Final Report
Comprehensive Air Quality Model with extensions (CAMx) inputs to Community Model for Air Quality (CMAQ) Inputs Converter

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1.0 INTRODUCTION

The Texas Commission on Environmental Quality (TCEQ) uses the Comprehensive Air Quality Model with Extensions (CAMx) for Ozone State Implementation Plan (SIP) modeling. Other researchers use the Community Multi-scale Air Quality (CMAQ) model and wish to use the best available emissions data for Texas, specifically those developed by TCEQ. The emission inputs to CAMx and CMAQ are not directly compatible. Providing the modeling community with an easier path to use Texas' emission inventory data will encourage all researchers and others conducting photochemical modeling to use TCEQ emissions. This will in turn make it much easier for TCEQ staff to understand and interpret research reports, incorporate new developments into TCEQ's modeling system, and ultimately lead to more robust conclusions that are based on the best available input data. The purpose of this project is to provide TCEQ with procedures and computer code for converting TCEQ's CAMx modeling files into a format that can be input to CMAQ.

Both CAMx and CMAQ models require emissions, meteorology, and initial and boundary condition (IC/BC) data as inputs. CAMx uses the *Urban Airshed Model (UAM)*-compatible format whereas CMAQ uses the hybrid Network Common Data Form- *Input/Output Applications Programming Interface (netCDF-I/O API*) file format. The CAMx User's Guide, available at the following web site: http://camx.com/files/camxusersguide_v6-00.pdf contains specifications of the CAMx input format. The CMAQ I/O API data structure is available in its operation guidance (UNC, 2012). Although the formats are different, the data contents are similar. Since CAMx emissions and IC/BC inputs carry all information necessary for CMAQ, converting CAMx modeling files for CMAQ is achievable. However, CMAQ requires extra meteorology input parameters (e.g., planetary boundary layer) from those available in CAMx meteorological inputs, so it is necessary that CMAQ meteorology inputs be prepared separately using the Meteorology-Chemistry Interface Processor (MCIP) distributed with CMAQ.

A suite of computer software that converts CAMx emissions and IC/BC modeling files into CMAQ format were developed (*hereinafter* referred to as CAMx-to-CMAQ converters) as described in Section 2 and 3 of this report. A complete CMAQ test case modeling database was constructed and a 13-day CMAQ simulation was run to test that the CMAQ inputs were generated correctly. The test case was built off the TCEQ's Rider 8 CAMx modeling database. The CMAQ results are presented and discussed in Section 4 and conclusions and recommendations are presented in Section 5.

2.0 CAMx TO CMAQ EMISSIONS CONVERTER

We developed computer software to convert CAMx format emissions files into CMAQ format emissions files. We tested the software by running a test case using the Rider 8 CAMx emissions files and inspecting the outputs to ensure a correct conversion. This section documents the capabilities of the software and presents results from the Quality Assurance (QA) tests that were performed to ensure that the software is converting the CAMx emissions files correctly. The QA tests were designed to focus on each specific step in the overall conversion process.

2.1 Software Overview

There are two types of emission files that CAMx and CMAQ use. The two-dimensional emissions file contains gridded fields of low-level (i.e., surface) emission rates for all emitted species to be modeled. The elevated point source emissions file contains emission rates for all elevated point sources, and for all emitted species, to be modeled. The CAMx elevated point source emissions file also contains stack parameters. CMAQ requires a separate stack groups file that identifies elevated source locations and stack parameters. We developed a suite of programs (called modules) that convert CAMx emission modeling files for CMAQ. Each module is responsible for carrying out one of the tasks (such as CAMx to CMAQ model species mapping and time-zone shifting). Module structure of the emission converter is illustrated in Figure 2-1.

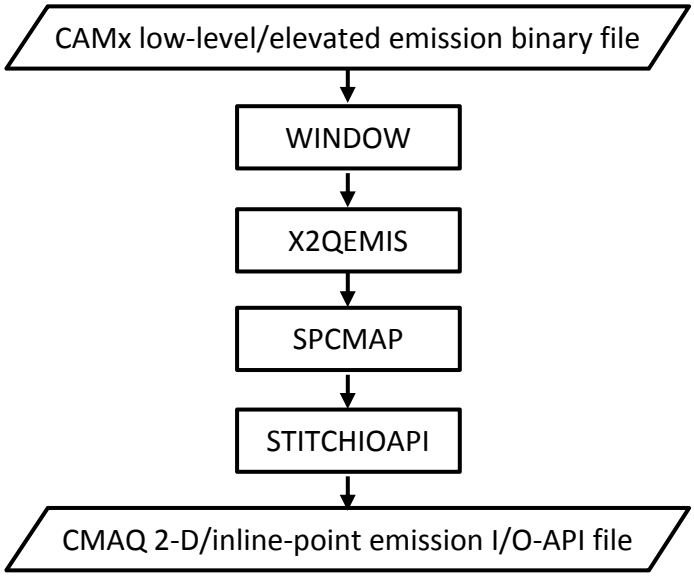


Figure 2-1. CAMx-to-CMAQ emission converter module structure

The functionality of each emission converter module is described below:

WINDOW

- Resize domain based on user-supplied information (e.g., exclude CAMx buffer cells)
- Disaggregate emissions to finer grid resolution as specified by user

X2QEMIS

- Convert from CAMx low-level/elevated emission binary file to CMAQ 2-D/inline-point emission I/O-API file
- Insert map projection parameters for the CMAQ file header based on user-supplied information
- Shift time zone from local time to UTC for CMAQ if needed
- Convert units from CAMx (per-hour emission rate) to CMAQ (per-second emission rate)
- Include special treatment for point sources with pre-calculated plume rise (e.g., fire emissions)

SPCMAP

- Map CAMx species to CMAQ (e.g., downgrade CB6 to CB05, map CAMx PM species to their CMAQ PM equivalents)

STITCHIOAPI

- Append an additional hour of emission data to store 25 hourly records in a daily emission file (CMAQ convention)
- Stitch multiple time-zone-shifted emission files into a midnight-to-midnight (in UTC) daily file

2.2 Software Capability

The specific conversion steps that are performed by the software are listed below. Each step was tested by comparing the CAMx emissions file and the resulting CMAQ emissions by explicitly focusing on that step.

- Temporal Conversion
  - Time zone shift
  - Include 25 hours per day (required by CMAQ, as opposed to 24 hours per day in CAMx input files)
- Chemical Species and Unit Conversions
  - Unit conversions from moles/hour for CAMx to moles/second for CMAQ for aerosol species
  - Species mapping (e.g., downgrade Carbon Bond 6 (CB6) to CB05, map CAMx Particulate Matter (PM) to its CMAQ PM equivalent
- Surface Level Emission – Spatial Grid Options
  - Resize domain based on user-supplied information (e.g., exclude CAMx buffer cells)
  - Disaggregate emissions to finer grid resolution as specified by user
- Point Source Emissions – Stack Options

- Retain CAMx point sources as CMAQ in-line point sources (point sources with dynamically calculated plume-rise)
- Set zero exit velocity for point sources with pre-calculated plume rise (e.g., fire)

- Emissions File Header Conversion
  - CAMx version 6.0 and later uses updated file headers that include additional meta data, such as map projection, grid specifications, time zone, and various field-specific flags. These meta data are needed by CMAQ. The converter is capable of handling the updated headers and the older headers used in previous versions of CAMx.

2.3 Quality Assurance

2.3.1 Temporal Conversion

CAMx supports the option to perform model simulations in different time zones, and often the emissions are prepared and CAMx is run using Local Standard Time (LST). In contrast CMAQ is always run using UTC. Therefore the conversion software has the capability to convert from an arbitrary time zone to UTC for CMAQ. The CAMx Rider8 emissions files were prepared in Central Standard Time (CST) for Texas, as shown in Table 2-1.

Table 2-1. Settings from CAMx control file for Rider8 Simulation.

```
!--- Model clock control ---
 Time_Zone = 6, ! (0=UTC,5=EST,6=CST,7=MST,8=PST)
Start_Date_Hour = 2006,06,03,0000, ! (YYYY,MM,DD,HHHH)
 End_Date_Hour = 2006,06,03,2400, ! (YYYY,MM,DD,HHHH)
Emiss_Grid(1) = '/model/input/tx/ei/bl06_06jun/reg2f/camx_cb6p_ei_lo.20060603.tx.bl06_06jun.reg2f.rpo_36km',
```

The figures in Figure 2-2 show VERDI visualizations of the time series of NO averaged across the entire 36 km modeling domain. The upper figure shows the CAMx surface level emissions in CST, and the lower figure presents the CMAQ surface level emissions shifted to UTC, both for June 3, 2006. Also, note that the CAMx emissions are 24 hours and the CMAQ emissions span 25 time periods. Note that VERDI incorrectly reports the units for the CAMx emissions as the VERDI default units of PPM instead of moles/hour, since the CAMx file does not include unit information in the header. The CAMx units should be interpreted as moles/hour instead of PPM. The CMAQ emissions are correctly interpreted by VERDI as moles/second.

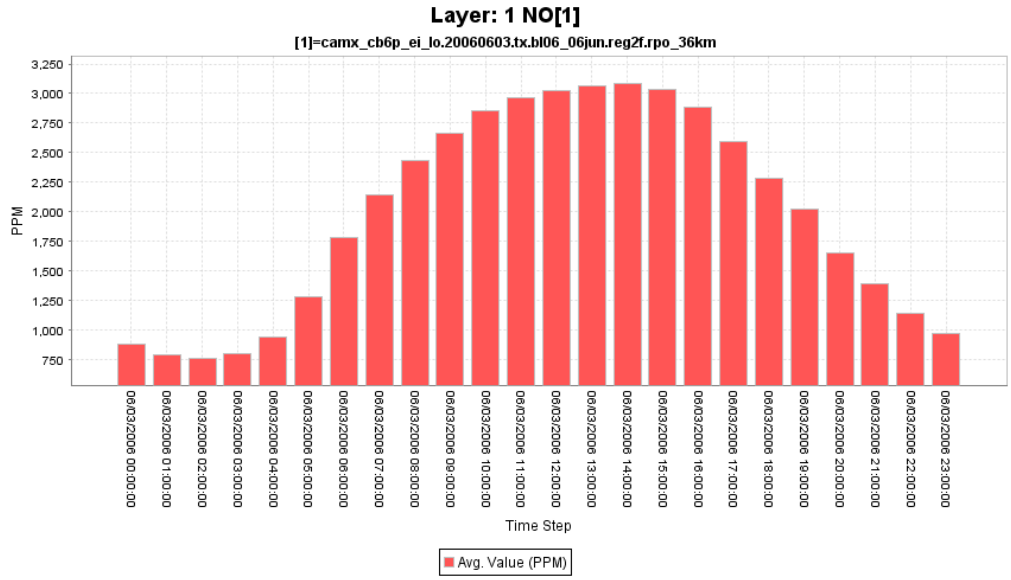
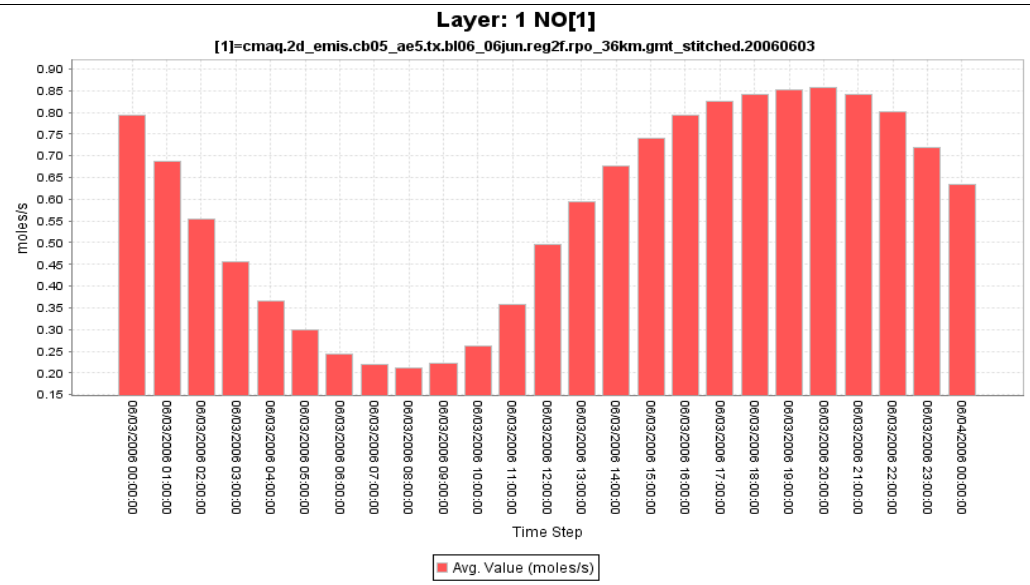
CAMx in CST **(= UTC - 6 hrs)**	
CMAQ in UTC	

Figure 2-2. VERDI visualization showing input CAMx-format and output CMAQ-format as time series bar plots. Average grid cell NO emission rate over the 36km domain.

2.3.2 Chemical Species and Unit Conversion

CAMx emission rate units are mol/time unit for gases and grams/time unit for aerosols. The emission time unit is typically, but not necessarily, one hour. The time interval of the emissions record matches the input frequency of the emissions as specified in the CAMx.in control file. For the Rider8 test case the time unit interval is one hour. CMAQ emissions are given in moles /second therefore the CAMx emissions were divided by 3600 to convert from an hourly emission rate to emissions every second. The color bar and maximum value of emissions in the

spatial plots presented in Figure 2-3 show that the unit conversion has been successfully applied when converting from CAMx to CMAQ.

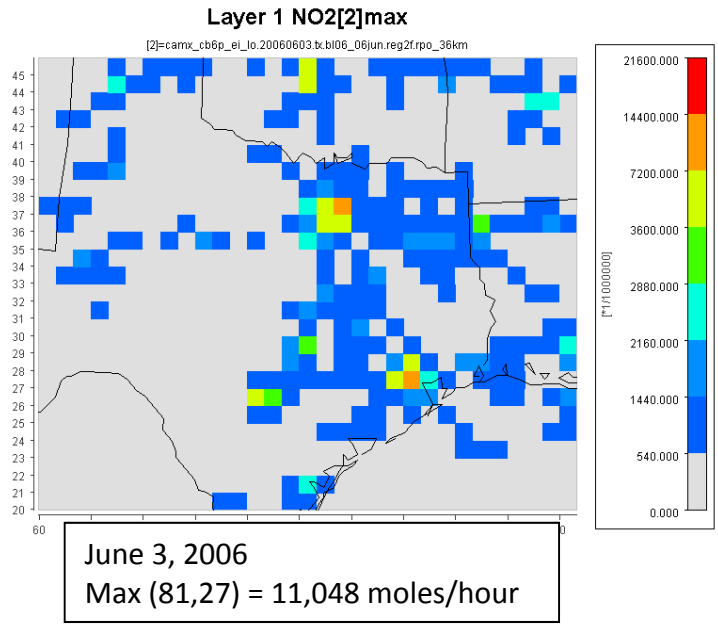
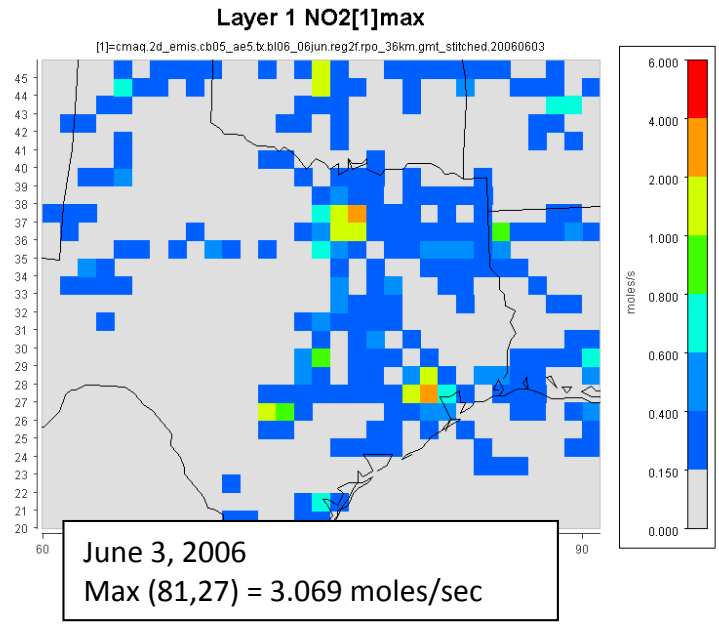
CAMx	
CMAQ	

Figure 2-3. VERDI spatial plot showing unit conversion for matched time zone for NO_2.

The CAMx to CMAQ species mapping for the species that are included in the Rider 8 emissions is shown in Table 2-2.

Table 2-2. CAMx to CMAQ species mapping. Species with different name conventions and/or non 1-to-1 mapping are highlighted in red.

