Daily Near Real-Time Ozone Modeling for Texas

WO 582-11-10365-FY14-16 Final Report

Prepared for:
Mark Estes
Texas Commission on Environmental Quality
121 Park 35 Circle MC 164
Austin, TX 78753

Prepared by:
Jeremiah Johnson,
Gary Wilson, DJ Rasmussen,
and Greg Yarwood
ENVIRON International Corporation
773 San Marin Drive, Suite 2115
Novato, California, 94998
www.environcorp.com
P-415-899-0700
F-415-899-0707

January 29, 2015

CONTENTS

TABLES

FIGURES

EXECUTIVE SUMMARY

ENVIRON is assisting TCEQ by deploying a near real-time (NRT) ozone modeling system that delivers model results each morning via a password-protected website. The NRT ozone modeling system uses the WRF meteorological model, CAMx air quality model and emissions data provided by TCEQ. Model configurations are similar to those used for TCEQ SIP modeling, with changes made to meet operational requirements. The NRT model also provides an opportunity to test model changes using sensitivity simulations. The intention is that SIP modeling performed by TCEQ and forecasting performed by ENVIRON will be synergistic and mutually beneficial. This report describes the implementation of the 2014 model including improvements to the system originally developed in 2013, and evaluation of the 2014 NRT ozone modeling system. We provide specific recommendations for future improvements.

The 2013 project found that overall, the NRT ozone modeling system performed well when high ozone was observed. Therefore, in the 2013 final report we emphasized decreasing the number of “false alarms” –ozone over-predictions when observed ozone is low to moderate. Very few high ozone events were observed in 2014, so the potential for false alarms was high. Despite this, the 2014 modeling improved overall ozone bias and error relative to the 2013 modeling.

Sensitivity Tests and Results

Table ES-1 describes the sensitivity simulations used in the 2014 NRT ozone modeling system. CAMx sensitivity simulations were run in parallel with the “base case” simulation. ENVIRON selected several sensitivity tests based on evaluation of 2013 and 2014 ozone performance to investigate potential improvements and measure impacts of different model configurations, by comparing the results of the sensitivity tests with the base case model. Five of these simulations were selected to run for an extended period of time – September 9 to October 20, 2014 – so that the simulations could be compared against one another and the base case.

The first of these five CAMx sensitivity tests uses the Wesely dry deposition scheme instead of the base case Zhang scheme. The next sensitivity test substituted date-specific 2014 NRT MOZART boundary conditions for the base case 2012 monthly-average GEOS-CHEM boundary conditions. For both GEOS-CHEM and MOZART we reduced by 10 ppb the ozone boundary condition for CAMx over the Gulf of Mexico. Several studies have attributed ozone depletion to Saharan dust, so we designed another sensitivity test that used MOZART boundary conditions but replaced the 10 ppb reduction of ozone boundary conditions with a reduction based on Saharan dust load as simulated by MOZART. The next CAMx sensitivity test used date-specific NRT fire emissions produced by NCAR for their NRT MOZART simulation. Analysis of the 2013 modeling results found a strong correlation between a lack of cloud cover in WRF and ozone over-predictions in CAMx. The final sensitivity test used a modified version of WRF developed by Dr. Kiran Alapaty’s research group at EPA that includes feedback of subgrid cloud information to radiation schemes in WRF, which was expected to reduce persistent ozone over-predictions.

The model performance evaluation shows that base case CAMx ozone tended to be higher than measured values. The over-prediction of daytime ozone concentrations appeared to be due in part to over-predictions of solar radiation in many cases, where WRF failed to accurately depict the timing and/or location of cloud cover. This continues to be an area which we will investigate, and we expect to gain additional information from other Texas projects.

The daily performance evaluations show that CAMx tended to over-predict ozone levels in the DFW and Houston areas during most days in September and October 2014. NRT MOZART boundary conditions, which include a flat 10 ppb ozone decrease, tended to reduce biases more than a similar run with ozone decreases based on the presence of dust. The effects from both runs were more pronounced in areas influenced by transport from the Gulf of Mexico. Wesely dry deposition improved ozone bias on some days where the base case had the highest positive biases. Where ozone impacts in DFW from near real-time fires were highest, ozone under-predictions were improved by the addition of fire emissions.

Saharan dust was frequently transported to Texas during the 2014 ozone season with TCEQ daily forecasts predicting Saharan dust events on 55 of the 92 days (60%) from June 1 through August 31, 2014. Since ozone impacts from dust in the sensitivity simulation appeared to be lower than what was observed or suggested by several studies, we plan to use a more refined approach that uses dust from MOZART to reduce ozone boundary conditions by a greater amount.

Wesely dry deposition also tended to decrease large positive ozone biases on most days. We propose that higher dry deposition velocities from lower surface resistances on these days cause the ozone reductions The Wesely simulation sometimes produces the largest positive biases on a given day. Further investigation is needed to determine the cause of these over-predictions.

We also observe some ozone over-predictions in the Houston area related to unrealistic ozone buildup offshore, which is then transported inland with the afternoon sea breeze. We plan to test and implement an iodine chemistry scheme in 2015, which will be simplified in order to accommodate operational time constraints.

Recommendations

We identify five categories in which improvements can be made to the NRT ozone modeling system in 2015: 1) boundary conditions, 2) solar radiation, 3) chemistry, 4) emissions, and 5) model configurations. We plan to improve boundary conditions by incorporating the NRT MOZART boundary conditions into the base model configuration and changing the flat 10 ppb decrease in ozone boundary conditions to 15 ppb. We also propose to modify the dust sensitivity by either including coarse dust in the adjustment or by using a larger scaling factor. We propose to improve solar radiation performance in the model by testing the Multi Scale Kain-Fritsch (MSKF) cumulus parameterization in WRF. Because photosynthetically active radiation (PAR) used in the MEGAN biogenics calculation does not currently account for attenuation caused by subgrid clouds, we propose to make adjustments to PAR within MEGAN. We observe that CAMx tends to over-predict ozone over the Gulf, due to a lack of halogen chemistry that destroys ozone. We recommend including iodine chemistry using a simplified scheme that can operate under the NRT system's time constraints. We plan to improve emissions in the model by incorporating new MEGAN input databases and source code, including NRT fire emissions, updating the anthropogenic emissions inventory, and re-speciating NOx emissions from ship plumes and fires. Finally, we address model configuration by using the Wesely dry deposition scheme and implementing 4 km domains covering the Houston-Galveston-Brazoria and Beaumont-Port Arthur (HGBPA) and Dallas-Fort Worth regions.

The website for the NRT ozone modeling system can be improved by applying the following: 1) dynamic charting of "zoom-able" ozone time series updated hourly in near real-time; 2) presenting ozone scatter plots at each CAMS site or Texas region with regression lines and correlation coefficients; 3) integrating Google maps for site selection; and 4) improving the presentation of model performance statistics.

Table ES-1. CAMx sensitivity simulations utilized in the NRT ozone modeling system. The sensitivity tests in the last five rows (FINN NRT Fires, Alapaty WRF, Wesely dry deposition, MOZART BCs, and MOZART BCs + dust O3) were selected to run for an extended period of time – September 9 to October 20, 2014.

Sensitivity Simulation	Description
Biogenic isoprene divided by 4	MEGAN biogenic isoprene emissions divided by 4
No anthropogenic emissions	CAMx run with natural emissions sources only
Isoprene Nitrates produce less NOx	In the reaction of INTR with OH the yield of NOx is reduced from 63% to 40%
Biogenic VOC divided by 2	MEGAN biogenic VOC emissions divided by 2
Southeast Louisiana NOx divided by 2	Anthropogenic NOx in Baton Rouge and New Orleans divided by 2
Stratiform Subgrid Clouds	Stratiform subgrid clouds diagnosed by WRFCAMx
HGBPA 4 km + Exp 12 km	Addition of 4 km domain over HGBPA and expansion of Rider 8 12 km domain to include Ohio River Valley and Southeastern states
DFW 4 km	Addition of 4 km domain over Dallas Fort Worth region
FINN Near Real-Time Fires	Latest fires data added to inventory
Alapaty WRF	WRF run with Alapaty modification, which feeds back subgrid cloud information to the radiation schemes in WRF
Wesely dry deposition scheme	Switch dry deposition scheme from Zhang to Wesely
MOZART BCs	Boundary conditions extracted from near real-time MOZART simulation.
MOZART BCs + dust O3	Same configuration as MOZART BC run, but used MOZART fine dust concentrations to scale ozone BCs and adjust photolysis rates in the model

1.0 BACKGROUND

Near real-time modeling presents a unique set of challenges not present in retrospective modeling. All steps in the process must be completely automated and run at a specific time each day, which coincides with model data availability. In addition, model configuration options must be chosen carefully in order to produce model results within the modeling time window. This time window has to account for potential delays inherent in the process, including data unavailability, slower than normal runtimes due to anomalous conditions (e.g. high winds, convective activity), etc.

The purpose of this study is to assist TCEQ by implementing and evaluating a near real-time (NRT) ozone modeling system for Texas. SIP modeling by TCEQ and NRT ozone modeling by ENVIRON will be synergistic and mutually beneficial. We evaluate model performance statistics for the base and sensitivity simulations to measure the impacts of different model configurations and identify areas for improvement.

We presented a complete overview of the 2013 project in Johnson et al. (2013). We found that the ozone model performed well when high ozone was observed. A general lack of cloud cover and stagnant conditions from WRF meteorology led to ozone over-predictions when observed ozone was low to moderate. Lessons learned from the sensitivity simulations run in 2013 have aided us in our design of the 2014 base model configuration, in terms of performance and reliability.

This report describes the various components of the development of the NRT ozone modeling system, and presents an evaluation of model results. First, we detail our modeling cycle in Section 2.1, including information about run schedule and data sources used. We then specify our WRF and CAMx configurations in Section 2.3, and describe our sensitivity tests and why they were selected in Section 2.4. Next, we present qualitative and quantitative analyses of model results in Section 3, including relative performance of the base case versus sensitivity tests. We also compare performance amongst different metropolitan regions in Texas to identify regions where the model is performing better or worse. Finally in Section 4, we discuss various recommendations as improvements to the NRT ozone modeling system, including additions to the website.

2.0 NEAR REAL-TIME OZONE MODELING SYSTEM

This section describes the various components of the development of the near real-time ozone modeling system. We detail our modeling cycle, including information about run schedule and data sources used. We then describe our WRF and CAMx configurations, CAMx sensitivity tests and finally, features of the NRT ozone modeling website.

2.1 Modeling Cycle

We utilize the modeling system as developed for the 2013 project, with updates to increase reliability and improve model performance. ENVIRON runs the NRT ozone modeling system for 79 simulation hours (3 full days from midnight to midnight in CST plus 7 hours to allow for 8-hour averages to be calculated for the third day). This simulation period is called a modeling cycle, and is run once per day. Table 2-1 details the hindcast and forecast sections of the WRF cycle initialized at August 1, 2014 00:00 CST and data sources used. The term initialization is used because the meteorological simulation is started from initial conditions at this time. ENVIRON uses 12 km NAM (North American Mesoscale) forecasting system data assimilation system (NDAS) analysis data (DiMego and Rogers, 2011) as initial conditions for the WRF meteorological model. This NDAS data is also used for boundary conditions and data assimilation during the WRF "hindcast" period. When WRF transitions to forecast mode, we then supply NAM forecast data (since observations and analyses are no longer available) to the WRF model, which we use for boundary conditions throughout the rest of the simulation period.

Table 2-2 presents nominal start times for each process in the modeling cycle. In order to supply WRF with the latest data available, ENVIRON utilizes NAM/NDAS data covering 00:00 UTC of the first modeled day (August 2 for a August 1 initialization). Accounting for possible delays in the upload of the NAM/NDAS data from NCEP (which are typically available before 22:00 CDT) and/or downloading the data, the WRF preprocessing steps begin at 23:30 CDT of the hindcast day (August 1). The WRF simulation and CAMx processing follow, with NRT images typically being uploaded by around 05:00 CDT of the first modeled day. We will consider removing the second day for a 2015 project in order to decrease overall model runtime.

Table 2-1. Description of data sources used for a WRF modeling cycle initialized at August 1, 2014 00:00 CST.

Simulation Start Time	Simulation End Time	Data Source	Description
August 1 00:00 CST (August 1 06:00 UTC)	August 1 18:00 CST (August 2 00:00 UTC)	NAM analysis data (NDAS)	WRF hindcast mode: NDAS used for initial conditions, boundary conditions, and data assimilation
August 1 18:00 CST (August 2 00:00 UTC)	August 4 07:00 CST (August 4 13:00 UTC)	NAM forecast data	WRF forecast mode: NAM used for boundary conditions

Table 2-2. Nominal run schedule for a modeling cycle initialized at August 1, 2014 00:00 CST.

Time (CDT)	Process
August 1 23:00	Download NDAS analyses and NAM forecast data
August 1 23:30	Run WPS (WRF Pre-processing System)
August 1 23:40	Begin WRF simulation
August 2 03:30	Run CAMx pre-processors
August 2 03:45	Begin CAMx base case model simulation
August 2 04:45	Run CAMx post processors
August 2 05:00	Upload forecast images for August 2-3, 2014 to www.airtomorrow.com

Model images were uploaded to the NRT ozone modeling website each morning from August 1 to October 31, 2014. Images for the current date and next date were generated for:

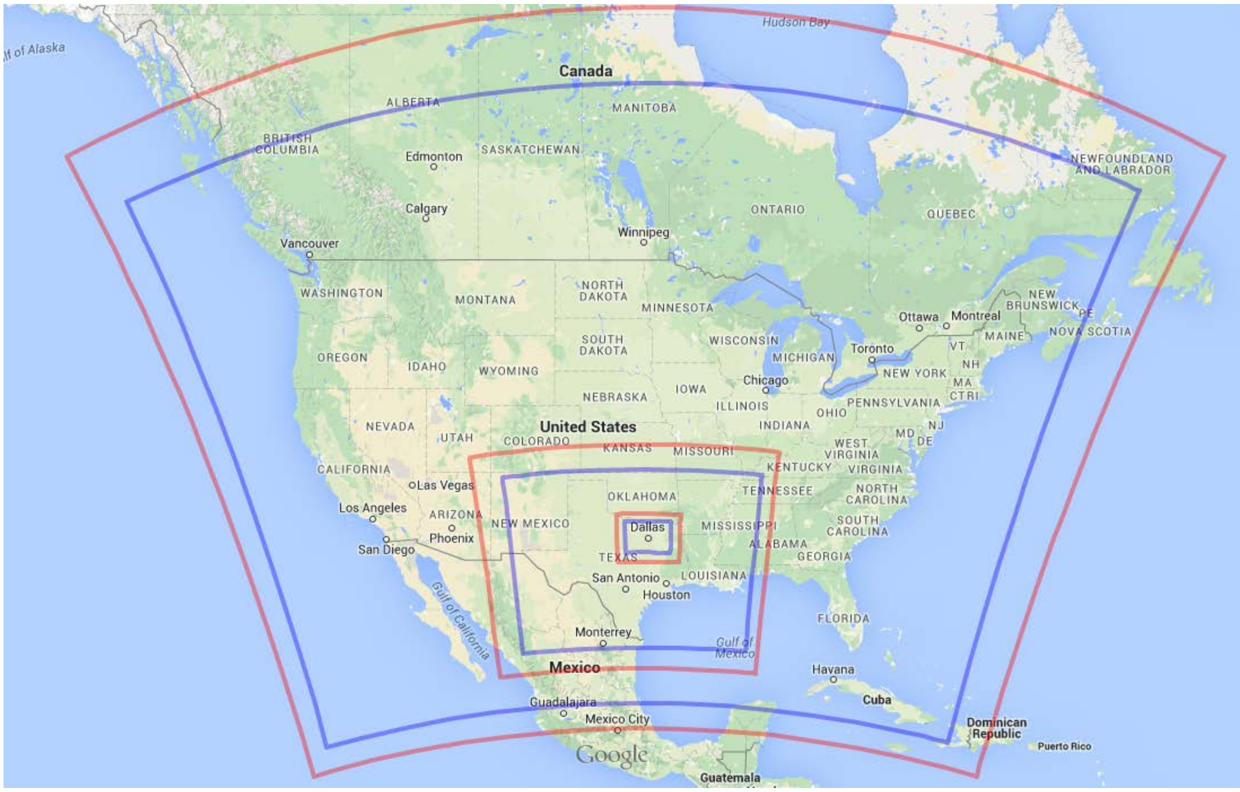
- Hourly ozone, NO, NOx, CO concentrations
- Daily maximum 1-hour and 8-hour average ozone concentrations
- Hourly 2-m temperature, PBL height, wind speed, wind vectors, incoming solar radiation

Each morning, all images above are uploaded to the site for later review. Users can select images for any modeling cycle for the base case and all sensitivity simulations.

