. Emissions Control Scenario Impacts on 2023 DVF at ozone sites in the Detroit, MI NAA

Site Name	DVC (ppb)	OTB Impact (ppb)	voccontrol Impact (ppb)	noxcontrol Impact (ppb)	hchocontrol Impact (ppb)	noxvoccontrol Impact (ppb)
East 7 Mile	74	2.211	0.300	0.093	0.068	0.400
Oak Park	73	2.659	0.161	0.157	0.008	0.326
New Haven	72	3.059	0.199	0.123	0.032	0.311
Port Huron	72	1.284	0.282	0.051	0.069	0.312
Ann Arbor	71	3.268	0.070	0.157	0.012	0.223
Towner St	69	2.312	0.081	0.151	0.020	0.230
Warren-Fire Station	69	2.592	0.153	0.162	0.018	0.304
Allen Park	68	1.259	0.181	0.140	0.096	0.305

* Sites Eliza Downwind and Eliza-Nr are not included here due to their invalid 2016-2018 DV.

Among the four sites with DVC in attainment of NAAQS, three of them have larger NOx controls impacts on DVF than the VOC controls and the HCHO controls. The Allen Park site however has larger VOC controls impact on DVF than the NOx controls, and its HCHO controls impact on DVF is also much larger than the NOx controls based on ppb ozone per ton of emissions reduction. Compared to the high DVC sites, all these four sites have smaller impacts of the NOx and VOC combined controls on DVF than the simple sum of the individual impacts of the NOx and VOC controls.

Many factors can possibly influence the magnitude of impact on DVF at a specific site from certain emission controls. These factors include the chemical environment near the site location, i.e. whether it is NOx limited or VOC limited, the relative distance between the site location and reduced emission sources, the terrain, geography, or local climate near the site.

Based on the above analysis we recommend VOC controls combined with NOx controls (including the accompanying HCHO control) for the SEMI region. This is mainly because the VOC controls have larger impact on reducing ozone concentrations at the SEMI ozone nonattainment sites according to the experiment results. At the same time, the experiment also indicated that the combination of VOC and NOx controls would enhance each other's impact on ozone reduction.

Section 7: Conclusions

The Georgia Tech team conducted high spatial resolution simulations of current (2016) and future (2023) year air quality in the SEMI region to evaluate emissions control strategies for mitigating surface ozone exceedances. We used the Comprehensive Air Quality Model with Extensions (CAMx, Ramboll, 2021) version 7.10 to conduct the ozone simulations for the 2016 ozone season (April 12 -September 25) on a 1.3-km horizontal resolution grid covering the entire SEMI region. The results from this study can assist the Michigan Department of Environment, Great Lakes, and Energy (Michigan EGLE) in demonstrating attainment of the 2015 O_3 NAAQS for the SEMI nonattainment area, i.e., the Detroit, MI NAA.

We improved the modeling inventories for the base year by incorporating the addition of undercounted formaldehyde (HCHO) emissions and volatile chemical product (VCP) VOC emissions, and by switching to the alternative biogenic emissions using the MEGAN program instead of BEIS3. Utilizing the updated emissions inventories, we conducted nine sensitivity tests for the base year 2016 to investigate the effect of improvements to the emissions inventory, specifically the enhancements of HCHO and VCP VOC emissions, on model performance.

The performance evaluation indicated that we should include additional HCHO emissions for the optimal base year simulation. We included the addition of VCP VOCs in the optimal configuration as well mainly for its better performance for MDA8 O_3 larger than 60 ppb, but one should keep in mind that the addition of VCP VOC emissions worsened the performance of VCP-related VOC species such as TOL and XYL at monitoring locations. The performance evaluation doesn't support the switch to the MEGAN biogenic emissions for the region, mainly due to the simulated lower O_3 levels and worsened performance of isoprene (using the default 2013 LAIv) or excessive terpene emissions (using the GLASS 2016 LAIv).

The performance evaluation also demonstrated that the optimal 1.3-km resolution ozone simulation of the SEMI region for the base year 2016 is acceptable to the US EPA based on model performance statistics.

We further prepared the future year base emissions for the 2023 on-the-book (OTB) simulation and the emissions-controlled inventories for control strategy assessment. We conducted four ozone season future year simulations to assess different emissions control scenarios. These four modeling experiments are aimed to assess impacts on projected future year ozone design values from 1) VOC emissions reductions resulting from Reasonably Available Control Technologies (RACT), especially those that reduce VCP VOC emissions from non-EGU point sources and Ozone Transport Commission (OTC)-derived rules for Architectural and Industrial Maintenance (AIM) coatings and Consumer and Commercial Products to reduce VOC emissions from non-point VCPs, 2) NOx emissions reductions resulting from Good Neighbor-like NOx RACT on non-EGU point sources, 3) the elimination of HCHO emissions from all stationary engines due to the adoption of oxycat or other controls in addition to any NOx emissions reductions obtained from the NOx RACT on the same engines at non-EGU point sources, and 4) NOx and VOC emissions reductions from the above NOx and VOC control strategies combined together. The results of experiments here in combination with the optimal base year simulation and the future year OTB simulation were then used to investigate the proposed control scenarios' impacts on projected future year design value (FDV), which can assist demonstration of modeled attainment of ozone NAAQS.

Among the ten sites in the Detroit, MI NAA, the 2016-2018 DV at four sites are in nonattainment of the 2015 ozone NAAQS. Among the four sites, the East 7 Mile site has the highest DVC at 74 ppb. With on-the-book controls applied, the projected DVFs are all in attainment of the NAAQS at under 71 ppb, except the East 7 Mile site which is still at 71.8 ppb. At the East 7 Mile site, the proposed VOC controls would further bring the 2023 DVF down by 0.3 ppb, while the proposed NOx controls would only bring the DVF down by 0.093 ppb, and the HCHO controls would decrease the DVF by 0.068 ppb, which however are approximately four times more effective than the NOx controls based on ppb ozone per ton of emissions reduction.

Based on the assessment results we recommend VOC controls combined with NOx controls (including the accompanying HCHO control as well) for the SEMI region. This is mainly because the VOC controls have larger impact on reducing ozone concentrations at the SEMI ozone nonattainment sites according to the experiments. At the same time, the experiment results also indicated that the combination of VOC and NOx controls would enhance each other's impact on ozone reduction.

Section 8: Data and Documentation Archive

We packed all the data and documents for this project on an external hard drive for product delivery. We also made a copy of the data and documents for our internal archive for the project. The delivery and the archived data both include all the model inputs, outputs, scripts, postprocessed data, tile plots, animations, time series plot and scatted plots, analysis datasheets etc., plus presentations and the final report. Among the model inputs and outputs, only the emissions files are zipped, the meteorology and air quality data are not. The delivery drive is labeled properly with a list of its contents inserted in the package.

An electronic Docket is available for accessing this final report conveniently:

http://semap.ce.gatech.edu/LADCO/SEMI_Modeling_Final_Report.pdf

Appendix A. References

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