CAMx Species and Mapping Factors	CMAQ Species
1 * ALD2 --->	ALD2
1 * ALDX --->	ALDX
1 * BENZ --->	BENZENE
1 * CO --->	CO
1 * ETH --->	ETH
1 * ETHA --->	ETHA
1 * ETOH --->	ETOH
1 * FORM --->	FORM
1 * HONO --->	HONO
1 * IOLE --->	IOLE
1 * ISOP --->	ISOP
1 * MEOH --->	MEOH
1 * NO --->	NO
1 * NO2 --->	NO2
1 * OLE --->	OLE
1 * PAR + 3 * ACET + 1 * BENZ + 1 * ETHY + 1 * KET + 1.5 * PRPA --->	PAR
1 * SO2 --->	SO2
1 * TERP --->	TERP
1 * TOL --->	TOL
1 * XYL --->	XYL
1 * NH3 --->	NH3
1 * NR + 5 * BENZ + 1.5 * PRPA --->	NR
1 * CH4 + 1 * ECH4 --->	CH4
1 * PSO4 --->	PSO4
1 * PNO3 --->	PNO3
1 * POA --->	POC
1 * PEC --->	PEC
1 * FPRM --->	PMFINE

To ensure the species mapping is functioning correctly for all species, an input Rider 8 CAMx emissions file and CMAQ output format emissions file were inspected for all species on a single grid cell and for a single hour. The corresponding hours were selected after accounting for the time zone shift. The CAMx and CMAQ emissions rates on grid cell i=81, j=27 of the 36km domain, at hour = 1am for CAMx, and at hour = 7am for CMAQ of the 36km domain, on June 3,

2006 are shown in Table 2-3. After applying the unit conversion and mapping shown in Table 2-2, the results are in agreement to 3 decimal places as shown in the last column of Table 2-3.

Table 2-3. Table showing emissions rates on grid cell i=81, j=27 at CAMx hour = 1am, and CMAQ hour = 7am, with conversion factors and differences.

CMAQ Species Name	Extracted CMAQ emissions	Mapping from CAMx Species	CAMx Species Name	Extracted CAMx Emissions	Unit Conversion Factor	Calculated CAMx emissions converted to moles/sec	QA Difference: (CMAQ-CAMX)/CMAQ
ALD2	2.26E-01	= 1 * ALD2	ALD2	8.15E+02	3600	2.26E-01	0.0002
ALDX	1.07E-01	= 1 * ALDX	ALDX	3.85E+02	3600	1.07E-01	-0.0004
BENZENE	2.28E-01	= 1 * BENZ	BENZ	8.19E+02	3600	2.28E-01	0.0000
CO	9.19E+01	= 1 * CO	CO	3.31E+05	3600	9.19E+01	0.0001
ETH	7.59E-01	= 1 * ETH	ETH	2.73E+03	3600	7.59E-01	-0.0001
ETHA	9.12E-01	= 1 * ETHA	ETHA	3.28E+03	3600	9.12E-01	0.0000
ETOH	3.02E-01	= 1 * ETOH	ETOH	1.09E+03	3600	3.02E-01	-0.0002
FORM	5.10E-01	= 1 * FORM	FORM	1.84E+03	3600	5.10E-01	0.0000
HONO	3.71E-02	= 1 * HONO	HONO	1.34E+02	3600	3.71E-02	0.0000
IOLE	3.50E-01	= 1 * IOLE	IOLE	1.26E+03	3600	3.50E-01	0.0003
ISOP	1.30E-02	= 1 * ISOP	ISOP	4.69E+01	3600	1.30E-02	-0.0003
MEOH	3.30E-01	= 1 * MEOH	MEOH	1.19E+03	3600	3.30E-01	-0.0003
NO	8.14E+00	= 1 * NO	NO	2.93E+04	3600	8.14E+00	-0.0001
NO2	7.76E-01	= 1 * NO2	NO2	2.80E+03	3600	7.76E-01	-0.0001
OLE	8.13E-01	= 1 * OLE	OLE	2.93E+03	3600	8.13E-01	0.0000
SO2	9.52E-01	= 1 * SO2	SO2	3.43E+03	3600	9.52E-01	0.0000
TERP	1.71E-01	= 1 * TERP	TERP	6.15E+02	3600	1.71E-01	0.0001
TOL	6.04E-01	= 1 * TOL	TOL	2.18E+03	3600	6.04E-01	-0.0001
XYL	3.94E-01	= 1 * XYL	XYL	1.42E+03	3600	3.94E-01	0.0002
NH3	3.06E+00	= 1 * NH3	NH3	1.10E+04	3600	3.06E+00	-0.0004
PSO4	1.32E+00	= 1 * PSO4	PSO4	4.76E+03	3600	1.32E+00	0.0001
PNO3	1.70E-01	= 1 * PNO3	PNO3	6.11E+02	3600	1.70E-01	0.0000
POC	2.45E+01	= 1 * POA	POA	8.84E+04	3600	2.45E+01	-0.0002
PEC	1.17E+01	= 1 * PEC	PEC	4.22E+04	3600	1.17E+01	-0.0003
PMFINE	7.68E+00	= 1 * FPRM	FPRM	2.76E+04	3600	7.68E+00	0.0001
PAR	3.68E+01	= 1 * PAR + 3 * ACET + 1 * BENZ + 1 * ETHY + 1 * KET + 1.5 * PRPA	-	132629.6	3600	3.68E+01	-0.0003
NR	2.12E+00	= 1 * PAR + 3 * ACET + 1 * BENZ + 1 * ETHY + 1 * KET + 1.5 * PRPA	-	7637	3600	2.12E+00	-0.0002
CH4	1.33E+02	= 1 * CH4 + 1 * ECH4	-	4.77E+05	3600	1.33E+02	-0.0001

2.3.3 Surface Level Emissions - Spatial Grid Options

The CAMx2CMAQ tool has the ability to window out a smaller domain from the CAMx domain and also to change the grid cell size. Grid cells can be aggregated to make a coarser grid or disaggregated to a finer grid cell size. For a finer grid cell size emissions will be uniform on all grid cells that originate from the same CAMx grid cell. As a test case, the Houston region of the CAMx 4km domain Rider8 surface level emissions file for June 3 2006 was windowed out and disaggregated to 2km resolution, based on the input variable settings in CAMx2CMAQ shown in Table 2-4.

Table 2-4. CAMx2CMAQ variable settings to window out a domain and decrease grid cell size.

```
set CONVERT_DOMAIN_GRID = Y
set BEG_COL_INDEX = 105
set END_COL_INDEX = 159
set BEG_ROW_INDEX = 55
set END_ROW_INDEX = 118
set MESH_FACTOR = 0.5
```

For the results of this test case comparison see the plots in Figure 2-4. The upper figure shows the daily maximum SO_2 CAMx emissions rate on June 3, 2006 on each grid cell in the entire Rider8 4km CAMx domain. The lower figure shows the daily maximum SO_2 CMAQ emission rate on the same day on each grid cell in the windowed out domain (around Houston), that were disaggregated to 2 km grid cell resolution. Note the maximum CAMx emissions rate around Houston on that day was 379 moles/hour/4km^2 grid cell, and the maximum CMAQ emissions rate in the same area on the same day was 0.026 moles/sec/2km^2 grid cell, which agrees with the CAMx emission rate to 2 significant digits. Note also that the CMAQ emissions are defined on a windowed out grid with new i/j cell definition, as shown on the x and y axes of the figure.

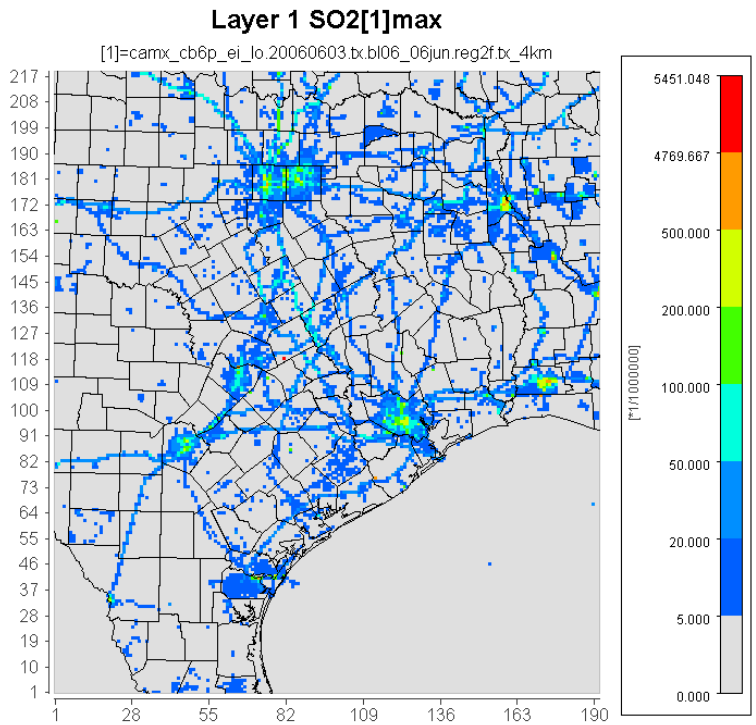
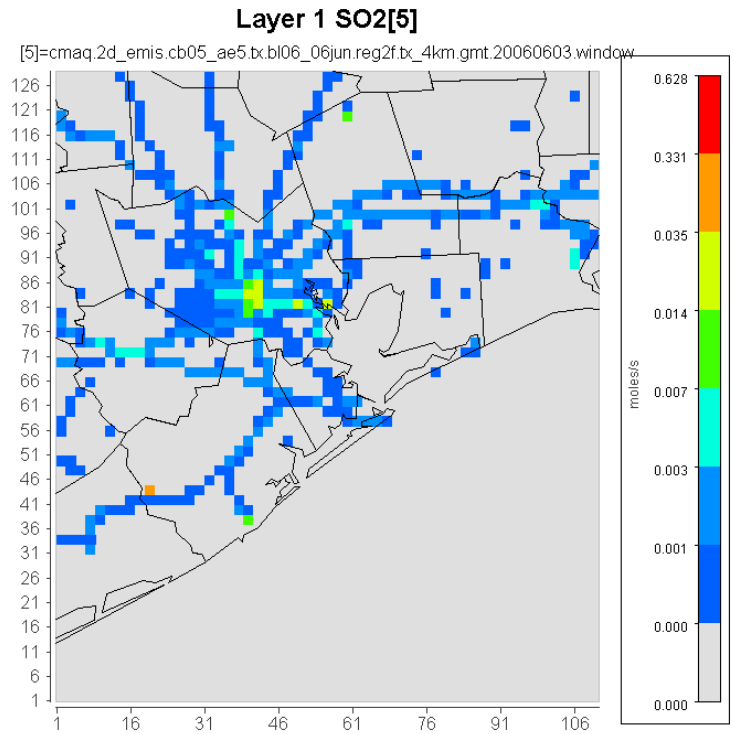
CAMx: **4km Rider8 File** **Maximum in Houston** **Area =** **379 moles/hr** **(per 4 km grid cell)**	
CMAQ: **Windowed out Houston area from 4km Rider8 file, disaggregated to 2 km grid cell resolution.** **Maximum in Houston Area =** **0.026 moles/sec (per 2 km grid cell).** Note: 0.026 mol/sec/2km^2 x 3600 sec/hr x 4 (=# 2km gridcells in 1 4km gridcell) = 374.4 moles/hr/4km^2	

Figure 2-4. Comparison of 4km CAMx grid cells and windowed 2 km CMAQ grid cells.

2.3.4 Point Source Emissions - Stack Options

2.3.4.1 Point Source Stack Parameter Inspection

To ensure the correct treatment was applied to the point source files, 6 stacks were selected from the 89,094 stacks in the Rider 8 files for close inspection. Stacks parameters for stacks listed with stack numbers: 1, 2, 3, 89092, 89093 and 89094 were chosen. Tools were used to convert the CAMx point source emissions binary file and the CMAQ point source emissions binary stack file to an ascii format so the stack parameters could be compared.

The CAMx stack parameters are shown in Table 2-5, and the corresponding CMAQ stack parameters are shown in Table 2-6. The stack X and Y coordinates, diameter, and temperature are identical in the CAMx and CMAQ files. For some stacks, the CAMx plume height is a negative value, the negative value is a flag used in CAMx to indicate that the internal plume rise calculation should be bypassed (e.g., for fires with pre-estimated plume height). For stacks without the plume height CAMx flag (i.e., stacks 1, 2, and 3), the CAMx plume height and the CMAQ stack height are the same, and velocity difference between CAMx and CMAQ are attributable to the different velocity units (meters/hour vs meters/second). For stacks with the plume height CAMx flag, (i.e., stacks 89092, 89093, and 89094), the CMAQ height is the absolute value of the CAMx plume height, and the velocity for those stacks was set to zero in order that the CMAQ internal plume rise calculation would calculate no additional plume rise.

Table 2-5. CAMX point source stack parameters inspection.

CAMx						
stk#	**xstk**	**ystk**	**diameter***	**temp**	**velocity**	**plume height****
	meters	meters	Meters	Kelvin	meters/hour	meters
skt1	133283.5	-1167476	-9.93E+00	4.08E+02	4.55E+04	1.52E+02
stk2	133637.3	-1166509	-7.26E+00	4.18E+02	1.46E+04	5.60E+01
stk3	133143	-1167232	-1.03E+01	4.08E+02	4.66E+04	1.83E+02
…	…	…	…	…	…	…
stk89092	-990000	-2034000	1.00E+00	1.00E+00	1.00E+00	-5.94E+01
skt89093	-990000	-1998000	1.00E+00	1.00E+00	1.00E+00	-5.94E+01
stk89094	-954000	-1926000	1.00E+00	1.00E+00	1.00E+00	-5.94E+01

* negative diameter is a CAMx flag for PiG function

** negative plume height is a CAMx flag to indicate no internal plume rise calculation should be performed

Table 2-6. CMAQ point source stack parameters inspection.

CMAQ						
stk#	**STKDM =**	**STKHT =**	**STKTK =**	**STKVE =**	**XLOCA =**	**YLOCA =**
	meters	meters	Kelvin	meters/sec	meters	meters
skt1	9.926	152	408.0	12.7	133283.5	-1167476
stk2	7.258	56	417.7	4.1	133637.2	-1166509
stk3	10.348	183	408.0	13.0	133143	-1167232
…	…	…	…	…	…	…
stk89092	1	59.4	1	0	-990000	-2034000
skt89093	1	59.4	1	0	-990000	-1998000
stk89094	1	59.4	1	0	-954000	-1926000

2.3.4.2 Point Source Total Emissions

An additional QA measure for the point source conversion routine that checked the preservation of total emissions was performed. The CAMx point source emissions file was converted to a gridded format viewable in VERDI, with all point sources within a single grid cell being assigned to and summed on that grid cell. The VERDI-generated time-series plot showing the average grid cell value of CH4 is presented in Figure 2-5. The emissions are highest at time step t = 14:00, with CH4 = 95.18 moles/hour. This corresponds to a total domain-wide CH4 of 1,577,704 moles/hour (=148 x 112 x 95.18). The CMAQ point file was directly loaded into VERDI since VERDI has the capability of viewing CMAQ inline point source files. For these files, a correct spatial representation is not possible, and each stack is treated as a single "grid cell". The time series of CMAQ CH4 is shown in the lower figure of Figure 2-5. The Central Standard Time to UTC time zone shift is apparent, as well as the additional 25th hour of emissions for CMAQ compared to CAMx. The daily peak emissions rate occurs at 20:00, and is 0.00491 moles/second on the average "grid cell". For CMAQ, the total emissions at that maximum time period are 437.5 moles/second (= 89094 stacks x 0.00491), which is equivalent to the CAMx emissions rate of 1,577,704 moles/hour, to 3 significant digits.

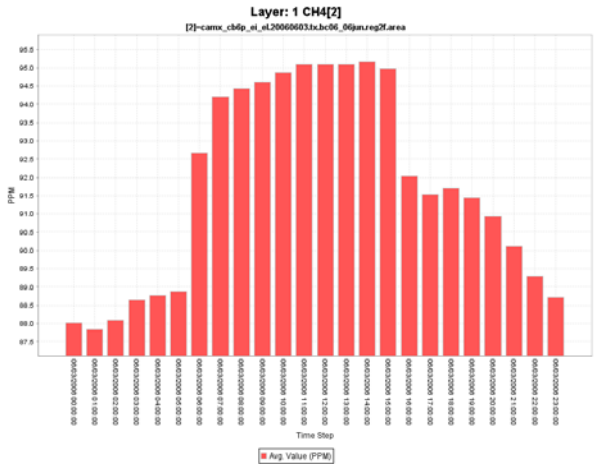
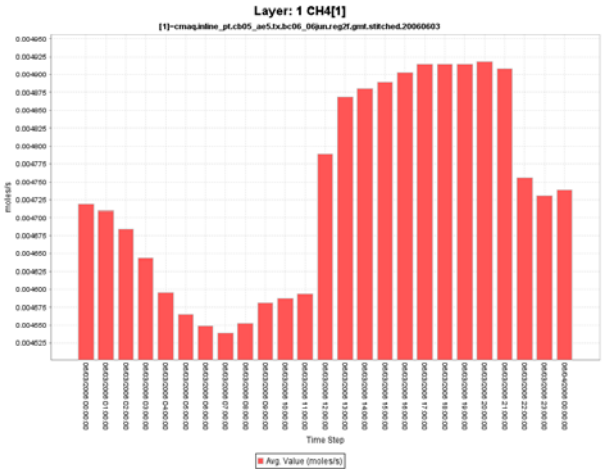
CAMx Max hour = 14:00, CH4 point emis rate = 95.18 moles /hr on average grid cell	
CMAQ Max hour = 20:00, CH4 point emis rate = 0.00491 moles/sec on average "grid cell"	

Figure 2-5. CAMx and CMAQ emission from all stacks.