ENVIRON has added an interactive ozone time series section to the site, which allows a user to view hourly ozone concentrations in near real-time. Ozone observations are downloaded from EPA's AIRNOW website (www.airnow.gov) at about 45 minutes past the hour in which the hourly measurement was recorded. The processing steps to extract model concentrations and make the plots at each CAMS monitor consumes about 5 minutes of time, which allows for a roughly 1-hour lag behind real time.

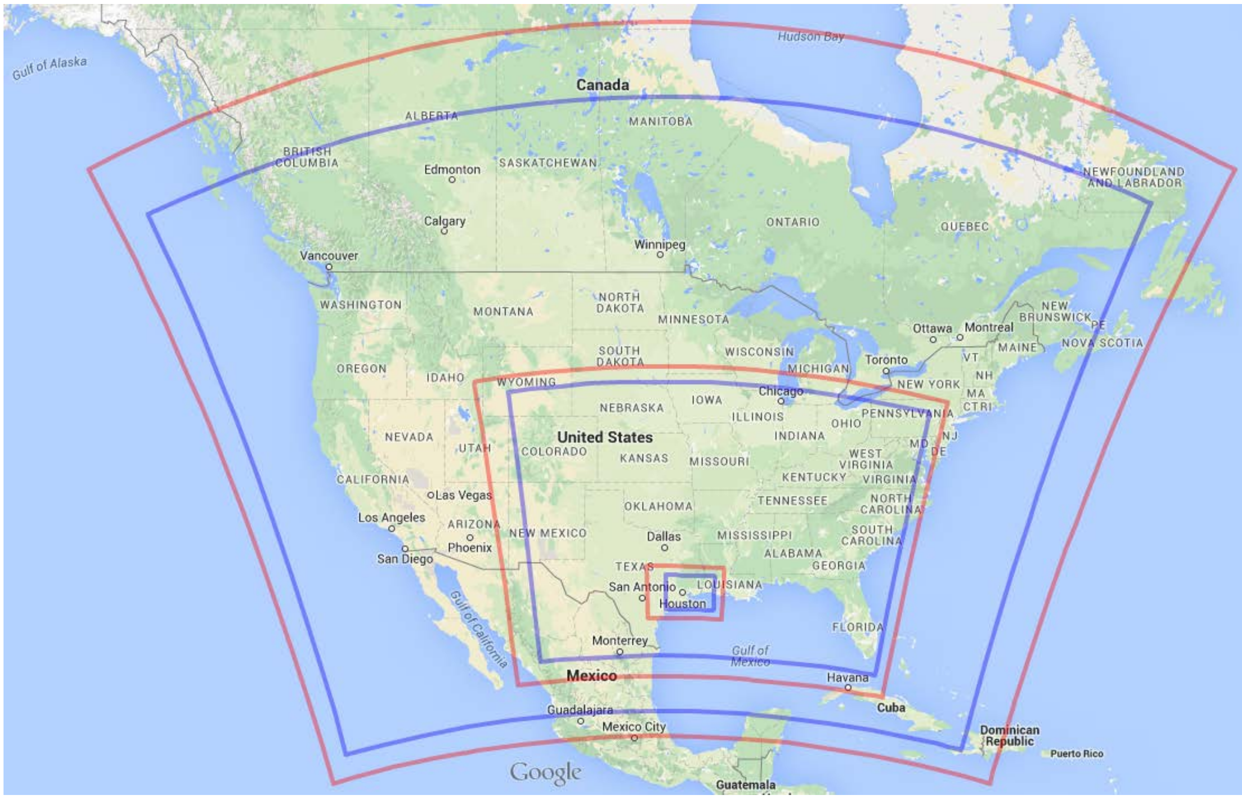
2.2 Modeling Domains

Figure 2-1 presents the 36/12 km WRF and CAMx modeling domains used for the NRT ozone modeling system. These domains are the TCEQ SIP domains, which have been used for other modeling efforts performed by ENVIRON. The 4 km WRF and CAMx domains shown in Figure 2-1 were used for the Dallas Fort Worth sensitivity simulation. An additional sensitivity simulation utilized expanded WRF and CAMx 12 km modeling domains and added 4 km WRF and CAMx domains centered over the Houston/Brazoria/Galveston-Beaumont/Port Arthur (HGBPA) region. We present the modeling domains used in this HGBPA simulation in Figure 2-2. The vertical layer mapping table from lowest 38 layers (43 total) in WRF to 28 layers in CAMx, is presented in Figure 2-3. As with the modeling domains, this layer mapping is from the TCEQ SIP modeling and other recent modeling work performed by ENVIRON.



WRF Domain	Range (km)		Number of Cells		Cell Size (km)	
	Easting	Northing	Easting	Northing	Easting	Northing
North America Domain	(-2916,2916)	(-2304,2304)	163	129	36	36
South US Domain	(-1188,900)	(-1800,-144)	175	139	12	12
Dallas Fort Worth Domain	(-204,252)	(-972,-624)	114	87	4	4
CAMx Domain	**Range (km)**		**Number of Cells**		**Cell Size (km)**	
	Easting	**Northing**	**Easting**	**Northing**	**Easting**	**Northing**
RPO 36km Domain	(-2736,2592)	(-2088,1944)	148	112	36	36
Texas 12km Domain	(-984,804)	(-1632,-312)	149	110	12	12
DFW 4km Domain	(-148,184)	(-904,-680)	83	56	4	4

Figure 2-1. WRF 36 km and 12 km and CAMx 36 km and 12 km modeling domains as used in the base model. WRF 4 km and CAMx 4 km domain turned on for Dallas-Fort Worth sensitivity simulation.

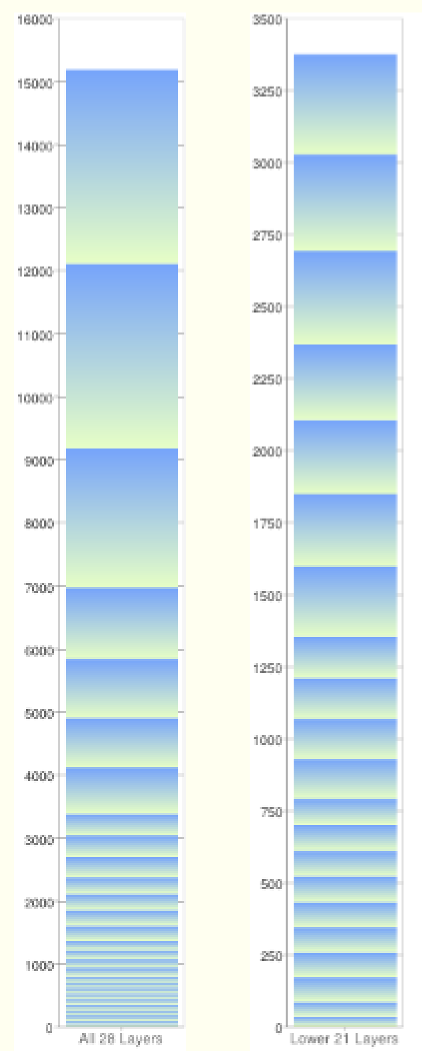


WRF Domain	Range (km)		Number of Cells		Cell Size (km)	
	Easting	Northing	Easting	Northing	Easting	Northing
North America Domain	(-2916,2916)	(-2304,2304)	163	129	36	36
Central/East US Domain	(-1188,1836)	(-1800,432)	252	186	12	12
HGBPA Domain	(-108,468)	(-1332,-936)	144	99	4	4
CAMx Domain	**Range (km)**		**Number of Cells**		**Cell Size (km)**	
	Easting	**Northing**	**Easting**	**Northing**	**Easting**	**Northing**
RPO 36km Domain	(-2736,2592)	(-2088,1944)	148	112	36	36
Texas 12km Domain	(-984,1740)	(-1632,336)	227	164	12	12
HGBPA 4km Domain	(32,400)	(-1264,-1004)	92	65	4	4

Figure 2-2. WRF 36 km, 12 km, and 4 km and CAMx 36 km, 12 km, and 4 km modeling domains as used in the HGBPA sensitivity simulation.

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 2-3. CAMx Model Layer Structure. TCEQ figure from http://www.tceq.texas.gov/airquality/airmod/rider8/modeling/domain.

2.3 Models, Configurations, and Data

We present a general overview of the input/output and processing streams for the near real-time ozone modeling system in Figure 2-4. A description of the inputs used and configuration of the WRF and CAMx models follows.

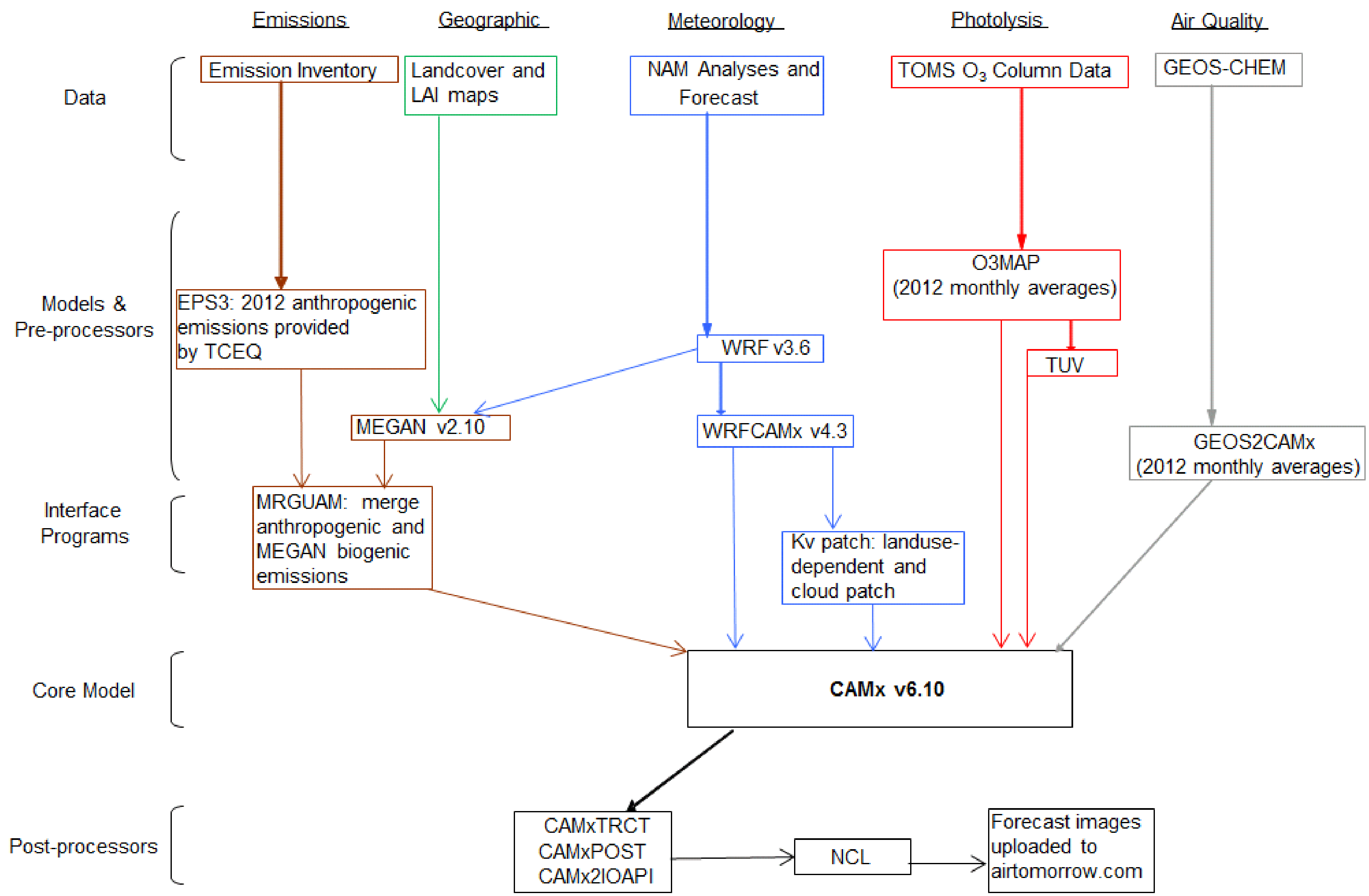


Figure 2-4. CAMx flow chart detailing input/output and processing streams for NRT ozone modeling system.

2.3.1 Meteorology

We are utilizing WRF v3.6 (released April 2014) for the NRT ozone modeling system, the latest version of the model currently available. We provide the WRF physics options in Table 2-3. This configuration is similar to that used for the TCEQ SIP modeling. We are using MPI (Message Passing Interface) for our WRF simulations, utilizing 48 of 64 available cores. Previous experience with WRF guided us to this configuration, as performance gains from either increasing the number of cores or using a hybrid MPI/OMP (Open MP) approach were found to be minimal for WRF, in contrast to CAMx.

Table 2-3. WRF v3.6 physics options used in the NRT ozone modeling system.

WRF Physics Option	Option Selected	Notes
Microphysics	WRF Single-Moment 6-class (WSM6)	A scheme with ice, snow and graupel processes suitable for high-resolution simulations.
Longwave Radiation	RRTMG	Rapid Radiative Transfer Model. An accurate scheme using look-up tables for efficiency. Accounts for multiple bands, and microphysics species.
Shortwave Radiation	RRTMG	Rapid Radiative Transfer Model. An accurate scheme using look-up tables for efficiency. Accounts for multiple bands, and microphysics species.
Surface Layer Physics	MM5 similarity	Based on Monin-Obukhov with Carslon-Boland viscous sub-layer and standard similarity functions from look-up tables
LSM	Noah	NCEP/NCAR land surface model with soil temperature and moisture in four layers, fractional snow cover and frozen soil physics.
PBL scheme	Yonsei University (YSU)	Non-local-K scheme with explicit entrainment layer and parabolic K profile in unstable mixed layer
Cumulus parameterization	1. Kain-Fritsch scheme 2. Alapaty WRF	1. Deep and shallow convection sub-grid scheme using a mass flux approach with downdrafts and CAPE removal time scale 2. Sensitivity simulation Alapaty WRF used a version of the code that includes feedback of subgrid cloud information to the radiation schemes

2.3.2 CAMx Configuration

ENVIRON selected CAMx version 6.10 (released April 2014) for the ozone forecasting system, the latest version of the model at the start of the project. The two most significant changes from version 6.0 include the update of the CB6 gas phase chemistry mechanism from CB6r1 to CB6r2.

Table 2-4 gives the CAMx configuration options that are currently in use. We utilize a hybrid MPI/OMP configuration for CAMx. We determined from model benchmarking that an 8 MPI slice x 4 OMP thread setup was the optimum configuration for this application. This configuration also allowed two sensitivity simulation to be run concurrently.

Table 2-4. CAMx v6.10 options used for the NRT ozone modeling system.

Science Options	Configuration	Comments
Model Code	CAMx Version 6.10	Released April 2014
Time Zone	Central Standard Time (CST)	
Vertical Layers	28 layers (model top approximately 100 mb)	Lowest 21 CAMx layers match lowest 21 WRF layers
Chemistry Gas Phase Chemistry Aerosol Chemistry	 CB6r2 (update from CB6r1) None	CB6r2 differentiates organic nitrates (ON) between simple alkyl nitrates that remain in the gas-phase (providing a reservoir of NO_2) and multi-functional ONs that can partition into organic aerosols (OA). ON present in OA are then assumed to undergo hydrolysis to nitric acid.
Plume-in-Grid	GREASD	Run-time consideration for NRT modeling
Photolysis Rate Adjustment	In-line TUV	Adjust photolysis rates for each grid cell to account for clouds. Certain photolysis Rates adjusted for temperature and pressure
Meteorological Processor Subgrid Cloud Diagnosis	WRFCAMx CMAQ-based	Sub-grid clouds diagnosed from WRF grid-resolved thermodynamic properties.
Horizontal and Vertical Transport Eddy Diffusivity Scheme Diffusivity Lower Limit	 K-Theory Kz_min = 0.1 m^2/s	Vertical diffusivity (Kv) fields patched to enhance mixing: 1. over urban areas in lowest 100 m (OB70 or "Kv100" patch) 2. in areas where convection is present, by extending the daytime PBL Kv profile through capping cloud tops (cloud patch)
Dry Deposition	1. Zhang et al. (2003) 2. Wesely (1989)	1. Utilizes 26 landuse categories and Leaf Area Index (LAI); used in base model 2. Run as a sensitivity simulation; utilizes 11 landuse categories and does not use LAI
Numerical schemes Gas Phase Chemistry Solver Horizontal Advection Scheme	Euler Backward Iterative (EBI) Piecewise Parabolic Method (PPM) scheme	

We are using the following CAMx inputs for the NRT ozone modeling system:

- Initial conditions extracted from GEOS-CHEM global 3-D chemical transport model simulation for 2012; only used for initial NRT ozone modeling cycle initialized on August 1, 2014 because subsequent cycles restart from previous cycle
- Boundary conditions extracted from GEOS-CHEM 2012 monthly averages; modifications made to increase unrealistically low CO concentrations and reduce impacts from 2012 wildfires in northern Manitoba. In addition, we perform a flat 10 ppb ozone reduction and apply various caps to ozone precursors over the Gulf of Mexico and Atlantic Ocean in order to deplete the ozone coming onshore, given in Table 2-5.

- NRT MOZART-4/MOPITT chemical forecasts from NCAR (http://web3.acd.ucar.edu/acresp/forecast) are used in the MOZART boundary conditions sensitivity. Chemical forecasts are run each day using MOZART-4, driven by GEOS-5 meteorology and including the standard (100 species) chemical mechanism (Emmons et al., 2010). The same caps listed in Table 2-5 are applied to the MOZART boundary conditions.
- The MOZART chemical forecasts also include fire emissions from the Fire INventory of NCAR (FINN), based on MODIS Rapid Response fire counts (Wiedinmyer et al., 2011). NCAR provides this data here: http://earthdata.nasa.gov/data/nrt-data/firms/active-fire-data. These fire emissions are used in the NRT fires sensitivity
- 2012 day-of-week specific anthropogenic emissions inventory with updates from 2013 oil and gas activity provided by TCEQ
- MEGAN v2.10 biogenic emissions using current WRF NRT modeling cycle meteorology
- WRFCAMx v4.3 using YSU Kv methodology
- Kv landuse patch up to 100 m and Kv cloud patch applied
- O3MAP: 2012 monthly averages from 1 degree TOMS satellite ozone column data
- Photolysis rates files generated using O3MAP 2012 monthly averages
- Land use / land cover inputs generated using USGS 24-category dataset; monthly LAI data from MODIS satellite
- Land use / land cover inputs mapped from 24 categories to 11 categories for Wesely dry deposition sensitivity

Table 2-5. Maximum concentration limits for ozone precursors applied to the 36 km boundary condition grid cells across the Gulf of Mexico, Caribbean Sea, and Atlantic Ocean south of Cape Hatteras.

Species	Description	Max. Concentration (ppb)
NO2	Nitrogen dioxide	0.05
CO	Carbon monoxide	150.0
N2O5	Dinitrogen pentoxide	0.001
HNO3	Nitric acid	0.25
PNA	Peroxynitric acid	0.001
H2O2	Hydrogen peroxide	0.5
NTR	Organic nitrates	0.01
FORM	Formaldehyde	0.25
ALD2	Acetaldehyde	0.05
ALDX	Propionaldehyde and higher aldehydes	0.02
PAR	Paraffin carbon bond (C-C)	1.0
OLE	Terminal olefin carbon bond (R-C=C)	0.01
ETHA	Ethane	1.0
MEPX	Methylhydroperoxide	0.1
PAN	Peroxyacetyl Nitrate	0.01
PANX	C3 and higher peroxyacyl nitrate	0.001
INTR	Organic nitrates from ISO2 reaction with NO	0.001

Species	Description	Max. Concentration (ppb)
ISOP	Isoprene	0.1
ISPD	Isoprene product (lumped methacrolein, methyl vinyl ketone, etc.)	0.1
TERP	Monoterpenes	0.05
ISP	Isoprene (SOA chemistry)	0.1
TRP	Monoterpenes (SOA chemistry)	0.05
TOL	Toluene and other monoalkyl aromatics	0.02
XYL	Xylene and other polyalkyl aromatics	0.01
SO2	Sulfur dioxide	0.1
PRPA	Propane	0.5
ACET	Acetone	0.25
KET	Ketone carbon bond (C=O)	0.05
BENZ	Benzene	0.1

2.4 Sensitivity Tests

Table 2-6 describes the sensitivity simulations used in the 2014 NRT ozone modeling system. CAMx sensitivity simulations were run in parallel with the "base case" simulation. ENVIRON selected several sensitivity tests based on evaluation of 2013 and 2014 ozone performance to investigate potential improvements and measure impacts of different model configurations, by comparing the results of the sensitivity tests with the base case model. Five of these simulations were selected to run for an extended period of time – September 9 to October 20, 2014 – so that the simulations could be compared against one another and the base case.

Table 2-6. CAMx sensitivity simulations utilized in the NRT ozone modeling system. The sensitivity tests in the last five rows (FINN NRT Fires, Alapaty WRF, Wesely dry deposition, MOZART BCs, and MOZART BCs + dust O3) were selected to run for an extended period of time – September 9 to October 20, 2014.

Sensitivity Simulation	Description
Biogenic isoprene divided by 4	MEGAN biogenic isoprene emissions divided by 4
No anthropogenic emissions	CAMx run with natural emissions sources only
Isoprene Nitrates produce less NOx	In the reaction of INTR with OH the yield of NOx is reduced from 63% to 40%
Biogenic VOC divided by 2	MEGAN biogenic VOC emissions divided by 2
Southeast Louisiana NOx divided by 2	Anthropogenic NOx in Baton Rouge and New Orleans divided by 2
Stratiform Subgrid Clouds	Stratiform subgrid clouds diagnosed by WRFCAMx
HGBPA 4 km + Exp 12 km	Addition of 4 km domain over HGBPA and expansion of Rider 8 12 km domain to include Ohio River Valley and Southeastern states
DFW 4 km	Addition of 4 km domain over Dallas Fort Worth region
FINN Near Real-Time Fires	Latest fires data added to inventory
Alapaty WRF	WRF run with Alapaty modification, which feeds back subgrid cloud information to the radiation schemes in WRF
Wesely dry deposition scheme	Switch dry deposition scheme from Zhang to Wesely
MOZART BCs	Boundary conditions extracted from near real-time MOZART simulation.
MOZART BCs + dust O3	Same configuration as MOZART BC run, but used MOZART fine dust concentrations to scale ozone BCs and adjust photolysis rates in the model

The first five CAMx sensitivity tests are designed to explore impact of emissions, with the goal of finding potential sources of persistent ozone over-predictions. The first CAMx sensitivity test reduced isoprene emissions from the MEGAN biogenic emissions model by a factor of four. Current modeling studies conducted by ENVIRON suggest that the MEGAN biogenic emissions model may be generating excessive isoprene emissions (ENVIRON and ERG, 2013). CAMx modeling performed for the 2013 modeling project demonstrated that ozone over-predictions were reduced and model performance statistics improved when MEGAN isoprene was reduced by a factor two. We wanted to determine if a further reduction in isoprene would reduce ozone over-predictions. This sensitivity, as well as a similar sensitivity which reduced all biogenic VOC by half, showed relatively small ozone impacts and so was replaced.

The next CAMx sensitivity simulation reduced Southeast Louisiana NOx emissions by half. We observed the base model frequently predicted very high ozone levels (exceeding 100 ppb) in Southeast Louisiana that appeared to be unrealistically high. These areas of elevated ozone are then sometimes transported into Texas via the Gulf leading to ozone over-predictions in HGBPA and nearby regions. The results of this test were promising, in that ozone levels were greatly reduced in Southeast Louisiana. But because we do not have any evidence that NOx emissions are overestimated in this area, we decided to discontinue the sensitivity

The next CAMx sensitivity simulation turned on stratiform sub-grid clouds. WRFCAMx diagnoses sub-grid cloudiness from grid-resolved thermodynamic parameters in a manner similar to that used in the Community Multiscale Air Quality Modeling System (CMAQ) model (Emery et al., 2010). Photochemical production of ozone is strongly influenced by the presence of clouds, which can both attenuate and enhance the actinic irradiance of ultraviolet (UV) and visible radiation responsible for photolysis. This sensitivity was designed to measure the impact of stratiform sub-grid cloudiness on surface ozone concentrations in Texas. We found minimal ozone impacts from this sensitivity over a roughly 2 week period, and decided to replace it with other sensitivities that were ready to be tested.

The next CAMx sensitivity simulation utilized an expanded 12 km domain and 4 km domain centered over the HGBPA region. The expanded 12 km domain covers most of the Eastern U.S. and therefore has many more grid cells than the Rider 8 domain used in the base model. Due to the extra computational cost imposed by the larger domain, WRF and CAMx runtimes roughly doubled and so this domain has been ruled out for inclusion in the 2015 project. Timing tests performed for the HGBPA 4 km show similar runtimes compared to a similarly sized 4 km domain covering the Dallas-Fort Worth region. Combined, these two 4 km domains roughly double model runtime over the base case, but we believe the potential benefits of the higher resolution warrant inclusion into the base configuration for 2015.

We developed and tested the following set of CAMx sensitivity simulations for the September 9 through October 20, 2014 period, in order to evaluate the ozone impacts relative to the base case simulation. We present an evaluation of these sensitivity simulations in Section 3.

The first of these simulations used date-specific 2014 NRT MOZART-4/MOPITT chemical forecasts from NCAR (http://web3.acd.ucar.edu/acresp/forecast). Chemical forecasts are run each day using MOZART-4, driven by GEOS-5 meteorology and including the standard (100 species) chemical mechanism (Emmons et al., 2010). We apply the same flat ozone decrease and ozone precursor caps to the MOZART boundary conditions are for the base case.

The MOZART chemical forecasts also include fire emissions from the Fire INventory of NCAR (FINN), based on MODIS Rapid Response fire counts (Wiedinmyer et al., 2011). NCAR provides this data here: http://earthdata.nasa.gov/data/nrt-data/firms/active-fire-data. We used these date-specific fire emissions as part of a CAMx sensitivity designed to examine the ozone impact of NRT fire emissions.

The next sensitivity used an updated version of WRF which includes feedback from the effects of sub-grid clouds on radiation (Alapaty et al., 2012). This is important because the radiation schemes in WRF are not aware of sub-grid cumulus clouds, thereby allowing the sun to shine through what should be cloudy sky. This has the effect of artificially increasing the amount of radiation reaching the surface, which has far-reaching effects. One of these effects has significant impacts on biogenic emissions. Results from the 2013 project showed that under-predictions of solar radiation in the afternoon hours led to persistent over-predictions of ozone. We anticipated that the Alapaty WRF sensitivity would reduce shortwave radiation at the surface, thereby decreasing positive ozone biases.

The next CAMx sensitivity simulation used the Wesely dry deposition scheme instead of the base case Zhang scheme. A recent study by Park et al., 2014 compared the Wesely and M3DRY dry deposition treatments in CMAQ. The study found that lower surface resistances employed by the Wesely scheme generated higher dry deposition velocities that correlated better with measurements made during a field campaign in forested areas of Colorado. We wanted to determine if we could increase ozone deposition velocities in a similar manner (thereby reducing positive ozone biases) by switching from Zhang to Wesely dry deposition in CAMx.

The last sensitivity test combined the MOZART boundary conditions simulation with a reduction of ozone boundary conditions in proportion to Saharan dust loading. There is evidence for Saharan dust depleting ozone during atmospheric transport, e.g., "ozone reductions of up to 40% have been observed in Saharan dust outflow (DeReus et al., 2000; Umann et al., 2003; Bonasoni et al., 2004)" in Fairlie et al. (2010). Fairlie et al. found no evidence for ozone depletion by Gobi desert dust during transport across the Pacific Ocean, and it may be that Saharan dust is effective in depleting ozone due to its mineral composition. Numerous studies have attributed ozone depletion to Saharan dust. Andrey et al., (2014) have the following statement:

> *"Cuevas et al. (2013), based on eight years of daily surface O_3 and PM_{10} (the concentration of particulate matter up to 10 um in size) at IZO*, found a negative logarithmic relationship between PM_{10} and surface O_3. The daily mean PM_{10} concentrations for clean conditions at IZO are normally <2 ug/m^3, whereas for dusty conditions, the PM_{10} concentrations fall within the 20 -300 ug/m^3 range (Rodríguez et al., 2009). Using this PM_{10}-O_3 relationship for summertime, Rodríguez et al. (2009) estimated an O_3 reduction of 40% for dusty conditions (PM_{10} = 20 ug/m^3) compared to O_3 levels in clean conditions (PM_{10} = 2 ug/m^3), which is approximately equivalent to our findings."*

*IZO is the subtropical high mountain Izãna station (2373 m a.s.l.) in the Canary Islands.