3.0 CAMx TO CMAQ IC/BC CONVERTER

This section documents the capabilities of the software to format initial and boundary conditions (IC/BCs) and presents results from the Quality Assurance (QA) tests that were performed to ensure that the software is converting the CAMx BC/IC files correctly.

3.1 Software Overview

The BC files contain gridded and time-dependent concentration fields on the lateral faces of the master grid boundary. The IC file contains gridded concentration fields on the master grid at the starting simulation hour. A suite of programs (called modules) that convert CAMx IC/BC modeling files for CMAQ was developed similarly to the emissions converter. Module structure of the IC/BC converter is illustrated in Figure 3-1.

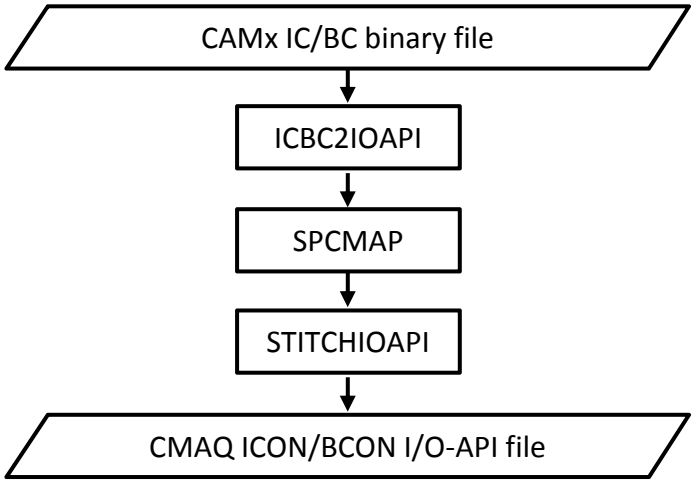


Figure 3-1. CAMx-to-CMAQ IC/BC converter module structure.

The functionality of each IC/BC converter module is described below:

ICBC2IOAPI

- Convert from the CAMx IC/BC binary file to the CMAQ ICON/BCON I/O-API file
- Insert map projection and vertical grid structure parameters for the CMAQ file header based on user-supplied information
- Shift time zone from local time to UTC for CMAQ if needed
- Add aerosol number and surface area concentration data for CMAQ based on the CMAQ pre-defined profile data

SPCMAP

- Map CAMx species to CMAQ (e.g., downgrade CB6 to CB05, map CAMx PM species to their CMAQ PM equivalents)

STITCHIOAPI

- Append additional hours of BC data to store 26 hourly records in a daily BC file

- Stitch multiple time-zone-shifted BC files into a midnight-to-midnight (in UTC) daily file

CAMx input file formats are explained in more detail in the CAMx User's Guide (ENVIRON, 2014) and CMAQ input file formats are explained in the CMAQ operation guidance (UNC, 2012)

3.1.1 Software Capabilities

The major conversion steps that are performed by the software are listed below. Each step was tested by comparing the CAMx IC/BC file and the resulting CMAQ IC/BC by explicitly focusing on that step.

- Temporal Conversion (for BCs only)
  - Time zone shift
  - Include 26 hours per day (as opposed to 24 hours per day in CAMx input files)
- Chemical Species
  - Species mapping (e.g., downgrade Carbon Bond 6 (CB6) to CB05, map CAMx Particulate Matter (PM) to its CMAQ PM equivalent
  - Add additional CMAQ species not available in CAMx BC/IC files
- File Header Conversion
  - CAMx version 6.0 and later uses updated file headers that include additional meta data, such as map projection, grid specifications, time zone, and various field-specific flags. These meta data are needed by CMAQ. The converter can handle both the current headers (CAMx6 and later) and the older headers (pre CAMx6).

3.2 Quality Assurance

3.2.1 Temporal Conversion

The CAMx Rider8 BC files were prepared in Central Standard Time (CST) for Texas, as shown in Table 3-1, so they were converted to UTC as required by CMAQ. In addition, each time step of CAMx BCs has concentrations averaged for the time step period while CMAQ uses instantaneous concentrations at the time step. For example, CAMx daily BC files typically have 24 hourly average concentrations (for 0:00-1:00, 1:00-2:00, etc.) while CMAQ daily BC files have 25 instantaneous concentrations at each hour (at 0:00, 1:00, 2:00, etc.). There is no single right way to map the 24 hourly average BCs back to the 25 instantaneous ones. Instead of using interpolation which tends to smooth out peak concentrations, this program simply assigns each average concentration to the mid-point of the time step period. Users need to append BCs of two additional hours (i.e., 23:30 the day before and 0:30 the day after) to cover one day period. This step is done by the STITCHIOAPI module.

Table 3-1. Settings from CAMx control file for Rider8 Simulation.

```
!--- Model clock control ---
 Time_Zone = 6, ! (0=UTC,5=EST,6=CST,7=MST,8=PST)
Start_Date_Hour = 2006,06,03,0000, ! (YYYY,MM,DD,HHHH)
End_Date_Hour = 2006,06,03,2400, ! (YYYY,MM,DD,HHHH)
Boundary_Conditions = '/model/input/tx/bcic/2006/camx_cb6_bc.20060603.geoschem.rpo_36km',
```

Figure 3-2 presents time series of ozone concentrations in grid cell i=65, j=1, and layer=1 of the 36km domain for June 3, 2006. The CMAQ BCs match well with the CAMx BCs but are shifted by half an hour (after shifted to UTC). Also, note that the CAMx BCs are 24 hours and the CMAQ BCs span 26 time periods.

Since ICs are not time-dependent, temporal conversion is not needed. Note that TCEQ's Rider8 IC file was prepared in CST (midnight) for Texas corresponding to 18:00 PM UTC.

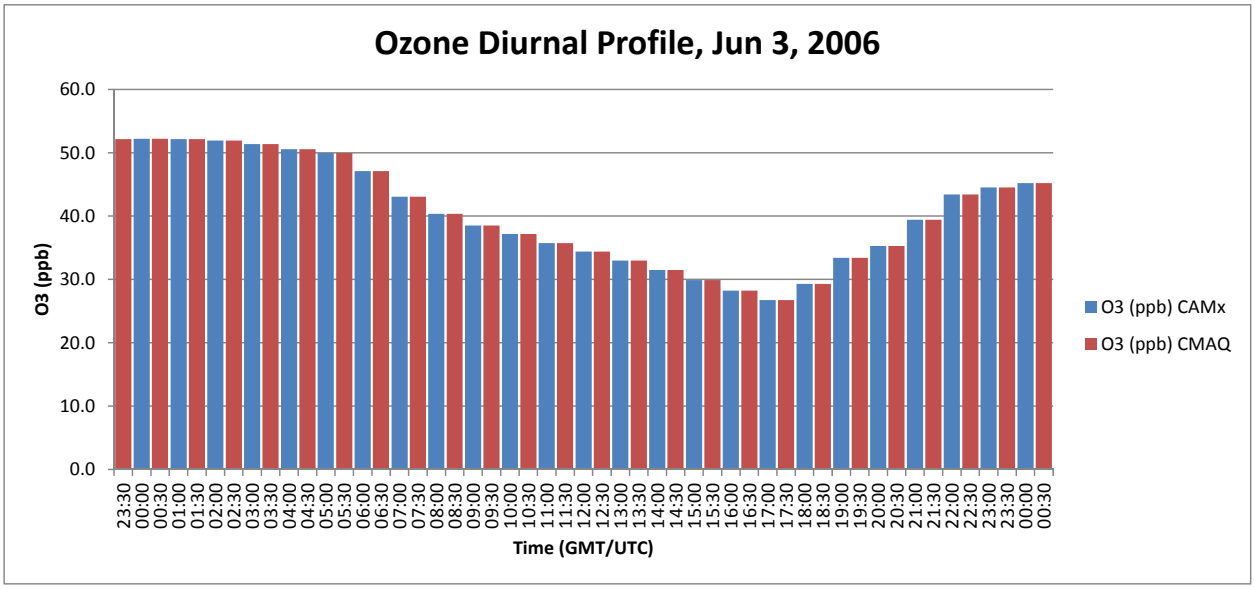


Figure 3-2. Ozone time series bar plot showing input CAMx-format and output CMAQ-format boundary conditions for grid cell i=65, j=1, and layer=1 of the 36km domain for June 3, 2006.

3.2.2 Chemical Species Mapping

The CAMx to CMAQ species mapping for the species that can be found in the IC/BC files are shown in Table 3-2. CMAQ requires additional species (i.e., aerosol number and surface area concentration) that are not available in CAMx IC/BC files, so they are obtained from the CMAQ pre-defined profile data (Table 3-3). Since the CMAQ profile data are only available for six specific sigma layers, the software interpolates this data for other sigma layers.

Table 3-2. CAMx to CMAQ species mapping for IC/BCs. Species with different name conventions and/or non 1-to-1 mapping are highlighted in red.

CAMx species and mapping factors	CMAQ's Default Profile	CMAQ species
1*AACD --->		AACD
1*ALD2 --->		ALD2
1*ALDX --->		ALDX
1*BENZ --->		BENZENE
1*CAT1 --->		CAT1
1*CO --->		CO
1*CRES --->		CRES
1*CRON --->		CRON
1*ETH --->		ETH
1*ETHA --->		ETHA
1*ETOH --->		ETOH
1*FACD --->		FACD
1*FORM --->		FORM
1*H2O2 --->		H2O2
1*HNO3 --->		HNO3
1*HONO --->		HONO
1*IOLE --->		IOLE
1*ISOP --->		ISOP
1*ISPD --->		ISPD
1*MEOH --->		MEOH
1*MEPX --->		MEPX
1*MGLY --->		MGLY
1*N2O5 --->		N2O5
1*NO --->		NO
1*NO2 --->		NO2
1*NO3 --->		NO3
1*NTR + 1*INTR + 1* NTR1 + 1*NTR2 --->		NTR
1*O3 --->		O3
1*OLE --->		OLE
1*OPAN --->		OPAN
1*OPEN --->		OPEN
1*PACD --->		PACD
1*PAN --->		PAN
1*PANX --->		PANX
1*PAR + 3*ACET + 1*BENZ + 1*ETHY + 1*KET + 1.5*PRPA --->		PAR
1*PNA --->		PNA
1*ROOH --->		ROOH
1*SO2 --->		SO2
1*SULF --->		SULF
1*TERP --->		TERP
1*TOL --->		TOL
1*XYL --->		XYL
1*NH3 --->		NH3
1*HCL --->		HCL
1*SQT --->		SESQ
0.5*CG1 --->		SV_TOL1
0.5*CG1 --->		SV_XYL1

CAMx species and mapping factors	CMAQ's Default Profile	CMAQ species
0.5*CG2 --->		SV_TOL2
0.5*CG2 --->		SV_XYL2
1*CG3 --->		SV_ISO2
1*CG4 --->		SV_ISO1
1*CG5 --->		SV_TRP1
1*CG6 --->		SV_TRP2
1*CG7 --->		SV_SQT
1*NR + 5*BENZ + 1.5*PRPA --->		NR
1*CL2 --->		CL2
1*CH4 + 1*ECH4 --->		CH4
1*HG0 --->		HG
1*HG2 --->		HGIIGAS
1*PSO4 --->		ASO4J
1*PNO3 --->		ANO3J
1*PNH4 --->		ANH4J
1*POA --->		AORGPAJ
1*PEC --->		AECJ
0.5*SOA1 --->		ATOL1J
0.5*SOA1 --->		AXYL1J
0.5*SOA2 --->		ATOL2J
0.5*SOA2 --->		AXYL2J
1*SOA3 --->		AISO2J
1*SOA4 --->		AISO1J
1*SOA5 --->		ATRP1J
1*SOA6 --->		ATRP2J
1*SOA7 --->		ASQTJ
1*SOPA --->		AOLGAJ
1*SOPB --->		AOLGBJ
1*NA --->		ANAJ
1*PCL --->		ACLJ
1*FPRM + 1*FCRS --->		A25J
1*CPRM --->		ACORS
1*CCRS --->		ASOIL
1*HGP --->		APHGJ
	1*NUMATKN --->	NUMATKN
	1*NUMACC --->	NUMACC
	1*NUMCOR --->	NUMCOR
	1*SRFATKN --->	SRFATKN
	1*SRFACC --->	SRFACC
	1*SRFCOR --->	SRFCOR

Table 3-3. CMAQ's default profile data for number and surface area concentrations.

Specie	Sigma Layer					
	0.98	0.93	0.84	0.6	0.3	0
NUMATKN	1.478E+09	1.470E+09	9.774E+08	9.655E+08	1.920E+08	9.584E+07
NUMACC	3.706E+08	3.412E+08	2.161E+08	1.693E+08	2.957E+07	1.416E+07
NUMCOR	2.350E+04	1.626E+04	6.338E+03	1.162E+03	2.025E+02	2.000E+02
SRFATKN	8.153E-07	8.112E-07	5.393E-07	5.327E-07	1.059E-07	5.288E-08
SRFACC	1.491E-05	1.373E-05	8.694E-06	6.815E-06	1.190E-06	5.697E-07
SRFCOR	2.640E-07	2.100E-07	1.160E-07	3.860E-08	8.530E-09	8.490E-09

To QA the species mapping for all species a set of Rider 8 CAMx IC/BC files was converted to CMAQ format IC/BC files and inspected for all species at a single grid cell and for a single hour (accounting for the time zone shift). The CAMx and CMAQ ICs on grid cell i=75, j=25, layer=1 of the 36km domain are shown in Table 3-4. The CAMx and CMAQ BCs on grid cell i=65, j=1, layer=1 of the 36km domain, at hour = 18pm on June 2 for CAMx, and at hour = 0:30am on June 3 for CMAQ, are shown in Table 3-5. After applying the mapping shown in Table 3-2, the results for both IC and BC are in agreement as shown in the last column of Table 3-4 and 3-5, respectively.

Table 3-4. Table showing CAMx and CMAQ ICs on grid cell i=75, j=25, layer =1 for June 3, 2006.