This logarithmic relationship of Cuevas et al. (2013) is not readily usable. Instead, we applied the following simple adjustment to ozone boundary conditions based on the summary statement of Andrey et al.:

$$\Delta O3\ (\%) = 2 \times FCRS(ug/m^3)$$

where FCRS (CAMx species representing fine dust) is capped at 20 ug/m^3 when the adjustment is applied. This adjustment results in a 40% reduction in ozone BCs when FCRS is 20 ug/m^3 or higher.

Ozone depletion by Saharan dust has previously been modeled in CAMx by adding irreversible uptake of ozone on dust surfaces with a reactive uptake coefficient (γ) of 5×10^{-5} based on literature review (Astitha and Kallos, 2009). For the purpose of sensitivity testing with the NRT modeling system, we are modifying ozone boundary conditions rather than modifying CAMx, but CAMx modifications are a possible future development if sensitivity tests suggest that ozone destruction by Saharan dust partly explains very low ozone (< 20 ppb) observed on the Texas coast during periods of persistent onshore flow.

3.0 MODEL EVALUATION

This section presents quantitative and qualitative evaluations of the CAMx ozone performance and its dependence on the accuracy of the meteorological fields and other factors. The objective was to evaluate the sensitivity simulations with respect to the base model to determine which configuration options help reduce overall ozone bias. This will help us to implement corrections to reduce discrepancies between observed and predicted ozone concentration patterns and peaks.

We note that we are examining a relatively short time period during an atypical ozone season. In fact, almost all regions in Texas recorded the lowest 4th highest daily maximum ozone concentrations over the past 10 years (Figure 3-1). The 2014 ozone season is characterized by frequent dust events and infrequent and/or short periods of elevated ozone. In particular, sensitivity to Gulf transport of ozone and Saharan dust may be reduced during a more typical ozone season.

In the sections below, we first provide results from the regional analysis of the base configuration, focusing on quantitative evaluation of the meteorological fields and ozone. We then describe the results of a solar radiation analysis by Texas region. Next, we present daily ozone bias statistics for all sensitivity simulations in the Dallas-Fort Worth and HGB regions, supplemented with qualitative analyses to highlight differences that are sometimes observed between statistics and time series at individual monitoring locations. Finally, we present an overall assessment of model performance, including our understanding of the possible reasons for poor performance on certain days in Dallas-Fort Worth and HGB.

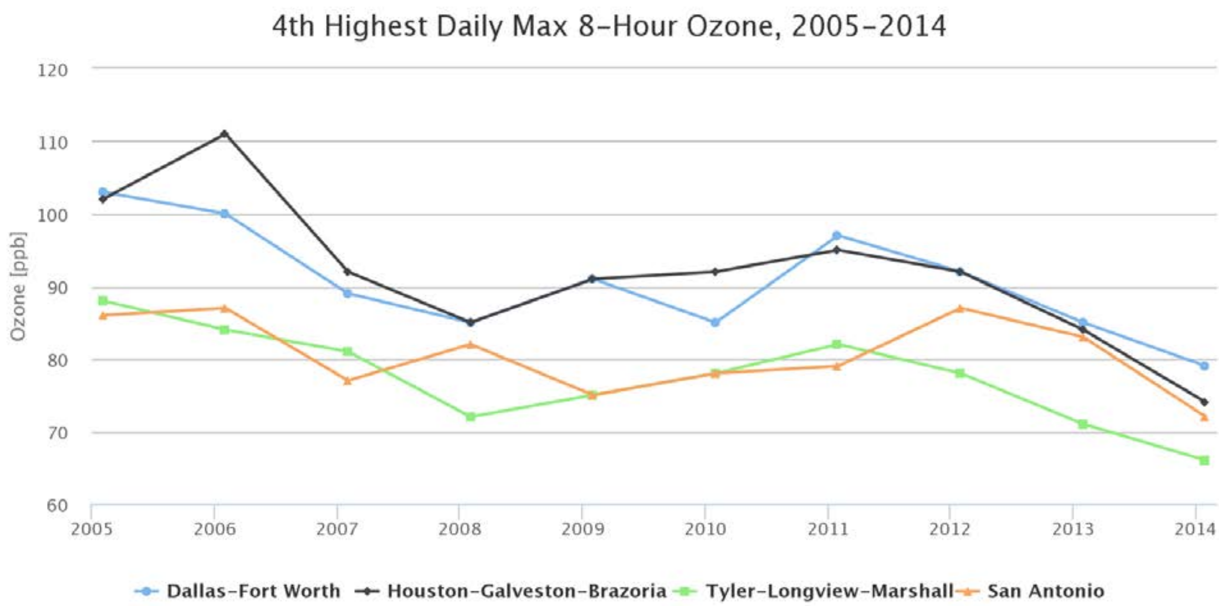


Figure 3-1. 4th highest daily maximum 8-hour ozone concentrations for the years 2005-2014 for the Dallas-Fort Worth, Houston-Galveston-Brazoria, Tyler-Longview-Marshall, and San Antonio metropolitan regions. Each data point represents the maximum concentration over all monitors in each region.

3.1 Model Performance Evaluation and Sensitivity Analysis

3.1.1 Statistics

The CAMx NRT ozone modeling website has been set up to compute model performance statistics for each CAMx run when observed data are available. Statistical metrics are computed for individual CAMS monitoring sites, major urban areas and the entire CAMS network.

The statistical metrics computed for CAMS monitoring locations are:

- Normalized Mean Bias (NMB)

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

where P_i and O_i are the predicted and observed values (O_i,P_i) in a data pair and N is the number of observed/modeled data pairs.

- Normalized Mean Error (NME)

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

- Correlation coefficient (r)

$$r = \frac{\sum_{i=1}^{N} P_i O_i - \frac{\left(\sum_{i=1}^{N} P_i\right)\left(\sum_{i=1}^{N} O_i\right)}{N}}{\sqrt{\left[\left(\sum_{i=1}^{N} P_i^2 - \frac{\left(\sum_{i=1}^{N} P_i\right)^2}{N}\right)\left(\sum_{i=1}^{N} O_i^2 - \frac{\left(\sum_{i=1}^{N} O_i\right)^2}{N}\right)\right]}}$$

The normalized mean bias and error replaced the mean normalized bias (MNB) and mean normalized error (MNE), respectively, which were originally posted on the website. The computation for MNB and MNE weigh predicted-observed pairings with smaller observed values more than pairings with higher observations; the normalized mean bias and error computations do not have such biases.

Statistical metrics were computed for:

- Hourly ozone, NO, NOx and CO
- Hourly temperature, wind speed, wind direction, total solar radiation

A 20 ppb threshold was applied to observed ozone concentrations; thresholds of 1 mph and 10 Watts/m^2 were employed for wind speed/direction and solar radiation, respectively. Since wind direction is an angular measurement, we correct for the switchover that occurs at 360° by taking adjusting the hourly bias in the following cases:

if $P_i - O_i > 180°$, $bias = P_i - (O_i + 360°)$

or

if $P_i - O_i < -180°$, $bias = (P_i + 360°) - O_i$

We evaluated model performance for the base simulation for the entire modeling period, August 1 through October 30, 2014. This evaluation includes 2-meter temperature, 10-m wind speed and wind direction, solar radiation, and ozone for the base simulation.

Since previous analyses of over-predictions of ozone appeared to be correlated with solar radiation over-predictions, we decided to evaluate solar radiation statistics for the base run versus a new sensitivity (subgrid cloud diagnosis turned on; no resulting CAMx simulation) and the Alapaty WRF run. We chose the September 9 through October 20 time period for this analysis. We start with September 9 so that the Alapaty sensitivity simulation results are available with consistent run configurations and spinup accounted for. This time period was also used to evaluate five CAMx sensitivity simulations against the base case, some of which were run retrospectively after the near real-time modeling had finished.

3.1.2 Regional Analysis of Base Configuration

We concluded from the 2013 project that poor performance for ozone on some days could be mostly attributed to inaccurate meteorology. Table 3-1 shows the model performance statistics for the meteorological variables covering August 1 to October 30 for all regions in Texas where air quality measurements are available. Note that the model performance statistics are computed for all hours (day and night), except for solar radiation.

The WRF simulations demonstrated considerable skill in predicting temperatures in all regions. The normalized mean bias and error were less than ±2 % and 6 %, respectively, in every region. In fact, all regions except Waco show NMB values less than ±1 %. It should be noted however, that with NME several times larger than NMB at most locations, it is likely that the very low biases are the result of mid-day over-predictions "cancelling out" overnight low under-predictions. We present an example of this phenomenon in Figure 3-2, which shows the temperature time series for the base model versus observations for a 48-hour period starting from 03:00 CST on August 2, 2014 at the Beaumont Downtown CAMS monitor.

Wind direction performance during the three month period showed respectable biases that were within ±8 % in all regions; the NME were between 20 % and 30 % in most regions. However, wind speed statistics were not as good. WRF tended to over-predict the wind speed in all but two areas, Corpus Christi and Waco. The Waco, Corpus Christi, and Dallas-Fort Worth regions had the lowest NMB (-6 % to 5 %) and the lowest NME (all near 30 %). The Tyler-Longview-Marshall area had the highest normalized mean bias and among the highest error, largely due to the fact that its average observed wind speed during the three month period was lower than all other regions. As noted in the 2013 project, the WRF predicted winds during the afternoon hours were frequently lighter than the observed winds on some days with poor model performance. Thus, the wind speed over-prediction bias from the model performance statistics is likely due to over-prediction of nocturnal winds. This has also been found in a WRF modeling study conducted by NOAA for TCEQ (Lee et al., 2012). In addition, recent WRF model performance efforts conducted by ENVIRON for a Northeast Texas June 2006 ozone episode show that inappropriate monitor siting at the Longview and possibly Karnack CAMS sites may play a role in inflating wind speed over-predictions under certain wind direction regimes. We are also investigating the use of MODIS/NLCD landcover information, which should serve to increase surface roughness in forested areas, which could reduce wind speed over-predictions.

The solar radiation performance statistics indicate an over-prediction bias in all areas. WRF performed best in the Austin and Waco regions (NMB for both regions of 1 %, NME of around 30 %) and tended to do worse near coastal regions like BPA and HGB. We will investigate a new

Multi Scale Kain-Fritsch cumulus parameterization in WRF that may improve characterization of fair weather cumulus clouds. We provide more details in Section 4.2. A statistical comparison of different solar radiation approaches is given below.

Ozone performance appears better for 2014 than 2013 although the comparison is not direct because observed ozone was generally lower in 2014 than 2013. For the August 1 to October 30, 2014 period the base case shows an NMB of 22% and NME of 29%, compared to NMB of 25% and NME of 36% for the 2013 project's "best case" configuration, which covered August 26 through October 15, 2013. Ozone performance is best for the El Paso, Waco, DFW, and San Antonio regions (NMBs from 9 to 13% and NMEs from 19 to 23%) and worst for the Harlingen, Tyler, Houston, and Beaumont regions (NMBs from 30 to 36% and NMEs from 34 to 40%).

Table 3-2 shows the results of a statistical analysis undertaken to examine the shortwave radiation impact of various subgrid cloud configurations and covers the September 9 through October 20, 2014 period. The "DIAG off" column is simply the WRF shortwave radiation (SWRAD) pass-through which has no influence from sub-grid clouds. "base" attenuates radiation for the presence of diagnosed subgrid clouds using algorithms from WRFCAMx. Finally, the "Alapaty" column uses radiation from the Alapaty WRF run. All hourly observed values < 10 W m^{-2} were screened out before calculating stats. The DIAG off SWRAD is biased high because cloudiness is under-represented. Note the implication that using SWRAD directly from WRF as input to MEGAN should be expected to bias high the resulting biogenic emissions. The base case improves bias but degrades correlation and error implying that the cloud diagnosis lacks skill (i.e., diagnosed clouds are frequently in the wrong place at the wrong time). The Alapaty WRF results show the best NME and r for almost all regions but also have the highest NMB for all regions. This result is counter-intuitive and further investigation would be needed to understand the Alapaty SWRAD results. However, we will soon obtain an update to the Alapaty WRF modifications and so believe further work on the current Alapaty scheme is not warranted.

Table 3-3 lists the model performance statistics for 1-hour ozone from September 9 to October 20, 2014 for the entire state of Texas and for each air quality region. This time period is the same as used for the shortwave radiation analysis above. The results are shown for the base case configuration and from five sensitivity simulations run during the same period – the Wesely dry deposition simulation (Wesely), the NRT MOZART boundary conditions simulation (MOZART), the MOZART BC simulation with ozone BCs adjusted for the presence of dust (Dust O3 MOZART), NRT FINN fires simulation (Fires), and the Alapaty WRF simulation (Alapaty). The Wesely and Dust O3 MOZART simulations were performed retrospectively.

All six runs over-predicted ozone in all regions. In the base case, the normalized mean error in most regions was only slightly larger than the mean normalized bias for some of the worst performing regions (HGB: NMB of 30%, NME of 35%, BPA: NMB of 32%, NME of 36%, and Tyler: NMB of 26%, NME of 29%), indicating that the errors in these regions were dominated by the positive bias. We observe larger discrepancies between NMB and NME for DFW (NMB of 10%, NME of 24%), El Paso (NMB of 12%, NME of 21%), and San Antonio (NMB of 14%, NME of 25%), indicating that negative biases are more prevalent in these regions. The worst performing regions all have biases greater than 30% (HGB, BPA, Laredo, and Harlingen).

The CAMx sensitivity with NRT MOZART boundary conditions demonstrates the lowest bias overall (18%) and in 7 of the 11 regions. The MOZART boundary conditions also produced the lowest NME overall (27%) and in 8 of the 11 regions. This sensitivity preserves the modifications to boundary conditions for ozone (including a flat 10 ppb decrease over the Gulf of Mexico) and ozone precursors; therefore, this test is a pure sensitivity to the MOZART boundary conditions. The two regions that show the most improvement over the base case – El Paso and Harlingen – are two regions influenced by boundary conditions; NMB was reduced 6 to 8% and NME by 4%. Since ozone is still over-predicted in all regions, we propose to increase the ozone boundary condition adjustment from 10 to 15 ppb over the Gulf of Mexico for NRT modeling performed in 2015.

The CAMx sensitivity with Wesely dry deposition scheme shows considerable improvement over the base case and produced the lowest NMB for the DFW, El Paso, Laredo, and Waco regions (NMB of 5%, 2%, 29%, and 6%, respectively). The Wesley simulation also shows slightly better NME statistics than MOZART BC for 3 regions (DFW, Harlingen, and Laredo), but they are all within 1% of the MOZART BC NME values in those regions. We propose to use the Wesely dry deposition scheme for NRT modeling performed in 2015 in order to further reduce ozone bias.

The CAMx sensitivity with MOZART boundary conditions and dust shows improvement over the base case, but they are smaller than those shown by the MOZART BC simulation. We note that there is an important difference in ozone boundary conditions from the prior sensitivity: the flat 10 ppb ozone decrease in Gulf of Mexico boundary conditions is removed in favor of the adjustment to ozone BCs for the presence of fine dust. Therefore, we can assume that the flat 10 ppb adjustment produces more realistic ozone concentrations over the Gulf. Analysis of Galveston ozone time series from Oct 1-3, 2014 (Figure 3-3) shows that this sensitivity decreases ozone by close to 10 ppb. We will design a new dust sensitivity simulation for 2015 where we will increase the ozone impact from dust. More information about the proposed dust simulation is provided in Section 4.2.

Next, we observe that including MODIS-detected NRT fire emissions from the FINN database increases positive ozone biases in all regions, by an average NMB and NME of around 1%. Skill is improved in all regions except Harlingen and Tyler. We intend to keep this configuration as a sensitivity going forward so that we can evaluate the ozone impacts of any large fire events that may occur in 2015.

Finally, we find that the Alapaty WRF simulation performed worst of all simulations, increasing positive biases in all regions. We anticipated an overall reduction in shortwave radiation from the feedback of subgrid cloud information to the radiation schemes in WRF, which should have led to lower ozone concentrations. The results of the shortwave radiation analysis showed that solar radiation NMB actually increased positive biases over the base case, but because a newer version of the scheme will be released soon, we don't believe further work on the current scheme is warranted. We expect to use the new version of the Alapaty scheme for a sensitivity simulation in 2015.

ENVIRON

Table 3-1. Model performance statistics by area for the base simulation for August 1, 2014 to October 30, 2014.

Region	2-m Temperature			10-m Wind Speed (Cutoff 1 mph)			10-m Wind Direction (Cutoff 1 mph)			Shortwave Radiation (Cutoff 10 W m^{-2})			Ozone (Cutoff 20 ppb)		
	NMB (%)	NME (%)	r	NMB (%)	NME (%)	r	NMB (%)	NME (%)	r	NMB (%)	NME (%)	r	NMB (%)	NME (%)	r
All	0.2	3.7	0.874	14.7	42.0	0.578	0.7	22.4	0.482	12.8	33.9	0.827	22.3	28.8	0.671
Austin	-0.3	3.6	0.922	24.8	50.6	0.538	3.3	21.8	0.395	1.0	28.6	0.843	22.4	27.2	0.673
Beaumont	-0.7	4.0	0.797	16.0	45.4	0.498	1.2	22.4	0.547	25.1	43.5	0.771	36.3	40.0	0.598
Corpus Christi	-0.2	2.7	0.891	-3.0	32.3	0.649	-6.1	19.3	0.543	14.0	35.5	0.817	25.3	29.4	0.702
Dallas Fort Worth	0.3	3.2	0.945	4.9	34.0	0.612	4.9	18.8	0.516	14.7	31.9	0.854	11.8	23.1	0.687
El Paso	-0.1	4.7	0.881	22.2	52.4	0.511	8.1	38.1	0.288	13.8	32.1	0.829	8.7	20.4	0.668
Harlingen	-0.7	2.9	0.859	21.3	38.7	0.632	-6.5	19.8	0.437	11.8	32.3	0.845	30.0	33.5	0.679
Houston	0.2	3.5	0.879	11.6	41.2	0.591	1.4	21.4	0.531	19.7	41.3	0.771	33.5	38.4	0.609
San Antonio	-0.8	3.2	0.930	19.5	43.1	0.584	-2.7	21.8	0.529	12.6	33.6	0.835	12.7	22.9	0.694
Tyler	0.9	3.1	0.949	36.2	49.3	0.632	6.1	21.3	0.519	14.5	31.6	0.862	31.4	33.8	0.665
Waco	3.4	5.8	0.691	-6.4	33.1	0.529	-2.6	19.5	0.510	0.9	28.1	0.846	11.1	18.8	0.733

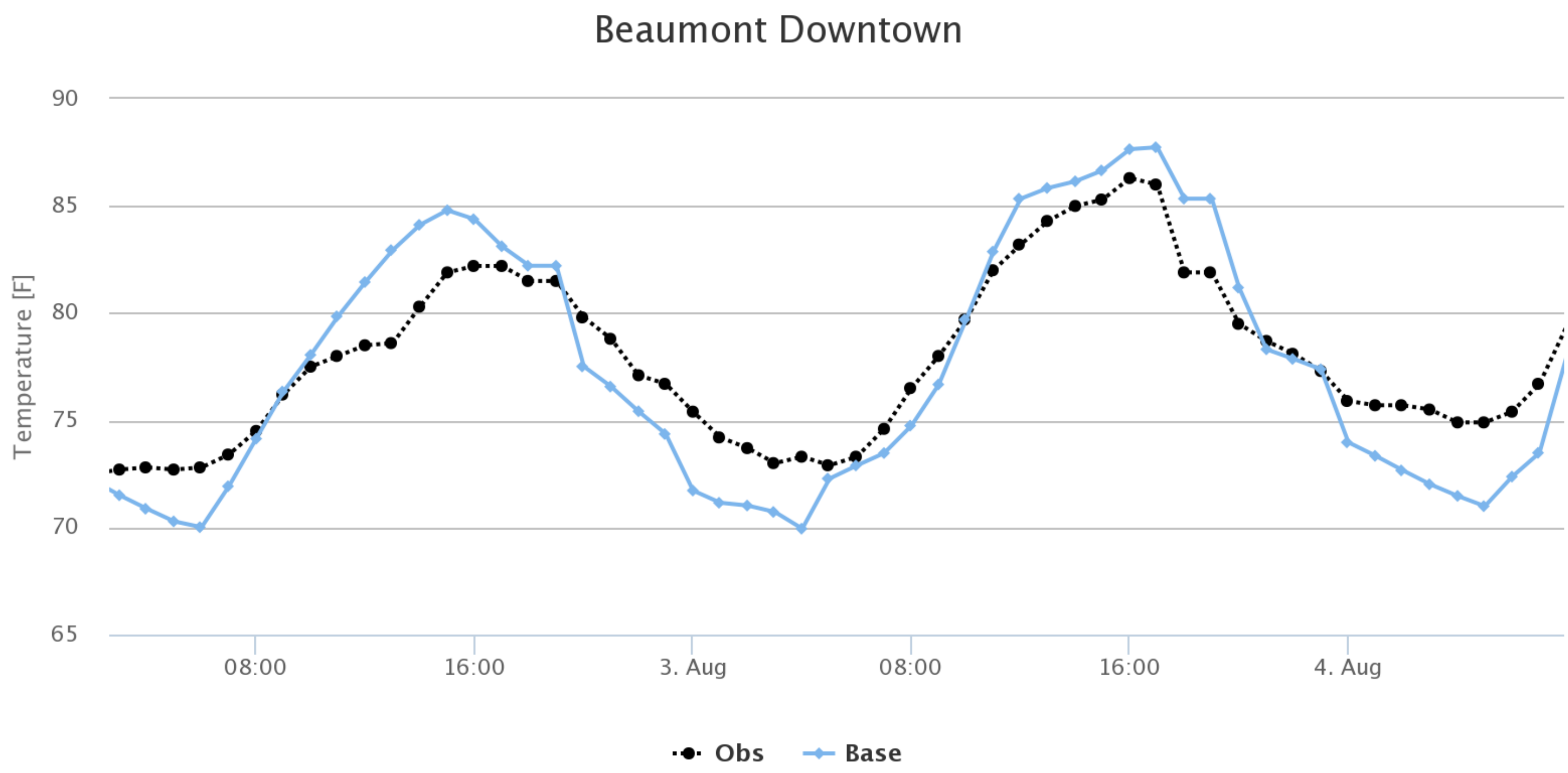


Figure 3-2. Observed (black) and base model (blue) temperature time series for August 2-4, 2014 at the Beaumont Downtown CAMS monitor.

Table 3-2. Model performance statistics by area for shortwave radiation (10 W m^{-2} cutoff) for September 9, 2014 to October 20, 2014 for WRF radiation pass-through (DIAG off), radiation attenuation from diagnosed subgrid clouds (base), and WRF radiation from the Alapaty simulation (Alapaty WRF). Best performing configuration for each statistic shown in bold.

	NMB (%)			NME (%)			r		
Region	**DIAG off**	**base (DIAG on)**	**Alapaty WRF**	**DIAG off**	**base (DIAG on)**	**Alapaty WRF**	**DIAG off**	**base (DIAG on)**	**Alapaty WRF**
All	12.0	**3.8**	20.0	37.3	39.9	**35.4**	0.793	0.738	**0.823**
Austin	**-0.7**	-7.3	8.1	33.2	36.8	**29.2**	0.794	0.726	**0.831**
Beaumont	24.3	**11.0**	30.0	44.5	46.6	**43.2**	0.752	0.693	**0.788**
Corpus Christi	16.4	**6.5**	22.4	41.3	46.2	**40.6**	0.777	0.690	**0.784**
Dallas Fort Worth	12.4	**9.0**	23.8	35.6	36.3	**35.2**	0.814	0.793	**0.842**
El Paso	10.9	**4.7**	20.7	30.0	**29.6**	30.5	0.866	0.836	**0.878**
Harlingen	10.4	**-2.1**	15.5	37.5	43.7	**36.6**	0.794	0.702	**0.800**
Houston	18.9	**5.6**	22.7	43.2	46.3	**39.7**	0.747	0.675	**0.787**
San Antonio	13.3	**5.6**	23.1	38.7	42.1	**35.3**	0.780	0.712	**0.827**
Tyler	11.5	**7.4**	23.6	34.2	36.2	**32.9**	0.818	0.781	**0.862**
Waco	**2.2**	-2.9	10.5	34.3	35.5	**30.5**	0.787	0.769	**0.830**

Table 3-3. Model performance statistics by area for ozone (20 ppb cutoff) for September 9, 2014 to October 20, 2014. Best performing configuration for each statistic shown in bold.

	NMB (%)						NME (%)						r					
Region	Base	Wesely	MOZART	Dust O3 MOZART	Fires	Alapaty	Base	Wesely	MOZART	Dust O3 MOZART	Fires	Alapaty	Base	Wesely	MOZART	Dust O3 MOZART	Fires	Alapaty
All	21.4	18.1	**17.7**	19.5	22.7	23.9	29.2	27.7	**26.9**	28.1	30.0	30.6	0.594	0.599	**0.616**	0.602	0.601	0.593
Austin	20.9	18.5	**17.1**	18.7	22.3	23.0	27.2	25.8	**24.6**	25.9	28.1	28.6	0.593	0.605	**0.623**	0.607	0.597	0.589
Beaumont	32.4	30.5	**29.5**	31.6	33.7	34.9	36.0	34.8	**34.0**	35.5	36.9	38.1	0.601	0.608	**0.618**	0.609	0.608	0.590
Corpus Christi	28.6	26.8	**24.6**	26.8	29.7	30.4	31.9	30.0	**29.2**	30.8	32.8	33.3	0.669	0.685	**0.686**	0.667	0.674	0.663
Dallas	10.1	**4.5**	7.0	8.6	11.5	13.1	24.0	**22.0**	22.2	22.9	24.5	24.8	0.620	**0.647**	0.641	0.634	0.628	0.624
El Paso	11.6	**2.1**	4.1	4.2	12.0	13.9	20.9	19.1	**17.3**	17.4	21.1	21.9	0.659	0.648	**0.692**	0.682	0.661	0.668
Harlingen	37.9	32.9	**32.2**	34.9	38.6	40.7	39.3	**34.8**	35.4	37.3	40.0	41.9	0.621	**0.688**	0.634	0.609	0.618	0.605
Houston	30.1	29.1	**27.0**	29.1	31.4	32.7	35.2	34.4	**32.9**	34.5	36.3	37.1	0.608	0.624	**0.630**	0.621	0.611	0.604
Laredo	35.5	**28.8**	31.6	33.6	36.5	37.8	37.1	**32.6**	33.4	35.3	38.0	38.8	0.656	0.621	**0.692**	0.655	0.659	0.676
San Antonio	13.6	11.1	**9.8**	11.8	14.9	16.0	25.0	23.3	**22.6**	23.9	25.4	25.9	0.591	0.618	**0.631**	0.610	0.599	0.587
Tyler	26.0	23.7	**22.5**	24.2	27.4	28.4	29.4	27.8	**26.9**	28.3	30.5	31.3	0.656	0.666	**0.677**	0.662	0.655	0.641
Waco	10.0	**5.9**	6.6	8.2	11.3	11.5	19.4	18.4	**18.0**	18.8	19.9	19.9	0.691	0.695	**0.709**	0.698	0.696	0.698

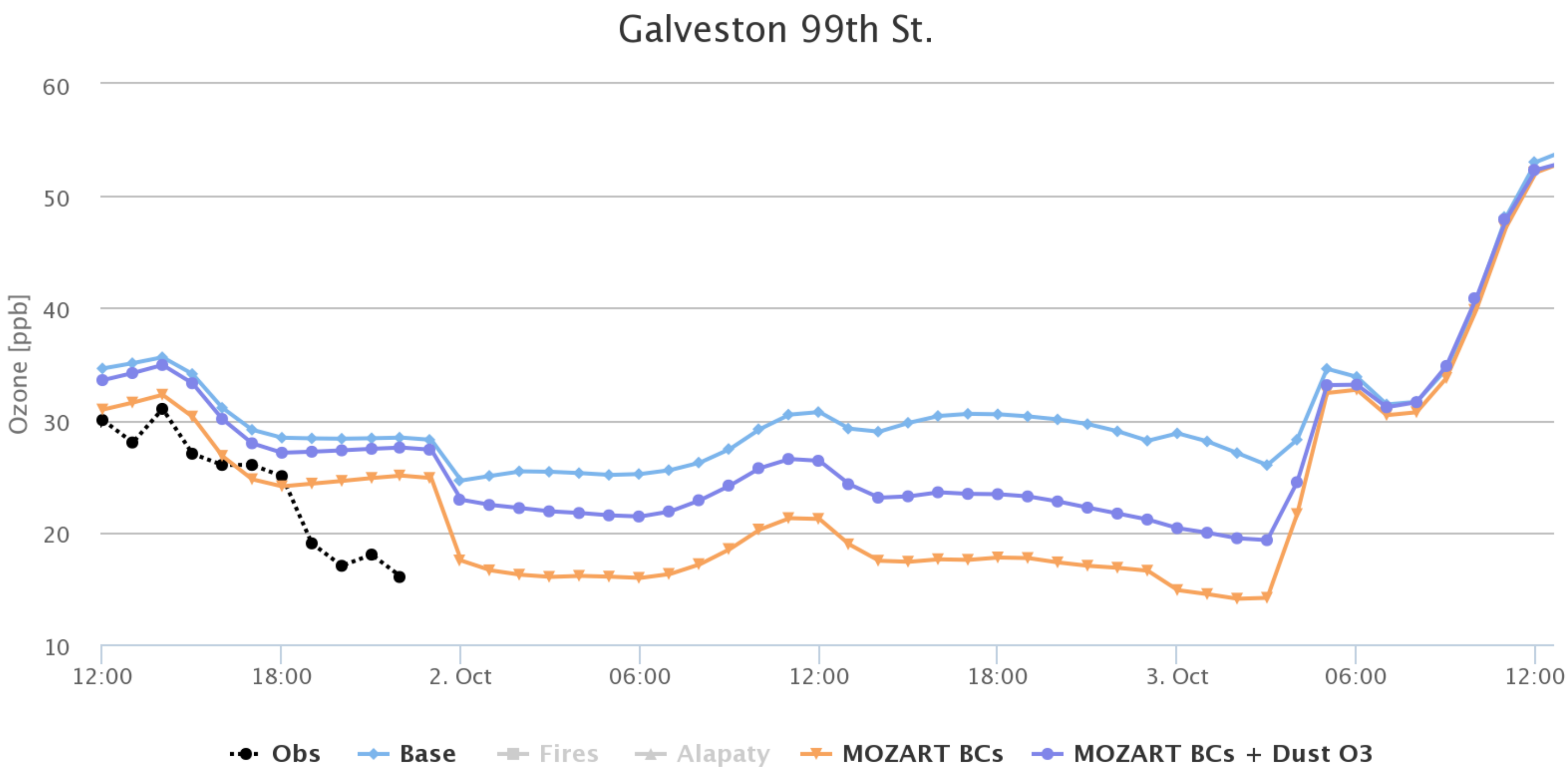


Figure 3-3. Ozone time series for observations (black), base case (cyan), MOZART boundary conditions (orange), and MOZART boundary conditions with adjustment to ozone boundary conditions from Saharan dust (purple) for October 1 12:00 CST through October 3 12:00 CST at the Galveston 99th Street CAMS monitor.