CMAQ Species Name	Extracted CMAQ ICs	Mapping from CAMx Species (or default profile)	Extracted CAMx ICs	QA Difference: (CMAQ-CAMX)/CMAQ
ALD2	7.13E-05	= 1*ALD2	7.13E-05	0.0000
ALDX	2.01E-05	= 1*ALDX	2.01E-05	0.0000
BENZENE	3.59E-05	= 1*BENZ	3.59E-05	0.0000
CO	1.19E-01	= 1*CO	1.19E-01	0.0000
ETHA	6.71E-04	= 1*ETHA	6.71E-04	0.0000
FORM	1.27E-03	= 1*FORM	1.27E-03	0.0000
H2O2	1.92E-03	= 1*H2O2	1.92E-03	0.0000
HNO3	3.68E-04	= 1*HNO3	3.68E-04	0.0000
ISOP	2.49E-06	= 1*ISOP	2.49E-06	0.0000
ISPD	1.69E-04	= 1*ISPD	1.69E-04	0.0000
MEPX	7.06E-04	= 1*MEPX	7.06E-04	0.0000
N2O5	6.17E-05	= 1*N2O5	6.17E-05	0.0000
NH3	1.60E-03	= 1*NH3	1.60E-03	0.0000
NO2	2.96E-03	= 1*NO2	2.96E-03	0.0000
NR	4.19E-04	= 1*NR + 5*BENZ + 1.5*PRPA	4.19E-04	0.0000
NTR	1.87E-05	= 1*NTR + 1*INTR + 1* NTR1 + 1*NTR2	1.87E-05	0.0000
O3	3.07E-02	= 1*O3	3.07E-02	0.0000
OLE	1.21E-04	= 1*OLE	1.21E-04	0.0000
PAN	4.90E-05	= 1*PAN	4.90E-05	0.0000
PANX	1.65E-05	= 1*PANX	1.65E-05	0.0000
PAR	8.92E-03	= 1*PAR + 3*ACET + 1*BENZ + 1*ETHY +	8.92E-03	0.0000

CMAQ Species Name	Extracted CMAQ ICs	Mapping from CAMx Species (or default profile)	Extracted CAMx ICs	QA Difference: (CMAQ-CAMX)/CMAQ
		1*KET + 1.5*PRPA		
PNA	1.57E-07	= 1*PNA	1.57E-07	0.0000
SO2	1.43E-03	= 1*SO2	1.43E-03	0.0000
SV_SQT	1.30E-05	= 1*CG7	1.30E-05	0.0000
SV_TRP1	9.69E-05	= 1*CG5	9.69E-05	0.0000
SV_TRP2	9.69E-05	= 1*CG6	9.69E-05	0.0000
TERP	5.48E-05	= 1*TERP	5.48E-05	0.0000
TOL	7.79E-05	= 1*TOL	7.79E-05	0.0000
XYL	4.84E-05	= 1*XYL	4.84E-05	0.0000
A25J	5.01E-01	= 1*FPRM + 1*FCRS	5.01E-01	0.0000
ACLJ	7.58E-01	= 1*PCL	7.58E-01	0.0000
AECJ	2.46E-01	= 1*PEC	2.46E-01	0.0000
ANAJ	4.84E-01	= 1*NA	4.84E-01	0.0000
ANH4J	8.96E-01	= 1*PNH4	8.96E-01	0.0000
ANO3J	7.53E-02	= 1*PNO3	7.53E-02	0.0000
AORGPAJ	5.00E-01	= 1*POA	5.00E-01	0.0000
ASO4J	2.54E+00	= 1*PSO4	2.54E+00	0.0000
ASOIL	1.03E+00	= 1*CCRS	1.03E+00	0.0000
ASQTJ	1.30E-02	= 1*SOA7	1.30E-02	0.0000
ATRP1J	2.94E-02	= 1*SOA5	2.94E-02	0.0000
ATRP2J	2.94E-02	= 1*SOA6	2.94E-02	0.0000
NUMACC	3.71E+08	= 1*NUMACC	3.71E+08	0.0000
NUMATKN	1.48E+09	= 1*NUMATKN	1.48E+09	0.0000
NUMCOR	2.35E+04	= 1*NUMCOR	2.35E+04	0.0000
SRFACC	1.49E-05	= 1*SRFACC	1.49E-05	0.0000
SRFATKN	8.15E-07	= 1*SRFATKN	8.15E-07	0.0000
SRFCOR	2.64E-07	= 1*SRFCOR	2.64E-07	0.0000

Table 3-5. Table showing CAMx and CMAQ BCs on grid cell i=65, j=1, layer =1 at CAMx hour = 18pm on June 2, and CMAQ hour = 0:30am on June 3.

CMAQ Species Name	Extracted CMAQ BCs	Mapping from CAMx Species (or default profile)	Extracted CAMx BCs	QA Difference: (CMAQ-CAMX)/CMAQ
ALD2	9.33E-05	= 1*ALD2	9.33E-05	0.0000
ALDX	1.84E-05	= 1*ALDX	1.84E-05	0.0000
BENZENE	2.93E-05	= 1*BENZ	2.93E-05	0.0000
CO	1.02E-01	= 1*CO	1.02E-01	0.0000
ETHA	5.41E-04	= 1*ETHA	5.41E-04	0.0000
FORM	1.35E-03	= 1*FORM	1.35E-03	0.0000
H2O2	2.07E-03	= 1*H2O2	2.07E-03	0.0000
HNO3	6.60E-04	= 1*HNO3	6.60E-04	0.0000
ISOP	6.72E-04	= 1*ISOP	6.72E-04	0.0000
ISPD	1.91E-04	= 1*ISPD	1.91E-04	0.0000
MEPX	6.31E-04	= 1*MEPX	6.31E-04	0.0000
N2O5	2.38E-09	= 1*N2O5	2.38E-09	0.0000
NH3	6.50E-04	= 1*NH3	6.50E-04	0.0000
NO2	1.86E-04	= 1*NO2	1.86E-04	0.0000
NR	2.91E-04	= 1*NR + 5*BENZ + 1.5*PRPA	2.91E-04	0.0000
NTR	2.02E-05	= 1*NTR + 1*INTR + 1* NTR1 + 1*NTR2	2.02E-05	0.0000
O3	5.22E-02	= 1*O3	5.22E-02	0.0000
OLE	5.06E-05	= 1*OLE	5.06E-05	0.0000
PAN	2.48E-04	= 1*PAN	2.48E-04	0.0000
PANX	4.58E-05	= 1*PANX	4.58E-05	0.0000
PAR	6.32E-03	= 1*PAR + 3*ACET + 1*BENZ + 1*ETHY + 1*KET + 1.5*PRPA	6.32E-03	0.0000
PNA	3.05E-06	= 1*PNA	3.05E-06	0.0000
SO2	3.22E-04	= 1*SO2	3.22E-04	0.0000
SV_SQT	2.10E-05	= 1*CG7	2.10E-05	0.0000
SV_TRP1	5.04E-05	= 1*CG5	5.04E-05	0.0000
SV_TRP2	5.04E-05	= 1*CG6	5.04E-05	0.0000
TERP	5.54E-05	= 1*TERP	5.54E-05	0.0000
TOL	2.26E-05	= 1*TOL	2.26E-05	0.0000
XYL	4.34E-06	= 1*XYL	4.34E-06	0.0000
A25J	2.58E-01	= 1*FPRM + 1*FCRS	2.58E-01	0.0000
ACLJ	3.53E-02	= 1*PCL	3.53E-02	0.0000
AECJ	1.21E-01	= 1*PEC	1.21E-01	0.0000
ANAJ	2.26E-02	= 1*NA	2.26E-02	0.0000
ANH4J	8.11E-01	= 1*PNH4	8.11E-01	0.0000
ANO3J	1.11E-01	= 1*PNO3	1.11E-01	0.0000
AORGPAJ	2.95E-01	= 1*POA	2.95E-01	0.0000
ASO4J	2.10E+00	= 1*PSO4	2.10E+00	0.0000
ASOIL	5.60E-01	= 1*CCRS	5.60E-01	0.0000
ASQTJ	1.67E-02	= 1*SOA7	1.67E-02	0.0000
ATRP1J	2.47E-02	= 1*SOA5	2.47E-02	0.0000
ATRP2J	2.47E-02	= 1*SOA6	2.47E-02	0.0000
NUMACC	3.71E+08	= 1*NUMACC	3.71E+08	0.0000
NUMATKN	1.48E+09	= 1*NUMATKN	1.48E+09	0.0000
NUMCOR	2.35E+04	= 1*NUMCOR	2.35E+04	0.0000
SRFACC	1.49E-05	= 1*SRFACC	1.49E-05	0.0000
SRFATKN	8.15E-07	= 1*SRFATKN	8.15E-07	0.0000
SRFCOR	2.64E-07	= 1*SRFCOR	2.64E-07	0.0000

To QA layer assignments, vertical profiles were inspected for ozone and all six CMAQ default species and for a single hour. The ozone vertical profiles for CAMx and CMAQ IC/BCs on the selected grid cell are shown in Figure 3-3. The vertical profiles for the six default species are shown in Figure 3-4 and 3-5. The results are in agreement for all species examined and confirm that the software appropriately interpolates default IC/BCs for all sigma layers.

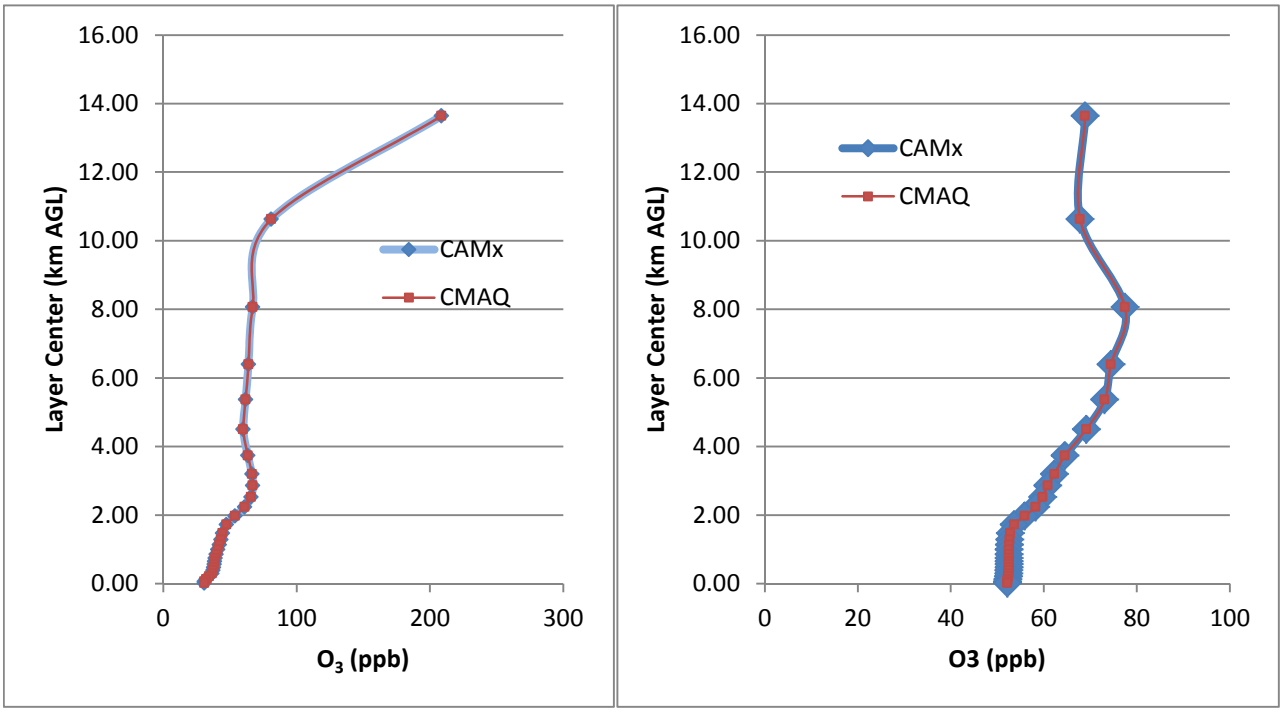
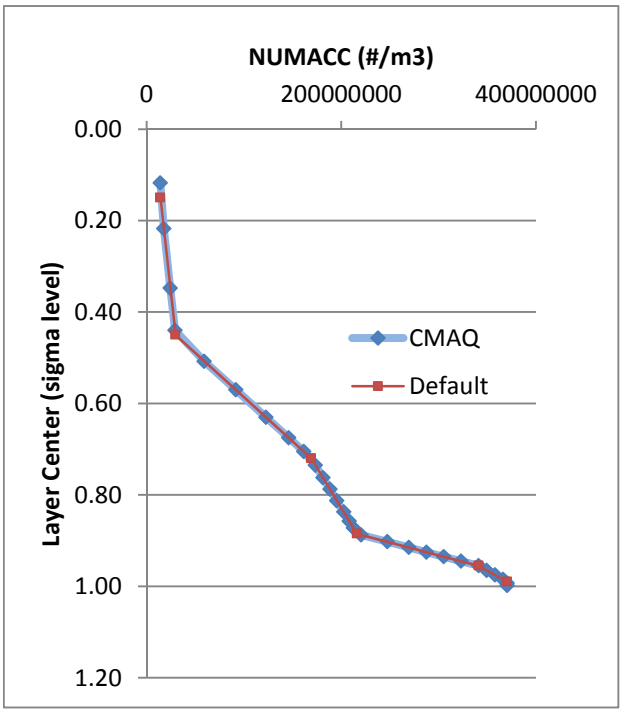
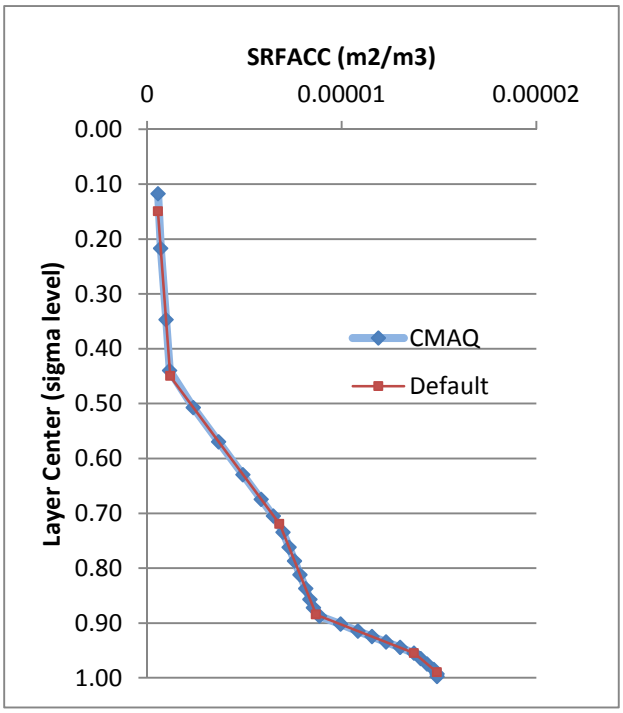
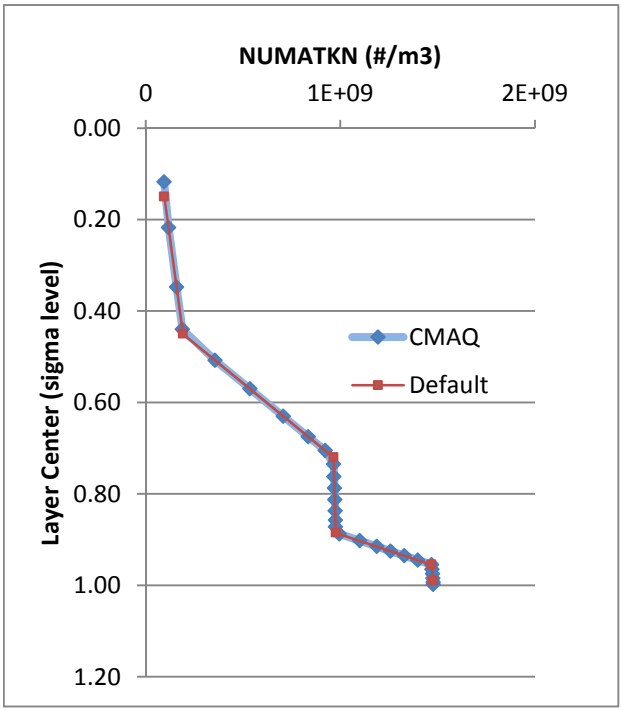


Figure 3-3. Vertical profiles plot showing matched CAMx and CMAQ ICs (left) and BCs (right) for ozone.