3.1.3 Analysis of Daily Statistics and Time Series in DFW and HGB

We examined daily statistics in two regions in Texas – Dallas and Houston. The top of Figure 3-4 shows time series of the ozone daily normalized mean bias in the DFW region in each of the six CAMx configurations – base case, Wesely dry deposition, near real-time fires, Alapaty WRF, MOZART boundary conditions, and MOZART boundary conditions with ozone reductions from the presence of dust. In addition, bars representing the highest observed 1-hour ozone for each date in the DFW region are faintly shown in the background to help identify the high ozone dates. Ozone bias was positive on most dates, though all runs showed negative bias for a 5-day period spanning Oct 14 through 18.

Analysis of the daily NMB statistics for the sensitivity runs matches the conclusions drawn from the episode total NMB for DFW. The NRT fires increased ozone bias on all days, though impacts are small (from near 0 to 2%) when wildfires are not active upwind of DFW. We observe the largest ozone impacts from fires during September 23-24, when fires increase ozone bias by 7% on each day. Alapaty WRF increased ozone bias on 36 of the 42 days, and by a larger average percentage than the NRT fires. Because most dates showed positive bias, Alapaty WRF was the worst performing simulation. MOZART boundary conditions sensitivity lowered ozone bias on almost all dates and was therefore the best performing simulation. The CAMx sensitivity with MOZART boundary conditions and dust shows improvement over the base case, but they are smaller than those shown by the MOZART BC simulation. As noted in Section 3.2.2, there is an important difference in ozone boundary conditions from the MOZART boundary conditions sensitivity: the flat 10 ppb ozone decrease in Gulf of Mexico boundary conditions is removed in favor of the adjustment to ozone BCs for the presence of fine dust. Wesely deposition usually predicted lower ozone than all other runs: therefore, Wesely deposition frequently displays the best model performance when ozone biases are highest in the base model, but also under-predicts ozone when the NMB in the base case is nearly zero, which occurs from September 22-27. Wesely deposition shows the highest NMB of all simulations during October 11-12, two very low ozone days.

As noted in Section 3.0, almost all regions in Texas recorded the lowest 4th highest daily maximum ozone concentrations over the past 10 years. The 2014 ozone season is characterized by frequent dust events and infrequent and/or short periods of elevated ozone. DFW only shows one multi-day period – September 23-26 – where peak 1-hour ozone exceeds 80 ppb during the September 9 through October 20, 2014 period. The base case exhibits good performance during this 4-day period: NMB is within ± 3 % for Sep 23-25 and is 16% on September 26. The Alapaty, MOZART BC and dust simulations all show similar performance. NRT fires shows larger NMB increases than is observed on most other days (NMB difference of +7% on September 23 and September 24); therefore, we conclude that fire emissions are leading to elevated ozone in this sensitivity. Wesely dry deposition demonstrates the worst performance of all sensitivities for September 23-25 (NMB of -15, -17, and -13%), but the best performance on September 26 (NMB of -1%).

We present hourly ozone time series for the base case and all sensitivity simulations for September 23-26, 2014 at the Fort Worth Northwest CAMS monitor in Figure 3-5. The base case simulation under-predicts peak ozone on September 23 (observed: 79 ppb, base case: 63 ppb) and 24 (observed: 83 ppb, base case: 71 ppb). NRT fires shows higher peak ozone concentrations than all other simulations on these two days (Sep 23: 70 ppb, Sep 24: 76 ppb). The NRT fires simulation only injects fire emissions during the “spin up” period. After model spin up, they are decreased to zero for the remainder of the simulation. This cutoff of fire emissions likely understates the ozone impacts from fire emissions when fires are active throughout the entire modeling cycle. All other sensitivity simulations’ peak ozone values are within 1-2 ppb of the base case.

In all cases, the highest NMB occurred on September 13, which was a low ozone date with the highest observed 1-hour ozone from all DFW monitors at only 33 ppb. The NMB for temperature over all DFW sites was 7%, one of the highest temperature biases of the entire episode. While the NMB for solar radiation over all DFW sites indicated very good performance (1%), some sites saw large over-predictions of solar radiation. Time series of solar radiation for the Fort Worth Northwest CAMS monitor (Figure 3-6) demonstrates large solar radiation over-predictions in the afternoon hours.

September 30 and October 11 are dates with high ozone biases that correspond to high NMB for solar radiation. On these dates, WRF failed to simulate sufficient cloud cover, resulting in more photochemical reactions and greater ozone production. NMB for solar radiation is only 2% for September 30, but similar to September 13, some individual sites show large over-predictions during the afternoon hours (Figure 3-7).

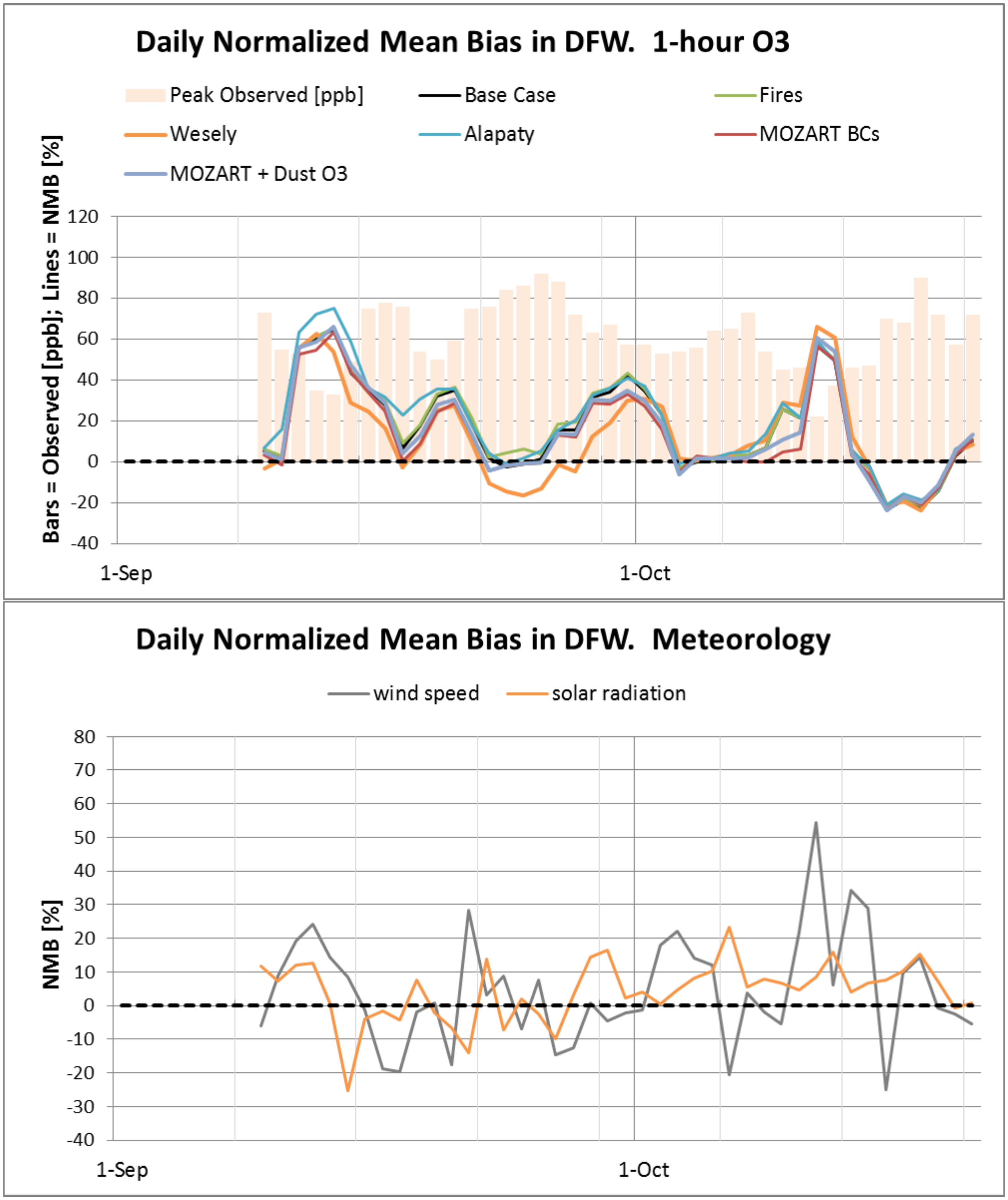


Figure 3-4. Time series of daily normalized mean bias for ozone (top) and meteorology (bottom) in DFW.

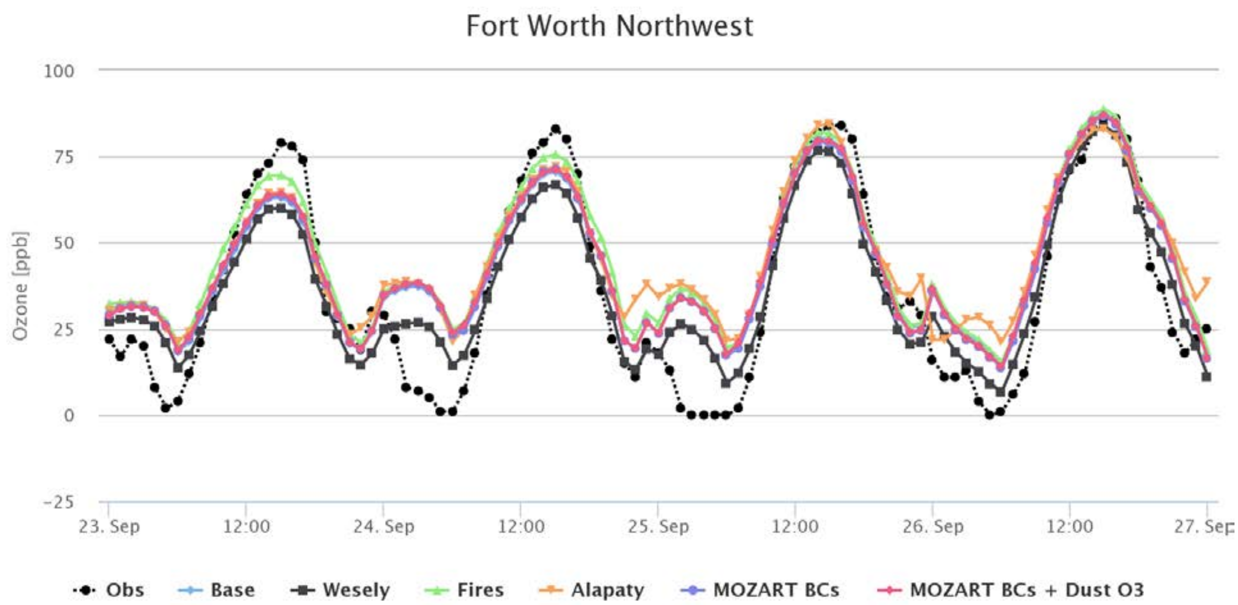


Figure 3-5. Time series of hourly ozone concentrations for September 23-26, 2014 at the Fort Worth Northwest CAMS monitor.

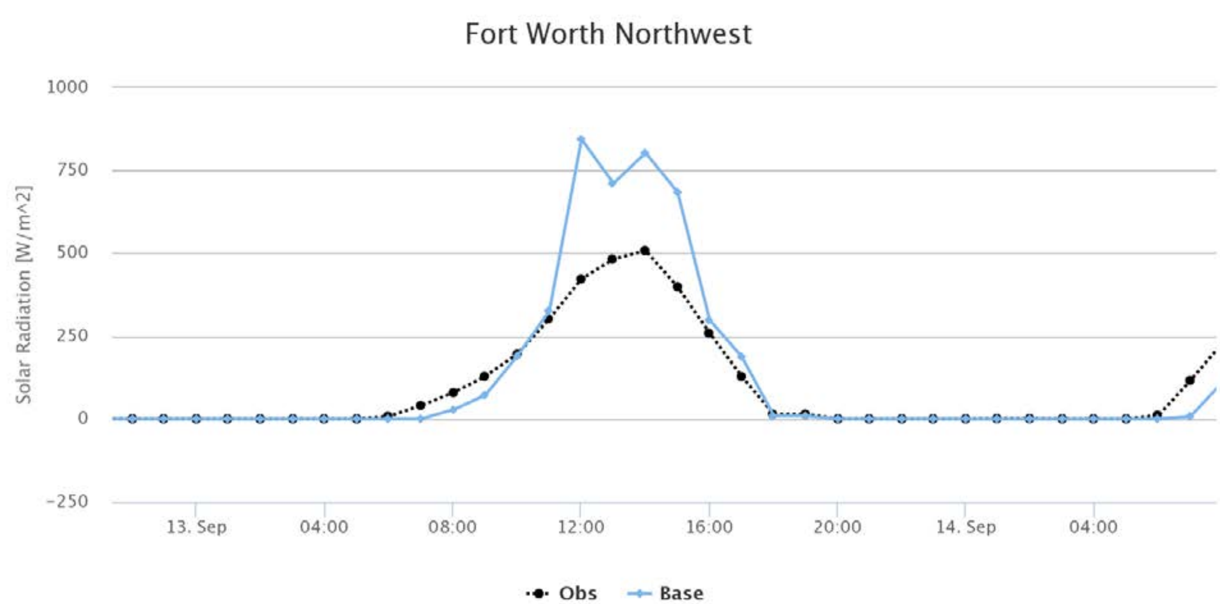


Figure 3-6. Time series of hourly observed (black) and base case modeled (blue) shortwave radiation for September 13, 2014 at the Fort Worth Northwest CAMS monitor.

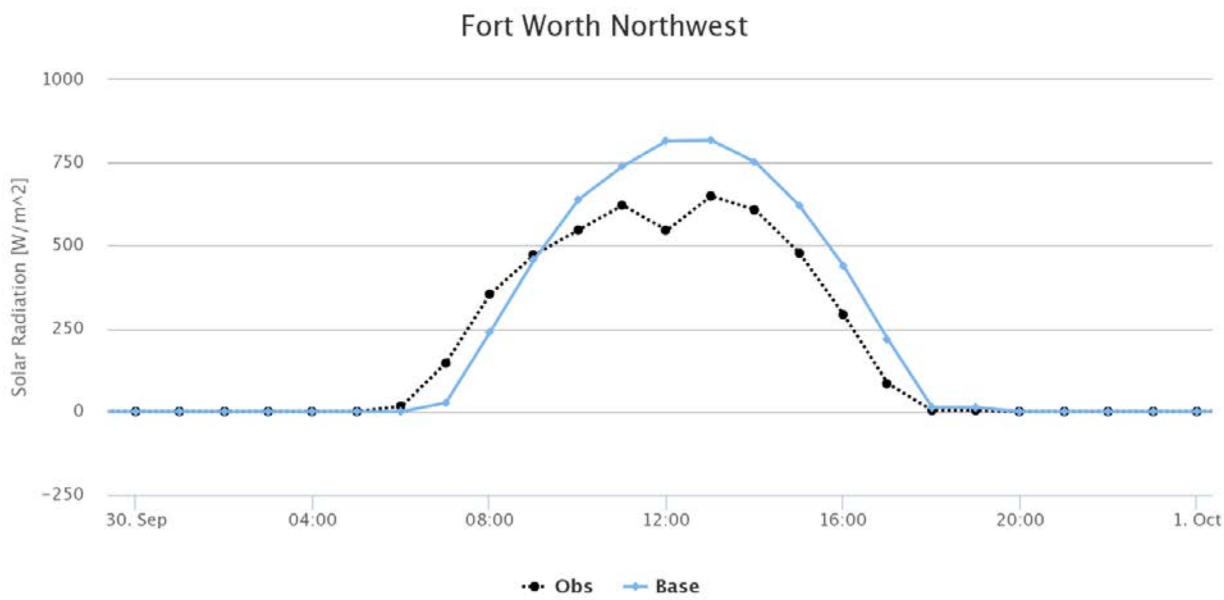


Figure 3-7. Time series of hourly observed (black) and base case modeled (blue) shortwave radiation for September 30, 2014 at the Fort Worth Northwest CAMS monitor.

The second region examined more closely is HGB, where Figure 3-8 shows time series of the daily ozone, wind speed, and solar radiation normalized mean biases. As with DFW, Alapaty WRF had the largest NMB values overall and NRT fires increased ozone bias when wildfires were active upwind of HGB. In contrast with DFW, MOZART BCs and the MOZART BC dust simulations show more pronounced NMB decreases from the base run due to proximity to the Gulf and therefore more impact from boundary conditions.

HGB has one multi-day period from August 1 – October 30, 2014 where peak observed ozone exceeds 80 ppb, October 11 and 12. (For comparison, HGB had 8 multi-day periods with peak ozone above 80 ppb from August 1 – October 15, 2013.) Normalized mean bias, error, and correlation coefficient (r) are presented for base case ozone and solar radiation for these two days in the last two rows of Table 3-4. The base case daily bias for October 19 and 20 (16% and 3%) both performed considerably better than the full 3 month period's NMB of 34%. The solar radiation bias was 11% on October 19 and near 0% on October 20. NME and pattern correlation for these two days are both improved over the 3 month period's stats.

We observe poor ozone model performance (NMB for base model ozone near or exceeding 60%) on September 13, 17, and 30. Statistics for these dates are also shown in Table 3-4. September 13 and 17 are both low ozone dates, where the 1-hour peak observed ozone is only 31 and 34 ppb, respectively. Observations at William P. Hobby airport (KHOU) show light rain in the morning of September 13, with overcast and mostly cloudy sky conditions present during all daylight hours. September 17 observations report thunderstorms and rain in the afternoon hours and mostly cloudy skies the rest of the day. Solar radiation bias is much higher on

September 13 (39%) and September 17 (75%) than for August 1 – October 30 (20%), indicating that the model did not simulate cloud conditions and/or precipitation patterns accurately. All simulations demonstrate poor performance on September 13, with NMB all exceeding 100% for all simulations. Performance of the MOZART boundary conditions and dust simulation show improvement over the base case for September 17: NMB is improved from 69% in the base case to 52% for the MOZART boundary conditions and 64% for the MOZART boundary conditions with dust simulation.

Ozone bias is also very high on September 30, where the base case NMB is 58%. NME is 59%, indicating that positive biases account for almost all of the error on this day. In contrast with September and 13 and 17, solar radiation NMB and NME are identical to those for the August 1 – October 30 period (NMB of 20% and NME of 41%). This indicates that solar radiation may not be the sole reason for ozone over-predictions on this day.

Figure 3-9 shows tile plots of 1-hour ozone concentrations for the base case (top left) and MOZART boundary conditions (top right) for September 30 16-17:00 CDT. The bottom panel of the figure shows CAMS observed hourly ozone for the same time period. Both models depict a small “ozone raft” feature along the coast between Galveston and Sabine. In the base model, ozone exceeds 80 ppb for several grid cells within the raft, while the MOZART boundary conditions are within 75-80 ppb. WRF winds then transport this ozone inland with the afternoon sea breeze, leading to elevated ozone in the HGB region. The CAMS observations (bottom) show ozone concentrations at or below 40 ppb along the Texas coast, although one monitor in Northwest Harris County (downwind of the Houston core and southeasterly sea breeze) recorded a value of 84 ppb. In fact, there was a wide range of ozone concentrations observed on September 30 in the HGB region. Figure 3-10 shows CAMS observed hourly ozone for the same time period as for Figure 3-9, but for the monitors surrounding the Houston core, including Galveston and Brazoria (top) and monitors within the Houston core (bottom). Areas of ozone above 50 ppb are concentrated to the north and northwest of downtown Houston.

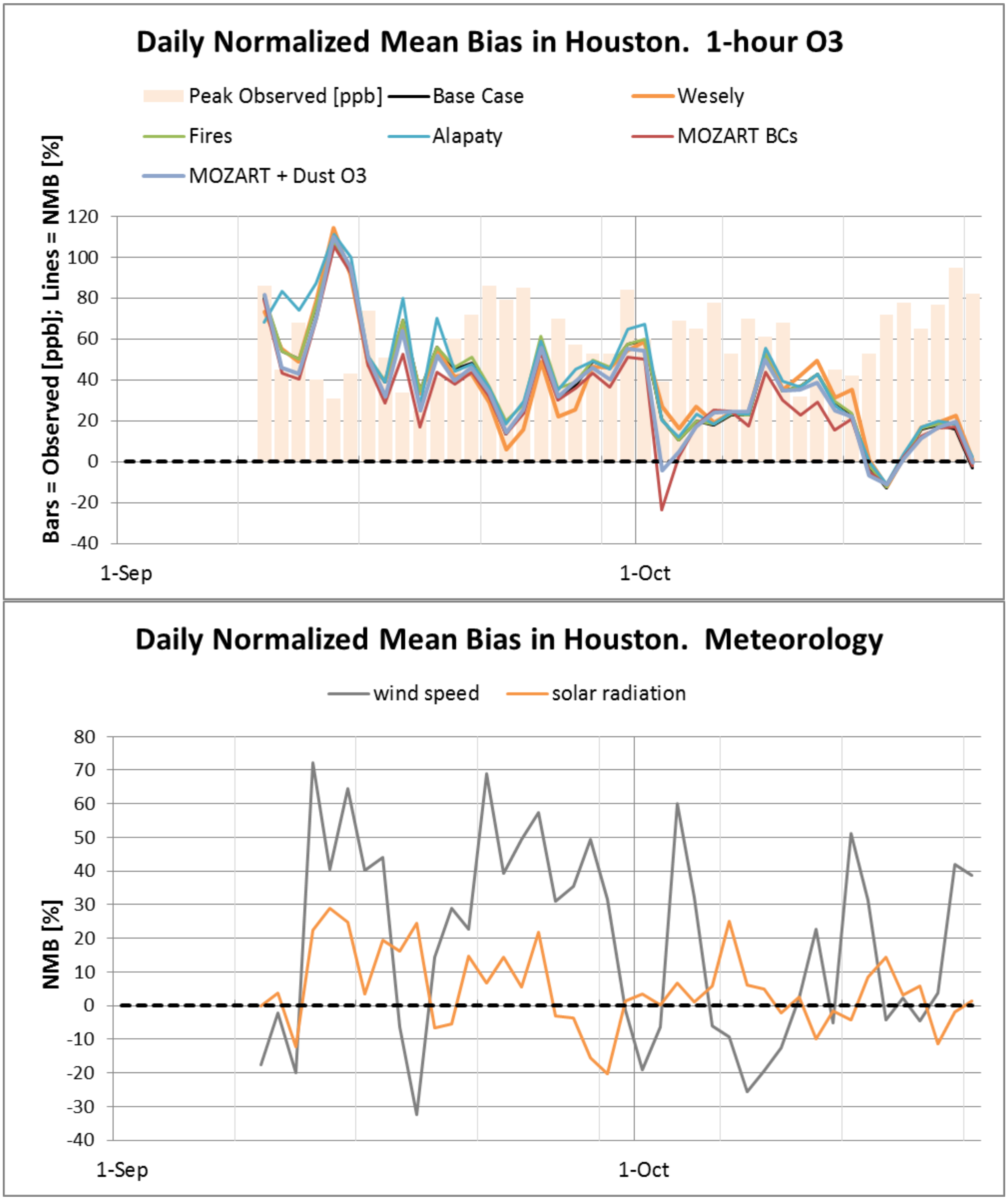


Figure 3-8. Time series of daily normalized mean bias for ozone (top) and meteorology (bottom) in HGB.

Table 3-4. Model performance statistics for selected dates for ozone (20 ppb cutoff) and solar radiation (10 W/m^2 cutoff) for the HGB region.

Date	Base Ozone				Solar Radiation			
	Peak Observed (ppb)	NMB (%)	NME (%)	r	Peak Observed (W/m^2)	NMB (%)	NME (%)	r
8/1/2014 - 10/30/2014	135	34	38	0.609	1093	20	41	0.771
9/13/2014	31	106	106	0.590	549	39	61	0.726
9/17/2014	34	69	71	0.297	823	75	101	0.394
9/30/2014	84	58	59	0.635	983	20	41	0.781
10/19/2014	95	16	20	0.826	817	11	31	0.862
10/20/2014	83	3	19	0.753	828	0	24	0.906

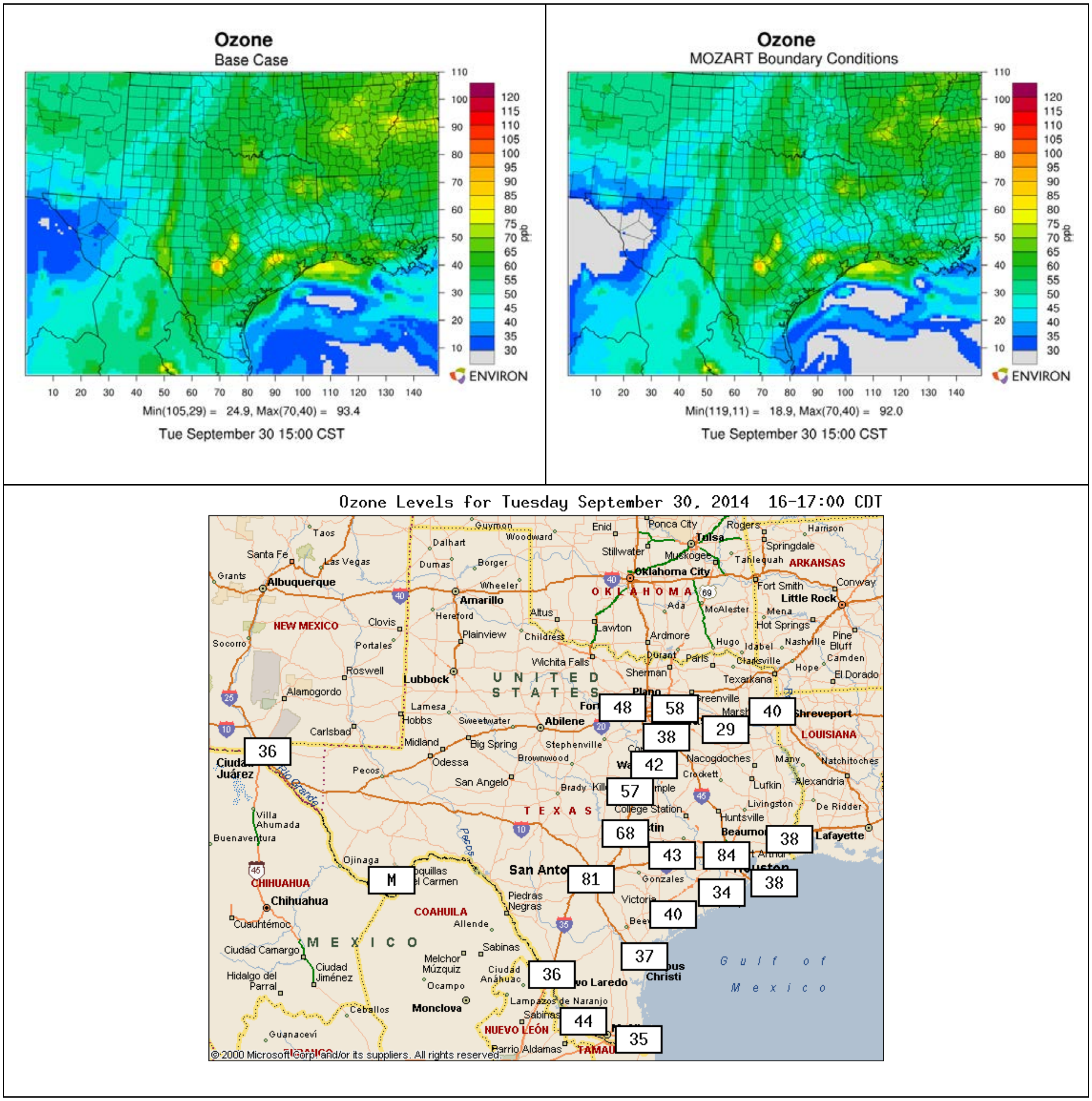
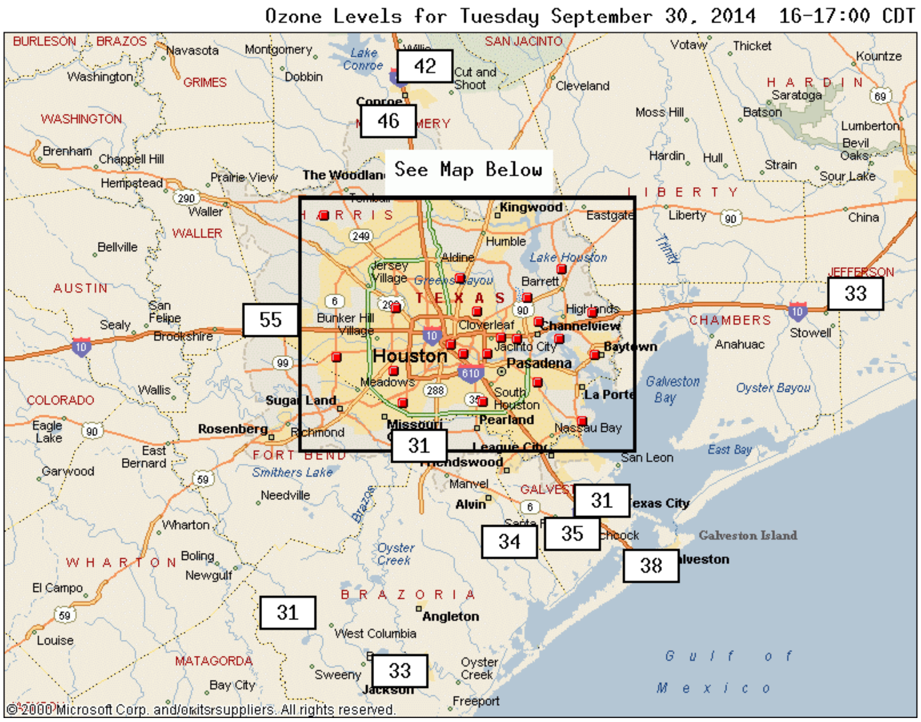


Figure 3-9. Hourly ozone concentrations for September 30, 2014 16-17:00 CDT for the base model (top left), MOZART boundary conditions simulation (top right), and observations at CAMS monitors (bottom).