NUMACC (#/m3)
0
200000000
400000000
0.00
0.20
0.40
0.60
0.80
1.00
1.20
Layer Center (sigma level)
CMAQ
Default


SRFACC (m2/m3)
0
0.00001
0.00002
0.00
0.10
0.20
0.30
0.40
0.50
0.60
0.70
0.80
0.90
1.00
Layer Center (sigma level)
CMAQ
Default


NUMATKN (#/m3)
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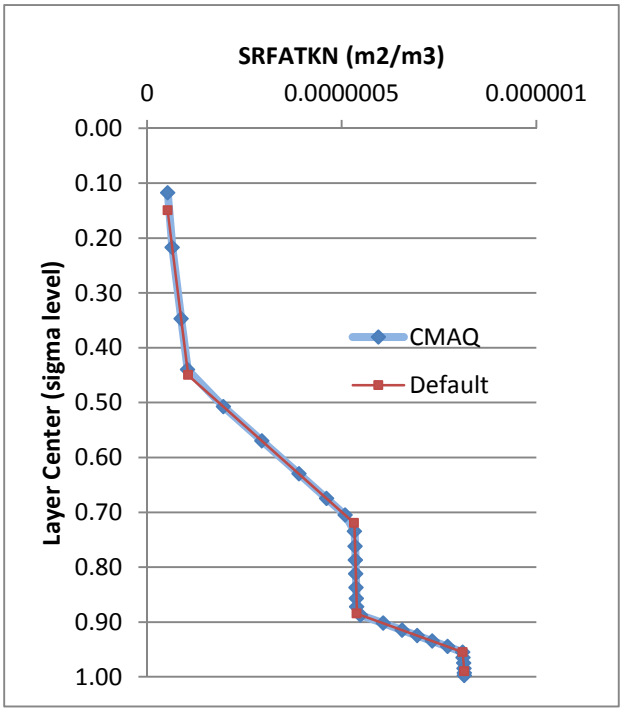
1E+09
2E+09
0.00
0.20
0.40
0.60
0.80
1.00
1.20
Layer Center (sigma level)
CMAQ
Default


SRFATKN (m2/m3)
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0.000001
0.00
0.10
0.20
0.30
0.40
0.50
0.60
0.70
0.80
0.90
1.00
Layer Center (sigma level)
CMAQ
Default

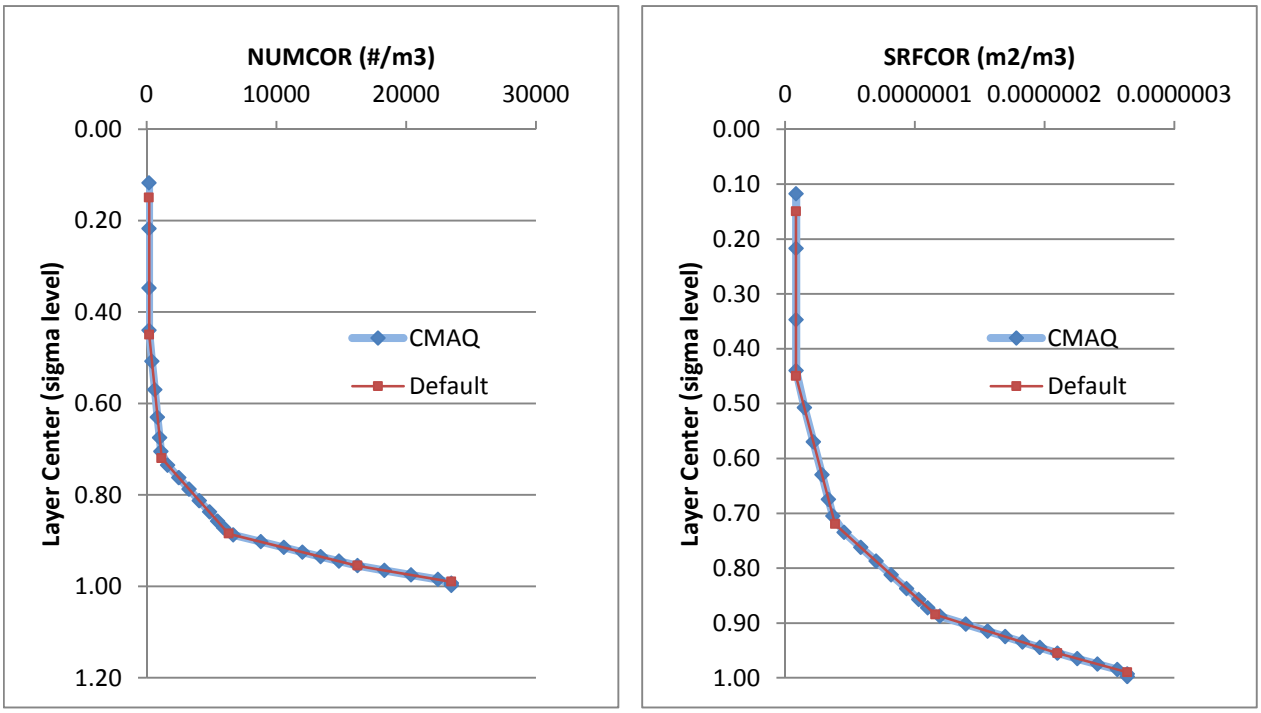
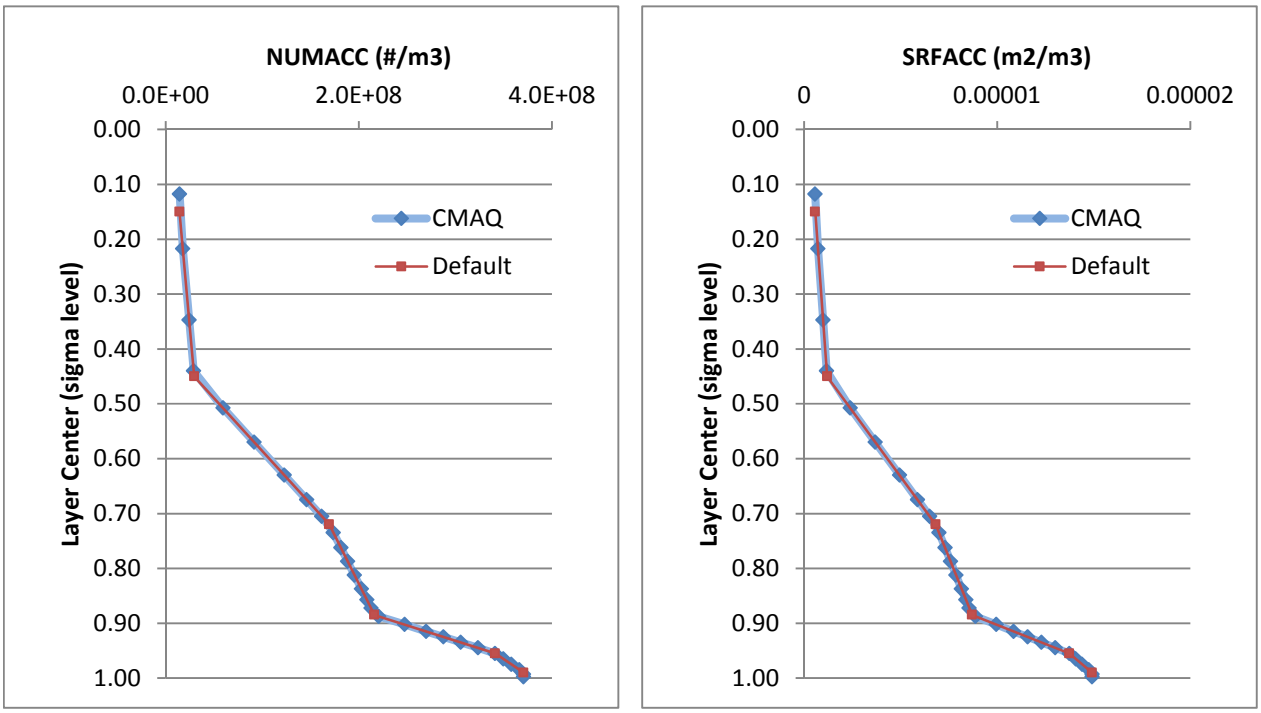


Figure 3-4. Vertical profiles plot showing matched default profile and CMAQ ICs for number and surface area concentration.



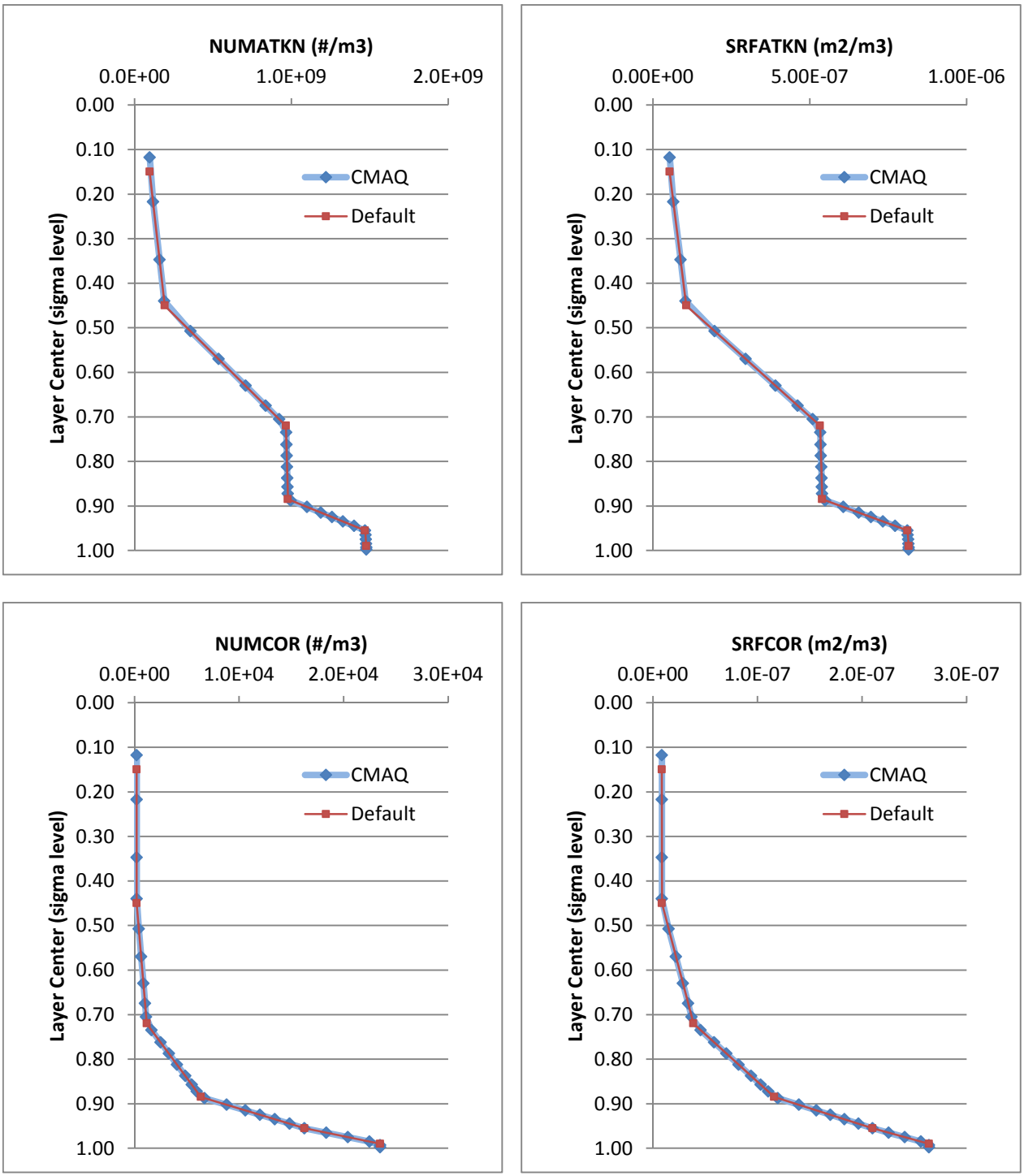


Figure 3-5. Vertical profiles plot showing matched default profile and CMAQ BCs for number and surface area concentration.

4.0 CMAQ TESTING

Functionality, interfacing, performance and design constraints for the CAMx-to-CMAQ converters were further evaluated through implementation in a CMAQ test simulation. We ran a test case using the Rider 8 CAMx files and inspected the outputs to ensure correct conversion. This section documents the CMAQ modeling setup and summarizes test case results, including maps of daily maximum average 8-hour ozone concentrations for all TCEQ modeling domains.

4.1 CMAQ Modeling Approach

We tested and evaluated the CAMx-to-CMAQ converters using the TCEQ's "Rider 8" CAMx modeling files and running the CMAQ model for May 25 – June 6, 2006. The CAMx emissions and IC/BCs files were obtained from TCEQ website (accessed in July 2014).

4.1.1 Rider 8" Model for June 2006

The TCEQ developed the CAMx "Rider 8" model for use by areas in Texas that are close to the National Ambient Air Quality Standard (NAAQS) for ozone but not designated as nonattainment areas. CAMx input data files were downloaded from: http://www.tceq.texas.gov/airquality/airmod/rider8/rider8Modeling. In summary, meterorological input data were developed using the Weather Research Forecasting (WRF) model and WRFCAMx interface; anthropogenic emissions were based on TCEQ data within Texas and data from EPA outside Texas; biogenic emissions were developed using MEGAN, and; boundary conditions for the outer 36 km grid were extracted from a GEOS-Chem global model simulation of 2006.

The Rider 8 nested modeling grids are shown in Figure 4-1 and the dimensions of grids are given in Table 4-1. The layer structure is defined in Figure 4-2 with 28 layers from the surface to 15 km and a surface layer depth of 34m. The outer 36 km grid covers the continental US (CONUS) and is the same grid that EPA and many States use for regional air quality modeling. The nested 12 km grid covers Texas and a substantial area that would typically be upwind of Texas during an ozone episode including adjacent States and the western Gulf of Mexico. The nested 4 km grid covers the Houston and Dallas ozone nonattainment areas and all of the near nonattainment areas in eastern Texas.

Table 4-1. TCEQ 36/12/4 km CAMx nested modeling grids for Rider 8 model of June 2006.

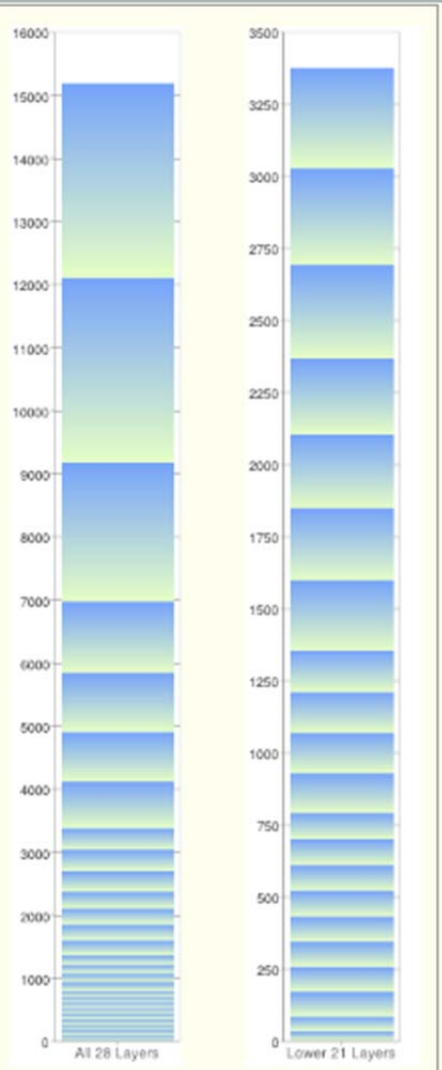
CAMx Grid	Grid Size (number of cells)		
	East-West	North-South	Layers
RPO 36km	148	112	28
Texas 12km	149	110	28
Texas 4km	191	218	28

Figure 4-1. TCEQ 36/12/4 km CAMx nested modeling grids for the Rider 8 model of June 2006. [1]

[1] TCEQ figure from http://www.tceq.texas.gov/airquality/airmod/rider8/modeling/domain.

Vertical Layer Structure

Corresponding WRF Layer	Layer Top (m AGL)	CAMx Layer	Layer Center (m AGL)	Thickness (m)
38	15179.1	28	13637.9	3082.5
36	12096.6	27	10631.6	2930.0
32	9166.6	26	8063.8	2205.7
29	6960.9	25	6398.4	1125.0
27	5835.9	24	5367.0	937.9
25	4898.0	23	4502.2	791.6
23	4106.4	22	3739.9	733.0
21	3373.5	21	3199.9	347.2
20	3026.3	20	2858.3	335.9
19	2690.4	19	2528.3	324.3
18	2366.1	18	2234.7	262.8
17	2103.3	17	1975.2	256.2
16	1847.2	16	1722.2	249.9
15	1597.3	15	1475.3	243.9
14	1353.4	14	1281.6	143.6
13	1209.8	13	1139.0	141.6
12	1068.2	12	998.3	139.7
11	928.5	11	859.5	137.8
10	790.6	10	745.2	90.9
9	699.7	9	654.7	90.1
8	609.7	8	565.0	89.3
7	520.3	7	476.1	88.5
6	431.8	6	387.9	87.8
5	344.0	5	300.5	87.1
4	256.9	4	213.8	86.3
3	170.6	3	127.8	85.6
2	85.0	2	59.4	51.0
1	33.9	1	17.0	33.9



AGL - Above Ground Level.

Figure 4-2. CAMx vertical layer structure for the Rider 8 model of June 2006. [2]

4.1.2 CMAQ Inputs

CAMx supports the option to perform model simulations in different time zones, and often the emissions are prepared and CAMx is run using Local Standard Time (LST). In contrast CMAQ is always run using UTC. Since the "Rider 8" CAMx emissions and IC/BCs files were prepared in Central Standard Time (CST) for Texas, they were converted to UTC for CMAQ. Meteorology inputs for CMAQ were prepared in UTC. More information on CMAQ inputs development is provided below.

[2] TCEQ figure from http://www.tceq.texas.gov/airquality/airmod/rider8/modeling/domain.

4.1.2.1 Emissions

The Rider8 CAMx-ready emissions files were converted into CMAQ-ready emissions files using the CAMx-to-CMAQ converters as described in Section 2. The tool converts both gridded surface level emissions and elevated point source emissions. CMAQ requires that emissions are provided for all emitted PM species including sulfate, nitrate, organic carbon, elemental carbon, and crustal material (fine and coarse). The Rider8 CAMx emissions files do not include coarse material (CAMx species: CPRM or CCRS; CMAQ species: PMC). To work around the limitation we added CMAQ PMC species to the emissions files but set the emissions to zero[3].

4.1.2.2 Initial and Boundary Conditions (IC/BCs)

The CMAQ CTM (CCTM) requires BC inputs to specify the assumed concentrations along the lateral edges of the 36 km modelling domain (see Figure 4-1). ICs also need to be specified for the start of the model simulation. The 12 km and 4 km domains are nested within the 36 km grid using one-way grid nesting, which means that the nested domains are run after the coarse domain and there is no feedback from the fine nests to the coarse domain. The IC/BCs for the 12 km CMAQ modelling domain were obtained by standard procedures for CMAQ, namely processing the CMAQ 36 km domain output using the CMAQ ICON/BCON processors to generate an hourly 12 km IC/BC input files. Similarly, the IC/BCs for the 4 km modelling domain were obtained from the 12 km modelling results.

For the 36 km domain, the Rider8 CAMx-ready IC/BC files were converted into CMAQ-ready IC/BC files using the CAMx-to-CMAQ converters (ENVIRON, 2014b). The Rider8 CAMx IC/BC files included many PM species (from GEOS-Chem) that were mapped to CMAQ PM species. Note that TCEQ's Rider8 IC file was prepared in CST (midnight) for Texas corresponding to 18:00 UTC.

4.1.2.3 Meteorology (MCIP)

The CMAQ Chemical Transport Model (CTM) meteorological inputs were generated by processing the WRF meteorological model output provided by TCEQ using the CMAQ Meteorological-Chemistry Interface Program (MCIP). MCIP provides the complete set of meteorological data required by CMAQ. The vertical layer mapping of the 38 WRF layers to 28 CMAQ layers is similar to the WRF-CAMx mapping shown in Figure 4-2 except that the CMAQ top layer extends to match the WRF top layer (i.e., sigma of 0.00) as required by MCIP. The MCIP Version 4.1 (released July 2012 together with CMAQ Version 5.0.1) was used.

The WRF output provided by TCEQ spanned May 24 0:00 UTC through June 7 23:00 UTC. MCIP calculates precipitation rates by subtracting the current hour's accumulated precipitation from the previous hour's (23:00), so the CMAQ starting date was set to be 1 day after the WRF starting date. MCIP also needs to include the first hour of the next day, so the CMAQ ending

[3] PMC was modified in the species mapping file used by CAMx-to-CMAQ converters :
PMC g/s 3
FPRM CPRM CCRS
0.0 1.0 1.0

date was set to be 1 day before the WRF ending date. As a result, MCIP can only run for May 25 through June 6.

4.1.2.4 Photolysis tables

The CMAQ JPROC processor was used to calculate clear-sky photolysis rates (or J-values) for each date. JPROC uses default values for total aerosol loading and date-specific data for total ozone column from Total Ozone Mapping Spectrometer (TOMS) satellites. TOMS data for the year 2006 are available daily from http://toms.gsfc.nasa.gov/eptoms/ep.html. The photolysis input table for the 12/4 km modeling was the same as the 36-km modeling.

4.1.2.5 Ocean mask file

CMAQ aerosol option AERO5 can compute sea salt emissions from both open ocean grid cells and surf zone grid cells. The Ocean file defines what fraction of each grid cell is on land, on the ocean, or on the surf zone where waves break against the shore. This file was created using the Spatial Allocator tool for the SMOKE emissions processor.

4.2 CMAQ Model Configuration

CMAQ version 5.0.1 was chosen for this work since it was the most updated version at the time work was initiated. The model configuration is shown in Table 4-2. The 36 km modeling used a 7 day spin up period starting on May 25. The 12 km and 4km grids used a 2 day spin up starting on May 30. All modeling domains were run through June 6.

Table 4-2. Model Configuration Options for the CMAQ Model.

Science Options	Configurations
Model Code	CMAQ Version 5.0.1 (July 2012)
Horizontal Grid Mesh	36/12/4 km
Vertical Grid Mesh	28 Layers
Initial Conditions	5 days full spin-up ; converted from CAMx IC file
Boundary Conditions	Converted from CAMx BC files
Emissions Processing	Converted from CAMx emission files
Gas-Phase Chemistry	CB05
Aerosol Chemistry	AE5 (With Sea Salt Emissions)
Meteorological Processor	MCIP Version 4.1
Horizontal Transport	PPM
Horizontal Diffusion	K-theory spatially varying
Vertical Advection Scheme	WRF
Vertical Eddy Diffusivity Scheme	ACM2
Diffusivity Lower Limit	Kzmin = 0.01 to 1.0 m2/s (PURB option) (KZMIN set to true)
Deposition Scheme	M3dry

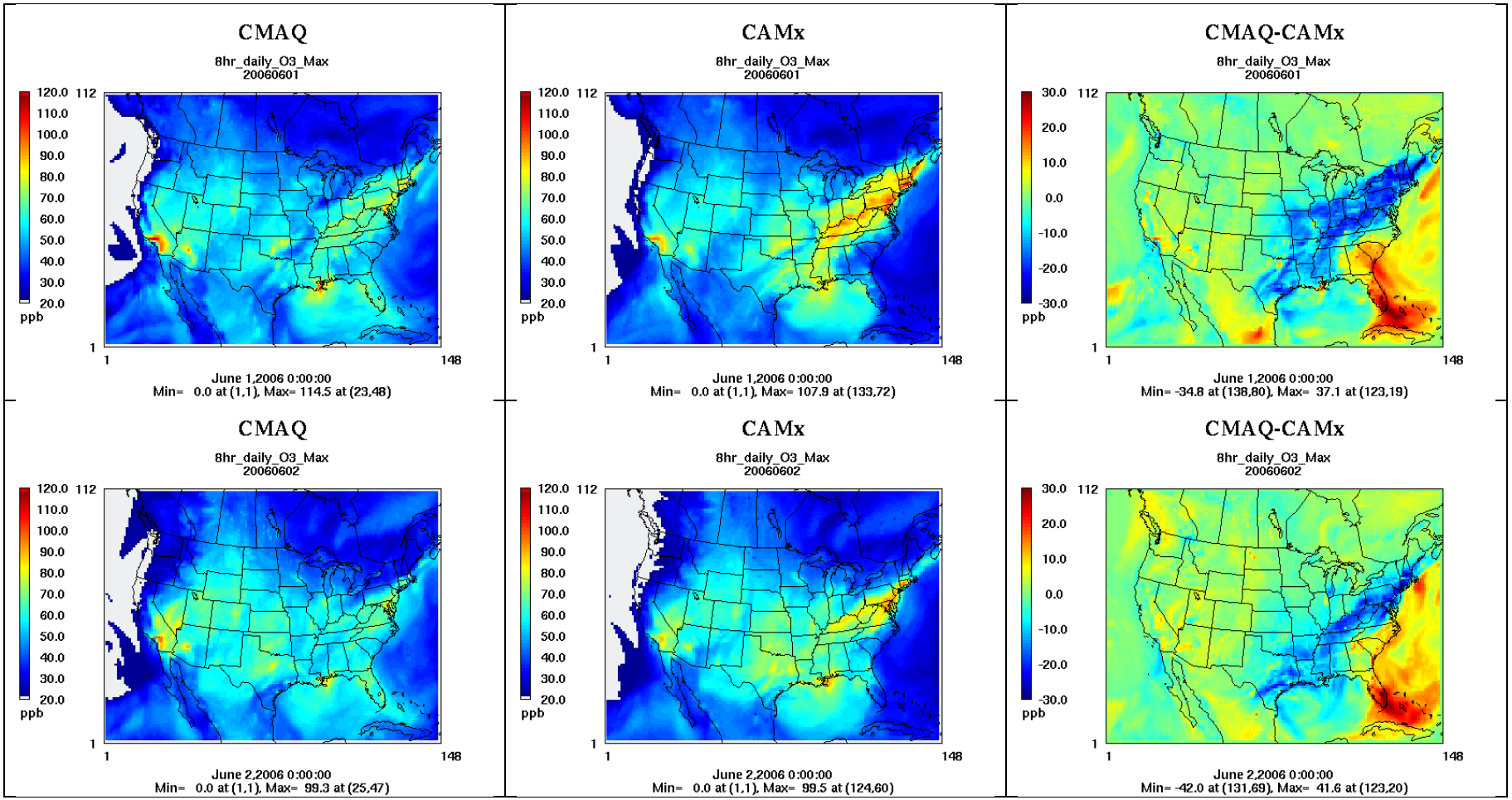
4.3 CMAQ Modeling Results

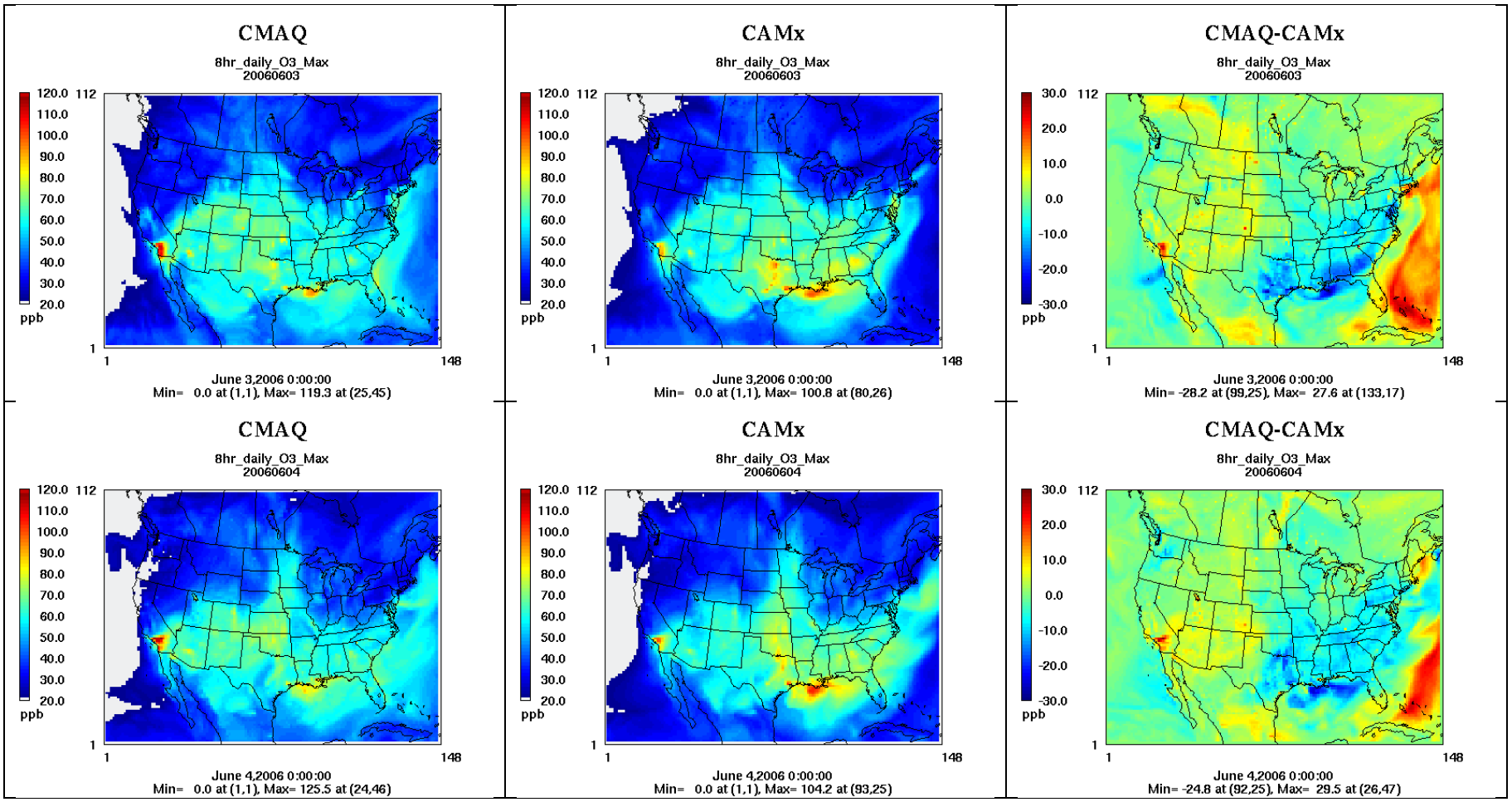
Daily CMAQ ACONC output files contained hourly average concentrations in UTC. The files were then converted to a CAMx average file format and time shifted from UTC to CST. Two consecutive daily CAMx average files were merged into a single file so that the 8-hour average concentrations could be computed for all 24 hours of the day. The daily maximum 8-hour (MDA8) ozone was computed using the CAMxPOST processor. We obtained the TCEQ's Rider 8 CAMx results from TCEQ's website and calculated MDA8 ozone for the same non-spinup modeling period, i.e., June 1-6.

The left and center columns of Figure 4-3 display spatial plots of the MDA8 ozone in each day during June 1-6, 2006, in the 36 km domain for CMAQ and CAMx runs, respectively. The right side shows the difference between the MDA8 ozone generated using CMAQ and that generated using CAMx. Figure 4-4 and 4-5 present similar plots for the 12 and 4 km domains, respectively.

The CMAQ simulation shows the MDA8 ozone exceeding 75 ppb, the current level of the ozone NAAQS, in several areas in the CONUS domain, mostly in the eastern states. High ozone concentrations (above 90 ppb) also occurred over water bodies close to major urban/industrial areas near the Great Lakes, Gulf Coast and the Northeast Seaboard, where emissions are transported over water and get confined in a shallow boundary layer. Texas ozone peaks exceeding 75 ppb were seen over the Houston and Dallas areas. The predicted-MDA8 ozone concentrations in Texas are higher with coarser grid resolution because artificial dilution of gridded emissions resulted in more productive ozone chemistry. Overall, the CMAQ results appear within a reasonable range.

CAMx results (Figure 4-3 to 4-5, center) show a similar spatial pattern of MDA8 ozone. However, the CAMx-predicted concentrations tend to be higher than CMAQ results in the central and eastern US but lower in the western US. In the 4 km domain, CMAQ-predicted MDA8 ozone concentrations were consistently lower in the eastern Texas especially near Houston with few exceptions. The highest ozone difference of 39 ppb occurred on June 2 in Houston where CAMx suggested ozone titration in the urban area whereas CMAQ predicted peak ozone exceeding 80 ppb. Another event when CMAQ estimated higher ozone compared to CAMx occurred on June 1 in Dallas with the maximum difference of 20 ppb. In contrast, CMAQ results were lower by 24 ppb and 32 ppb on June 5 and 6, respectively, as a result of lower ozone concentrations in the Houston-Galveston ozone plumes. What led to these differences is unclear and follow-up investigation is recommended.


CMAQ
8hr_daily_O3_Max
20060601
June 1,2006 0:00:00
Min= 0.0 at (1,1), Max= 114.5 at (23,48)
CAMx
8hr_daily_O3_Max
20060601
June 1,2006 0:00:00
Min= 0.0 at (1,1), Max= 107.9 at (133,72)
CMAQ-CAMx
8hr_daily_O3_Max
20060601
June 1,2006 0:00:00
Min= -34.8 at (138,80), Max= 37.1 at (123,19)
CMAQ
8hr_daily_O3_Max
20060602
June 2,2006 0:00:00
Min= 0.0 at (1,1), Max= 99.3 at (25,47)
CAMx
8hr_daily_O3_Max
20060602
June 2,2006 0:00:00
Min= 0.0 at (1,1), Max= 99.5 at (124,60)
CMAQ-CAMx
8hr_daily_O3_Max
20060602
June 2,2006 0:00:00
Min= -42.0 at (131,69), Max= 41.6 at (123,20)
ppb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20060603
June 3,2006 0:00:00
Min= 0.0 at (1,1), Max= 119.3 at (25,45)
CAMx
8hr_daily_O3_Max
20060603
June 3,2006 0:00:00
Min= 0.0 at (1,1), Max= 100.8 at (80,26)
CMAQ-CAMx
8hr_daily_O3_Max
20060603
June 3,2006 0:00:00
Min= -28.2 at (99,25), Max= 27.6 at (133,17)
CMAQ
8hr_daily_O3_Max
20060604
June 4,2006 0:00:00
Min= 0.0 at (1,1), Max= 125.5 at (24,46)
CAMx
8hr_daily_O3_Max
20060604
June 4,2006 0:00:00
Min= 0.0 at (1,1), Max= 104.2 at (93,25)
CMAQ-CAMx
8hr_daily_O3_Max
20060604
June 4,2006 0:00:00
Min= -24.8 at (92,25), Max= 29.5 at (26,47)
ppb

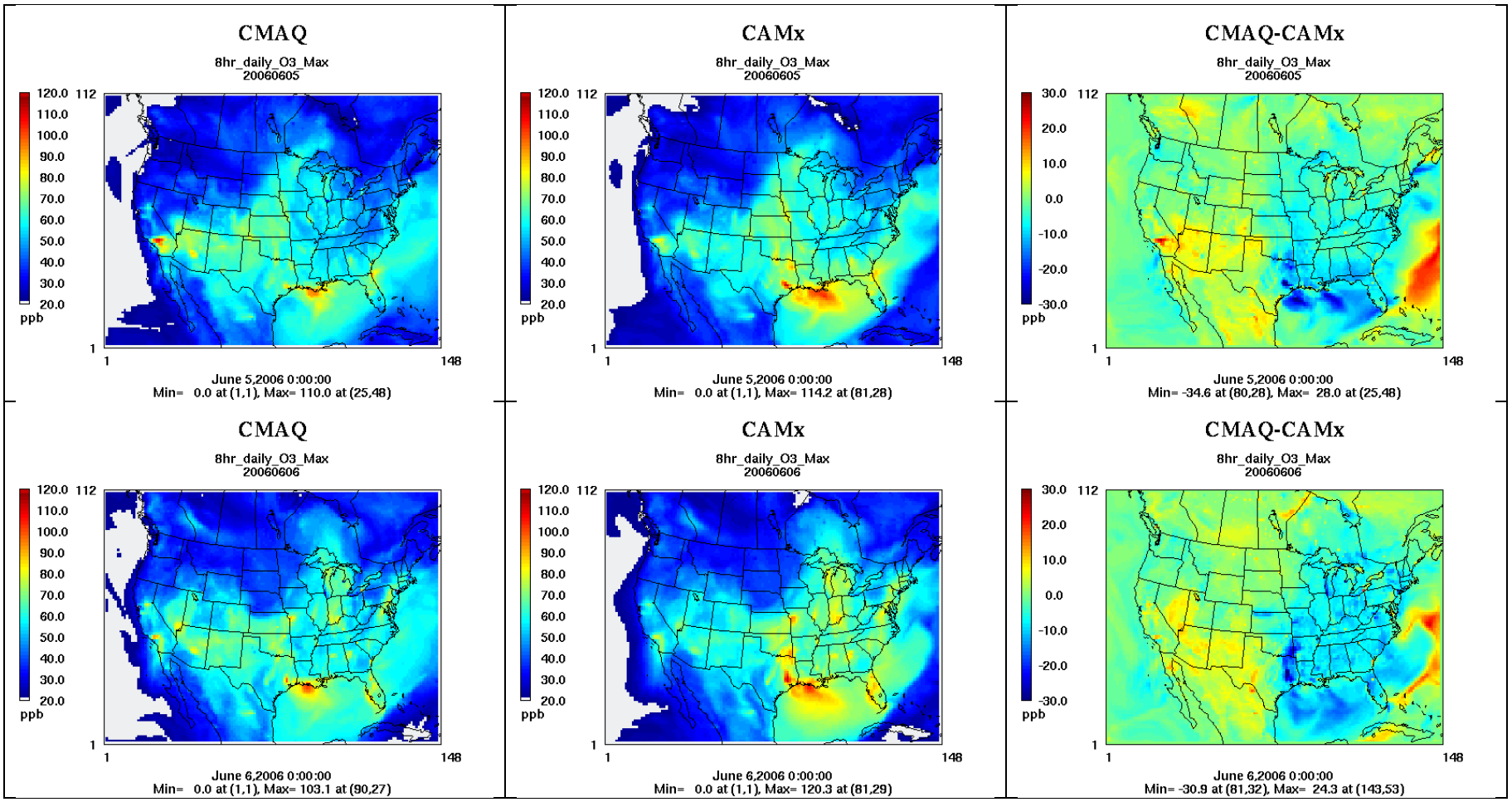
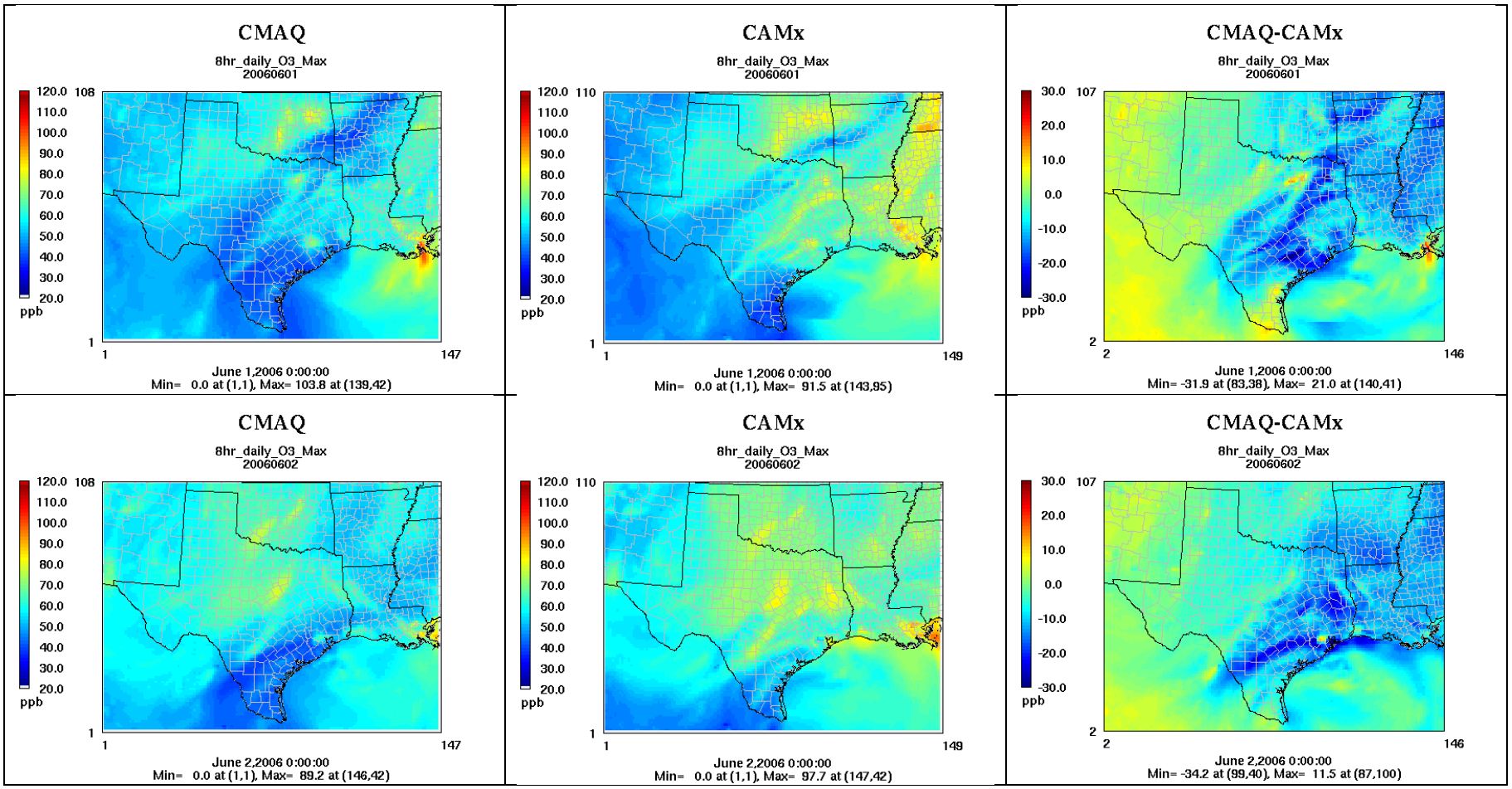
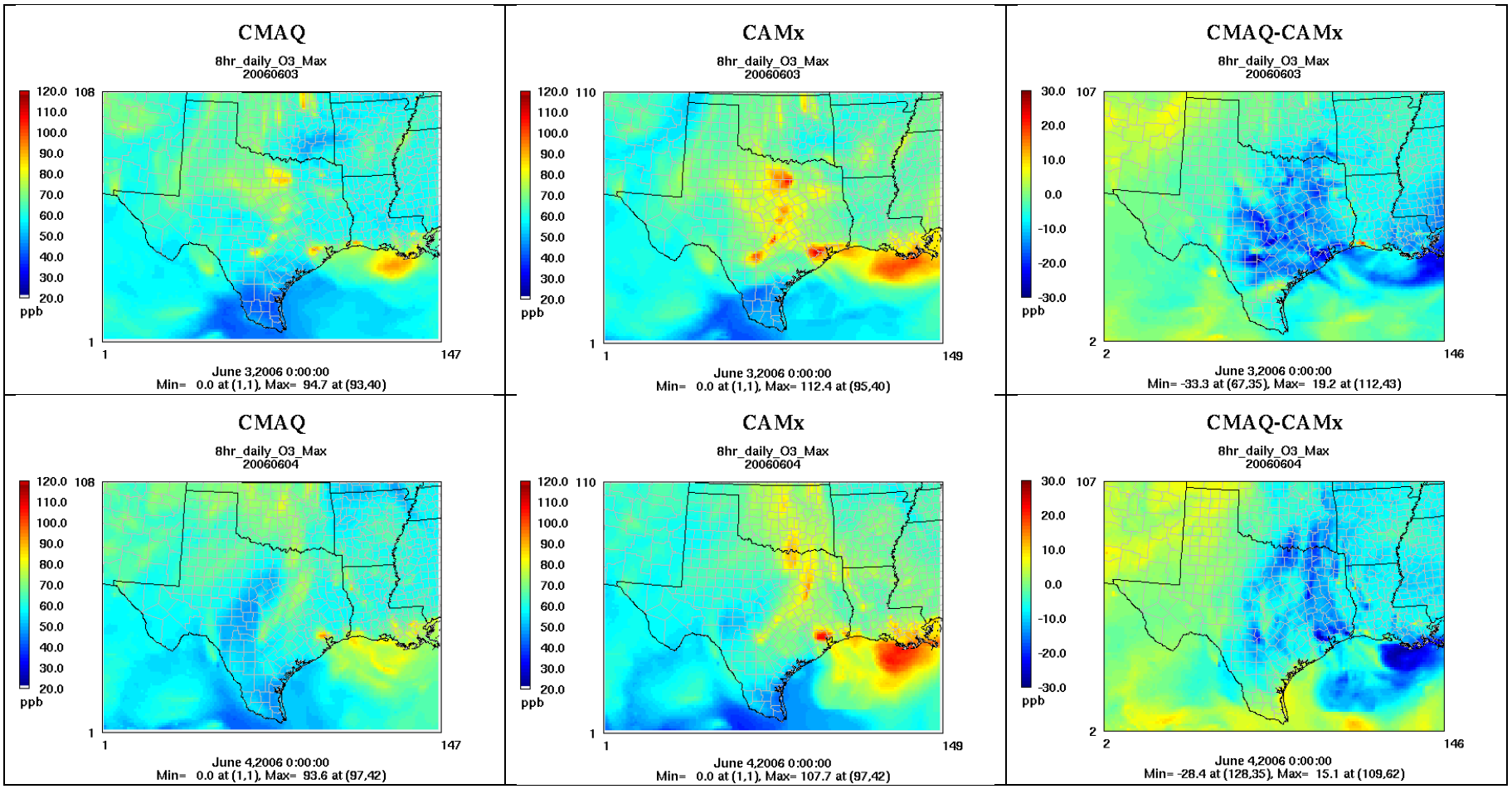


Figure 4-3. Maps of daily maximum 8-hour ozone in the 36 km domain from CMAQ (left), CAMx (middle) and the differences between CMAQ and CAMx results (right).


CMAQ
8hr_daily_O3_Max
20060601
June 1,2006 0:00:00
Min= 0.0 at (1,1), Max= 103.8 at (139,42)
CAMx
8hr_daily_O3_Max
20060601
June 1,2006 0:00:00
Min= 0.0 at (1,1), Max= 91.5 at (143,95)
CMAQ-CAMx
8hr_daily_O3_Max
20060601
June 1,2006 0:00:00
Min= -31.9 at (83,38), Max= 21.0 at (140,41)
CMAQ
8hr_daily_O3_Max
20060602
June 2,2006 0:00:00
Min= 0.0 at (1,1), Max= 89.2 at (146,42)
CAMx
8hr_daily_O3_Max
20060602
June 2,2006 0:00:00
Min= 0.0 at (1,1), Max= 97.7 at (147,42)
CMAQ-CAMx
8hr_daily_O3_Max
20060602
June 2,2006 0:00:00
Min= -34.2 at (99,40), Max= 11.5 at (87,100)
ppb


CMAQ
8hr_daily_O3_Max
20060603
June 3,2006 0:00:00
Min= 0.0 at (1,1), Max= 94.7 at (93,40)
CAMx
8hr_daily_O3_Max
20060603
June 3,2006 0:00:00
Min= 0.0 at (1,1), Max= 112.4 at (95,40)
CMAQ-CAMx
8hr_daily_O3_Max
20060603
June 3,2006 0:00:00
Min= -33.3 at (67,35), Max= 19.2 at (112,43)
CMAQ
8hr_daily_O3_Max
20060604
June 4,2006 0:00:00
Min= 0.0 at (1,1), Max= 93.6 at (97,42)
CAMx
8hr_daily_O3_Max
20060604
June 4,2006 0:00:00
Min= 0.0 at (1,1), Max= 107.7 at (97,42)
CMAQ-CAMx
8hr_daily_O3_Max
20060604
June 4,2006 0:00:00
Min= -28.4 at (128,35), Max= 15.1 at (109,62)
ppb

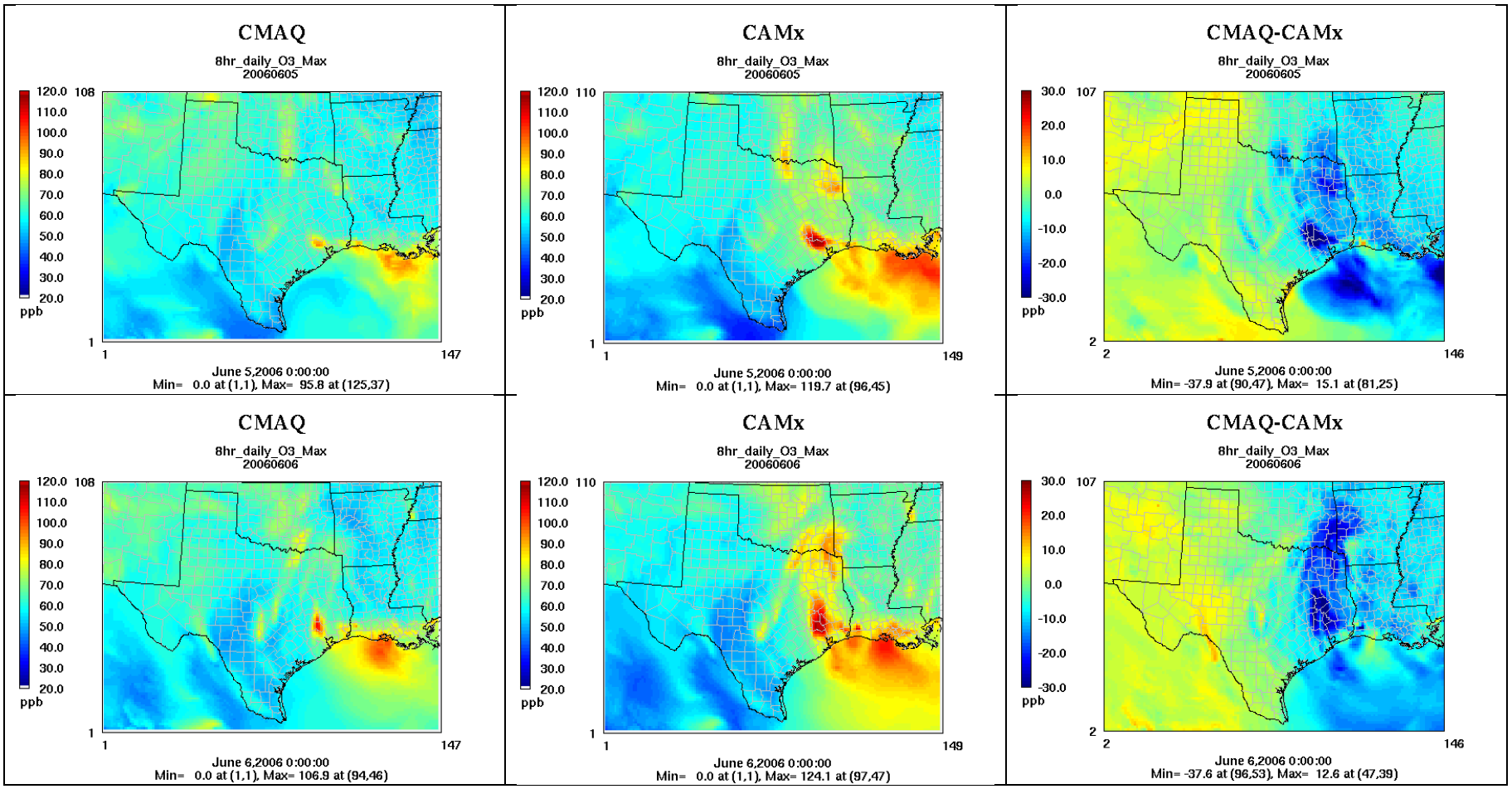
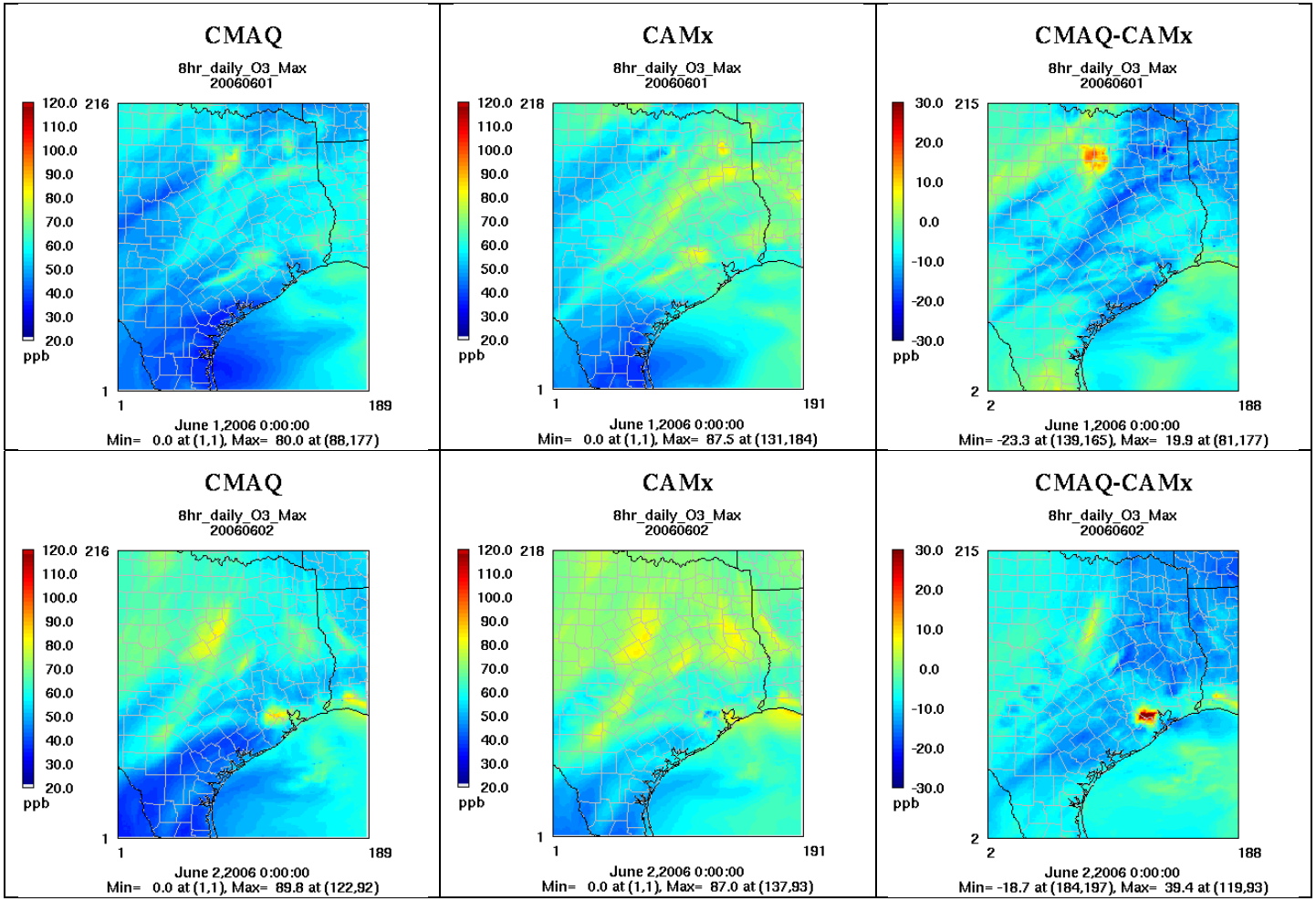
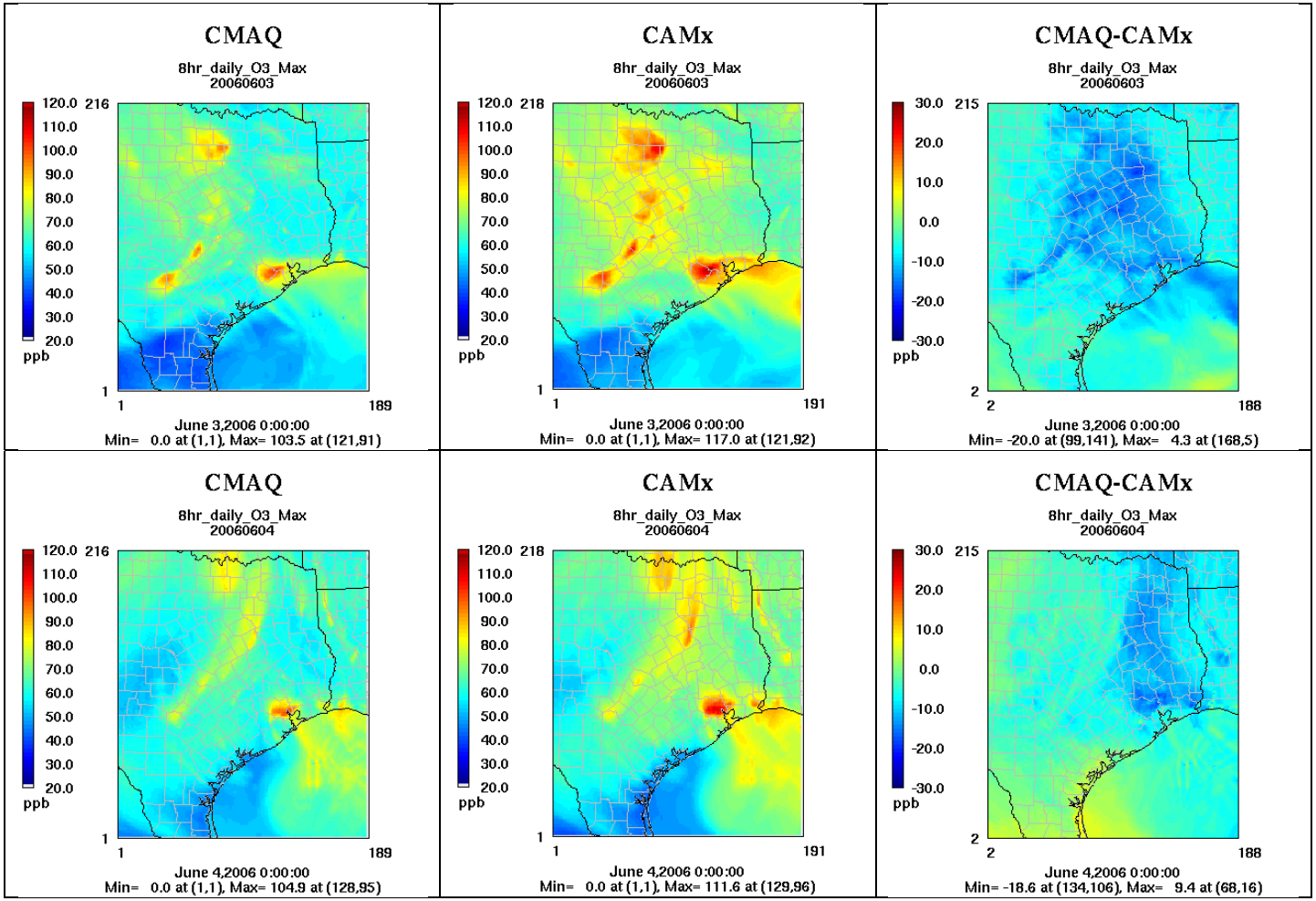


Figure 4-4. Maps of daily maximum 8-hour ozone in the 12 km domain from CMAQ (left), CAMx (middle) and the differences between CMAQ and CAMx results (right).


CMAQ
8hr_daily_O3_Max
20060601
120.0 216
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
ppb
1
1
189
June 1,2006 0:00:00
Min= 0.0 at (1,1), Max= 80.0 at (88,177)
CAMx
8hr_daily_O3_Max
20060601
120.0 218
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
ppb
1
1
191
June 1,2006 0:00:00
Min= 0.0 at (1,1), Max= 87.5 at (131,184)
CMAQ-CAMx
8hr_daily_O3_Max
20060601
30.0 215
20.0
10.0
0.0
-10.0
-20.0
-30.0
ppb
2
2
188
June 1,2006 0:00:00
Min= -23.3 at (139,165), Max= 19.9 at (81,177)
CMAQ
8hr_daily_O3_Max
20060602
120.0 216
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
ppb
1
1
189
June 2,2006 0:00:00
Min= 0.0 at (1,1), Max= 89.8 at (122,92)
CAMx
8hr_daily_O3_Max
20060602
120.0 218
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
ppb
1
1
191
June 2,2006 0:00:00
Min= 0.0 at (1,1), Max= 87.0 at (137,93)
CMAQ-CAMx
8hr_daily_O3_Max
20060602
30.0 215
20.0
10.0
0.0
-10.0
-20.0
-30.0
ppb
2
2
188
June 2,2006 0:00:00
Min= -18.7 at (184,197), Max= 39.4 at (119,93)


CMAQ
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20060603
120.0 216
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
ppb
1
1
189
June 3,2006 0:00:00
Min= 0.0 at (1,1), Max= 103.5 at (121,91)
CAMx
8hr_daily_O3_Max
20060603
120.0 218
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
ppb
1
1
191
June 3,2006 0:00:00
Min= 0.0 at (1,1), Max= 117.0 at (121,92)
CMAQ-CAMx
8hr_daily_O3_Max
20060603
30.0 215
20.0
10.0
0.0
-10.0
-20.0
-30.0
ppb
2
2
188
June 3,2006 0:00:00
Min= -20.0 at (99,141), Max= 4.3 at (168,5)
CMAQ
8hr_daily_O3_Max
20060604
120.0 216
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
ppb
1
1
189
June 4,2006 0:00:00
Min= 0.0 at (1,1), Max= 104.9 at (128,95)
CAMx
8hr_daily_O3_Max
20060604
120.0 218
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
ppb
1
1
191
June 4,2006 0:00:00
Min= 0.0 at (1,1), Max= 111.6 at (129,96)
CMAQ-CAMx
8hr_daily_O3_Max
20060604
30.0 215
20.0
10.0
0.0
-10.0
-20.0
-30.0
ppb
2
2
188
June 4,2006 0:00:00
Min= -18.6 at (134,106), Max= 9.4 at (68,16)

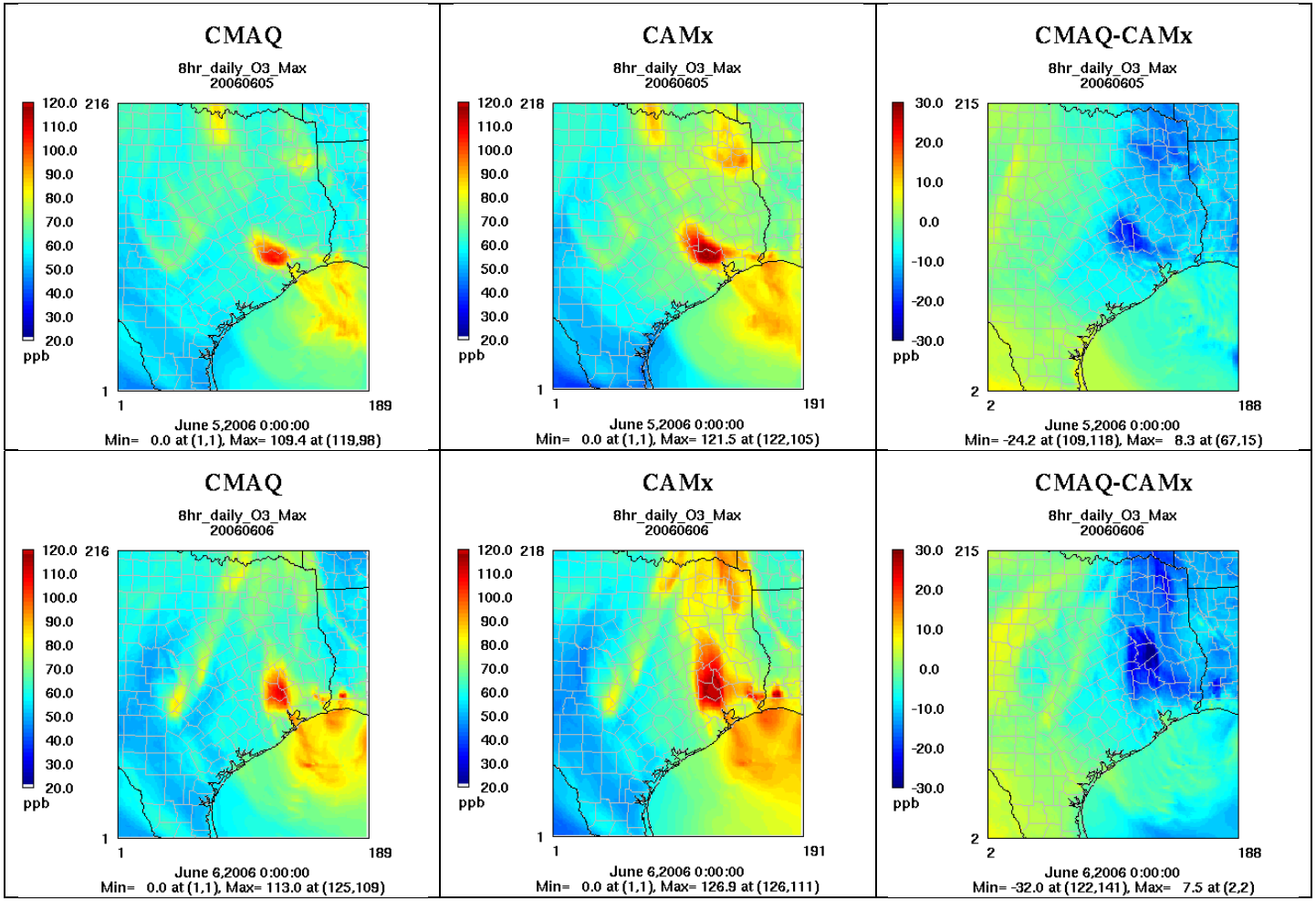

Figure 4-5. Maps of daily maximum 8-hour ozone in the 4 km domain from CMAQ (left), CAMx (middle) and the differences between CMAQ and CAMx results (right).

5.0 CONCLUSIONS AND RECOMMENDATIONS

In project FY14-20, ENVIRON developed software to convert CAMx-ready emissions and IC/BC files into CMAQ-ready files. We performed a series of Quality Assurance (QA) procedures to test each individual component of the software using emissions and IC/BC data from the TCEQ's Rider 8 database. The results of the QA tests demonstrate that all components of the software tool are functioning correctly. Functionality, interfacing, performance and design constraints for the CAMx-to-CMAQ converters were further evaluated through implementation in a CMAQ test simulation. We prepared other CMAQ inputs including meteorology, photolysis rates table, and an ocean mask file, and ran CMAQ for May 25 – June 6, 2006. Maps of daily maximum average 8-hour ozone concentrations for all TCEQ modelling domains were produced for each simulation day and compared to the Rider 8 CAMx results.

The CMAQ testing found no systematic problems with the modeling inputs that would prevent the CMAQ model from giving reasonable results. The CMAQ and CAMx results show comparable spatial pattern of the 8-hour ozone. These results demonstrate that the CAMx-to-CMAQ software functions correctly.

The CMAQ and CAMx results, although similar spatially, have some differences in magnitude. The CAMx-predicted concentrations tend to be higher than CMAQ results in the central and eastern US but lower in the western US. In the 4 km domain, CMAQ-predicted MDA8 ozone concentrations were consistently lower in the eastern Texas especially near Houston. Understanding these ozone differences will be important for TCEQ staff to interpret modeling work performed with CMAQ using TCEQ's modeling inputs. We speculated that the most likely possibilities leading to these variances are differences in: 1) chemical mechanism (CB6 in CAMx versus CB05 in CMAQ); 2) cloud cover; and 3) boundary layer depth. We recommend a follow-up investigation to help understand ozone differences predicted by CAMx and CMAQ.

The TCEQ runs CAMx with only gas-phase species (no aerosols) for ozone modeling studies. This approach is not possible with CMAQ which must always simulate both gases and aerosols. The fact that the TCEQ has been including many aerosol species (i.e., all components of $PM_{2.5}$) in emission files helped with running CMAQ. However, CMAQ requires that PM components be present in emission files and the absence of coarse PM (i.e., the difference PM_{10} minus $PM_{2.5}$) from TCEQ's emission files prevented CMAQ from running. This problem was circumvented by adding a coarse PM species with zero emissions to the CMAQ formatted emissions. In the future, we recommend that TCEQ include estimates of coarse PM in emissions files.

Since the Rider 8 CAMx database aimed to help ozone planning efforts, our evaluation of the CMAQ PM results was limited. Spatial maps of hourly $PM_{2.5}$ show elevated concentrations near Houston and Longview that are mainly attributable to high crustal material. We recommend a follow-up review of PM precursor emissions and model performance evaluation of PM species.

6.0 REFERENCES

ENVIRON (2014) User's Guide to CAMx version 6.10, available at http://www.camx.com/

University of North Carolina at Chapel Hill (UNC), 2012. Operational Guidance for the Community Multiscale Air Quality (CMAQ) Modeling System. Prepared in cooperation with the Community Modeling and Analysis System Institute for the Environment, Chapel Hill, NC., February, http://www.airqualitymodeling.org.