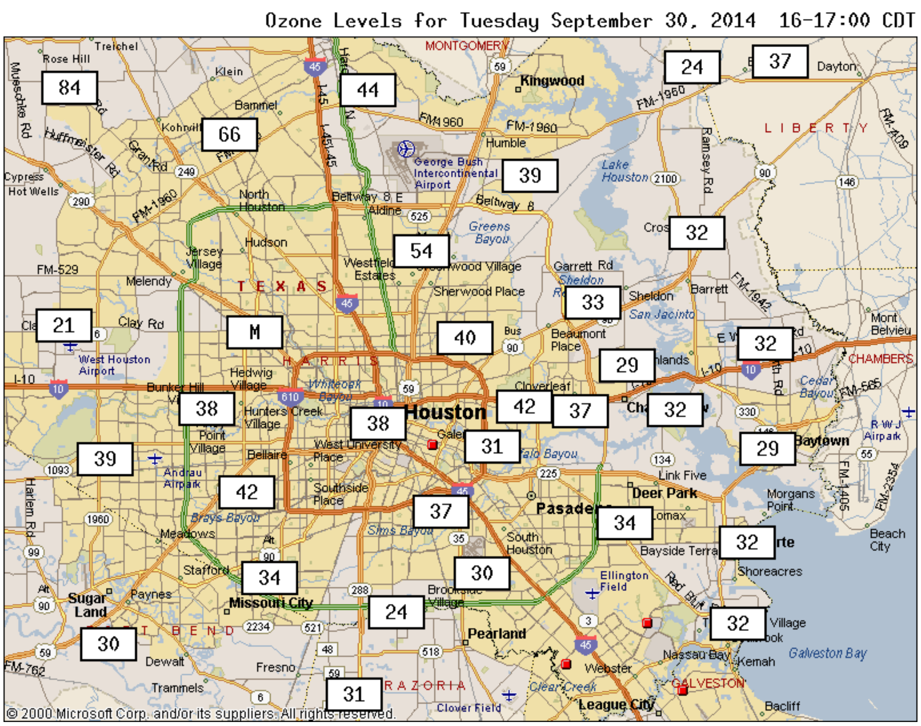


Figure 3-10. Observed hourly ozone concentrations for September 30, 2014 16-17:00 CDT for the Galveston Brazoria region (top) and Houston core (bottom).

3.2 Overall Assessment

3.2.1 Meteorological Performance Summary

The model performance evaluation shows that base case CAMx modeled ozone tended to be higher than measured values. The over-prediction of daytime ozone concentrations appeared to be due in part to over-predictions of solar radiation in most cases, where WRF failed to accurately depict the timing and/or location of cloud cover. This continues to be an area which we will investigate, and we expect to gain additional information from other Texas projects.

In Northeast Texas, wind speed bias was higher than any other region. We have observed this result in other Texas projects and we are currently investigating the use of an alternate landuse database – 2006 National Land Cover Database (NLCD) – which should serve to increase surface roughness and decrease wind speeds. Additionally, we are investigating to what extent CAMS monitor siting issues impact wind performance.

We observe that temperature and solar radiation statistics can be misleading. For temperature, very small bias values often result from over-predicted afternoon peaks “cancelling out” under-predicted early morning low temperatures. For solar radiation, poor performance during peak ozone production hours (roughly 10 AM through 3 PM) may be masked by low biases present during the early morning and late afternoon hours. We will investigate alternate methodologies for calculating and presenting meteorological statistics that are more appropriate for ozone production.

3.2.2 Sensitivity Analysis Summary

The daily performance evaluations show that CAMx tended to over-predict ozone levels in the DFW and Houston areas during most days in September and October 2014. NRT MOZART boundary conditions, which include a flat 10 ppb ozone decrease, tended to reduce biases more than a similar run with ozone decreases based on the presence of dust. The effects from both runs were more pronounced in areas influenced by transport from the Gulf of Mexico. Wesely dry deposition improved ozone bias on some days where the base case had the highest positive biases. Where ozone impacts in DFW from near real-time fires were highest, ozone under-predictions were improved by the addition of fire emissions.

Model performance for ozone benefitted from using near real-time MOZART boundary conditions (the base case used 2012 monthly averaged GEOS-CHEM boundary conditions), especially in areas where Gulf transport is frequent. GEOS-CHEM and MOZART tend to over-estimate ozone over the Gulf of Mexico, so we apply a flat 10 ppb ozone decrease to boundary conditions over the Gulf for both simulations. Since we did not apply this flat decrease in ozone boundary conditions to the dust simulation (we instead reduced ozone boundary conditions for the presence of fine dust), we were able to observe the effects of the flat ozone decrease. The results of this evaluation show that there is potential for further reductions in ozone bias; therefore, we plan to use a 15 ppb decrease in 2015.

Saharan dust was frequently transported to Texas during the 2014 ozone season with TCEQ daily forecasts predicting Saharan dust events on 55 of the 92 days (60%) from June 1 through August 31, 2014. Since ozone impacts from dust in the sensitivity simulation appeared to be lower than what was observed, we plan to use a more refined approach that uses dust from MOZART to adjust ozone boundary conditions.

Wesely dry deposition also tended to decrease ozone biases on most days. We propose that higher dry deposition velocities from lower surface resistances on these days cause the ozone reductions. The Wesely simulation sometimes produces the largest positive biases on a given day. Further investigation is needed to determine the cause of these over-predictions.

We also observe some ozone over-predictions in the Houston area are related to unrealistic ozone buildup offshore, which is then transported inland with the afternoon sea breeze. We plan to test and implement an iodine chemistry scheme in 2015, which will be simplified in order to be run operationally.

The near real-time ozone modeling project can benefit TCEQ's SIP modeling by identifying areas for improvement. We stated in the previous phase of the project that the reduction of "false alarms" – ozone over-predictions that occur when observed ozone is low to moderate – was the most significant issue to remedy. Very few high ozone events were observed in 2014, so the potential for false alarms was high. Despite this, the 2014 modeling improved overall ozone bias and error relative to the 2013 modeling. We propose to implement changes from the sensitivity simulations that we found beneficial into the 2015 base configuration as well as measure the impact of new configurations in the 2015 sensitivity simulations. We discuss specific recommendations for improving the NRT ozone modeling system in Section 4.

4.0 RECOMMENDATIONS FOR IMPROVEMENTS TO NEAR REAL-TIME OZONE MODELING SYSTEM

4.1 Specific Recommendations for Base Model Configuration

Our base model configuration for 2015 will combine the best performing simulations from the 2014 project. We present five recommendations for incorporating into the base model configuration in Table 4-1, ranked in order of importance.

Table 4-1. Specific recommendations for improvements in model configuration and/or input data sources for the NRT ozone modeling system's base configuration.

Recommendation	Importance
NRT MOZART-4/MOPITT chemical forecasts	High
Wesely dry deposition scheme	High
Change flat decrease in ozone BCs over the Gulf from 10 to 15 ppb	High
4 km grids over Houston and Dallas-Fort Worth	High
Updated anthropogenic emissions inventory	Medium

4.1.1 High Importance:

The most important recommendation is the addition of near real-time MOZART-4/MOPITT chemical forecasts. Results from this sensitivity simulation show improved ozone performance over the base case, which used 2012 monthly averaged GEOS-CHEM boundary conditions. We also propose to change the flat decrease in ozone BCs over the Gulf form 10 to 15 ppb. We propose that a more aggressive decrease in ozone over the Gulf will further improve ozone model performance when observed ozone is low or moderate.

Another important recommendation is the addition of the Wesely dry deposition scheme. The Wesely sensitivity tended to reduce large positive ozone biases on most days. We propose that higher dry deposition velocities from lower surface resistances on these days cause the ozone reductions.

Another important recommendation is the addition of 4 km domains over Houston and Dallas-Fort Worth. Results of timing tests show that adding 4 km domains over DFW and Houston roughly double total runtime of the entire daily modeling cycle. Model hardware may be upgraded by the time the next phase of the project begins and model timing tests will need to be conducted. We will use the results of these tests to determine whether to use 2-way or 1-way nesting. The 1-way nested approach will consume more time overall, but results for the 12 km domain could be posted to the web site early in the morning, before the 4 km simulations begin.

4.1.2 Medium Importance:

We also recommend using an updated anthropogenic emissions inventory. Currently, we are utilizing a seasonal 2012 emissions inventory with updates for 2013 oil and gas activity. We anticipate that TCEQ will provide an updated emissions inventory for use during the 2015 ozone season, and we would suggest using month-specific emissions for this modeling.

4.2 Specific Recommendations for Sensitivity Simulations

We recommend several model improvements to be used in sensitivity simulations in Table 4-2, ranked according to importance.

Table 4-2. Specific recommendations for improvements in model configuration and/or input data sources for the NRT ozone modeling system's sensitivity simulations.

Recommendation	Importance
Modify 2014 dust sensitivity by including coarse dust in the adjustment or use larger scaling factor	High
Include iodine chemistry using a simplified scheme	High
Updates to MEGAN	High
Update WRF to use Multi Scale Kain-Fritsch cumulus parameterization across all domains	High
Adjust PAR used in biogenics calculation to account for subgrid clouds	Medium
Near Real-Time (NRT) fire emissions	Medium
Re-speciate NOx emissions from ship plumes and fires	Medium
Expanded 12 km domain	Medium
Lightning NOx emissions	Low
Aircraft cruise emissions	Low

4.2.1 High Importance:

We observed that the dust sensitivity simulation, which used MOZART fine dust concentrations to scale ozone boundary conditions and adjust photolysis rates in the model, reduced ozone by close to 10 ppb on select days when observed ozone is low to moderate. Because ozone is still over-predicted on these days, we propose to increase the ozone impact from dust by either including coarse dust in the adjustment or by using a larger scaling factor.

ENVIRON recently developed a chemical mechanism for ozone depletion by halogens that reduces ozone over the Gulf of Mexico and therefore tends to improve ozone model performance in Texas. Iodine emissions are the main contributor to the modeled ozone destruction. The full halogen mechanism incurs a substantial run-time penalty in CAMx. Therefore, we recommend developing a simplified chemical mechanism for ozone destruction by iodine for testing in the NRT model.

We recommend testing a new version of MEGAN for the 2015 project. ENVIRON is currently developing a revised version of the standard high-resolution plant functional type (PFT) database for Texas and surrounding regions utilized by MEGAN. In addition, ENVIRON will use aircraft measurement data to modify isoprene and monoterpene emission factor maps. Average values based on the aircraft flux measurements will be used to calibrate the landcover scale emission factors for PFT types within different ecoregions. We expect this new version of MEGAN to be available sometime in July 2015.

We also recommend using the Multi Scale Kain-Fritsch cumulus parameterization in WRF, an update to the scheme used in the Alapaty WRF sensitivity simulation in 2014. ENVIRON has acquired a development version of the scheme from Dr. Kiran Alapaty's research group at EPA and is currently testing it. Alapaty's group expects the finalized version of the code to be included in the next public version of WRF (v3.7) available in Spring 2015. We will implement this scheme for several Texas projects over the next several months and compare with previous WRF simulations to determine how the new scheme simulates the timing and placement of cloud cover and precipitation. Because the new scheme is scale aware, it does not have the restriction of being used at grid resolutions coarser than 10 km. This should help to promote consistency between model solutions of various grid sizes.

4.2.2 Medium Importance:

We are currently using WRF's estimate of incoming solar radiation at the surface as a proxy for photosynthetically active radiation (PAR), since more accurate satellite data commonly used in retrospective simulations cannot be used in near real-time applications. PAR flux strongly influences the production of isoprene emissions in plants, and is therefore crucial to the MEGAN biogenic emissions calculations.

Emissions from moving ships form plumes that are diluted slowly to the spatial scale of a CAMx grid cell. Overly rapid dilution of NOx emissions in ship plumes may over-estimate the amount of ozone formed subsequently. Algorithms have been developed that approximate the chemical processing of NOx in ship plumes by converting a portion of the NOx to nitric acid. We propose to evaluate the potential importance of NOx processing within concentrated ship plumes by re-speciating NOx emissions from ships steaming in open water.

Another proposed sensitivity is using the NRT fire emissions from the MOZART-4/MOPITT chemical forecasts (http://earthdata.nasa.gov/data/nrt-data/firms/active-fire-data). We would like to examine the ozone impact of wildfires throughout the ozone season, so that we can measure the influence of any significant fire events in 2015. We note that the approach used in the 2014 sensitivity zeros out the fire emissions at the end of the spin-up period. We have discovered that NCAR uses a different approach for their chemical forecasts: they assume that the fire emissions persist throughout the entire modeling cycle. We may implement and evaluate this approach if we determine that ozone impacts from fire emissions are understated in 2015.

As part of the HGBPA sensitivity, we used expanded WRF and CAMx 12 km domains to cover much of the Eastern U.S. While this larger domain would be helpful for characterizing long range ozone production and transport, including the additional grid cells in this larger domain roughly doubles total model runtime. With the additional 4 km grids over Houston and DFW a high priority, an expanded 12 km domain will not be feasible in the short term.

4.2.3 Low Importance:

Finally, we recommend the use of lightning NOx and aircraft cruise emissions. This item is ranked lowest because these emissions sources, while important in the mid- to upper-troposphere, typically have small impacts on ozone near the surface. Lightning NOx parameterization is an active area of current research. Most parameterizations are dependent on convective precipitation, which has these major limitations:

- meteorological models typically demonstrate poor performance simulating the timing and location of convection
- these methods cannot be used for simulations without convective parameterizations, where convection is assumed to be explicitly resolved (usually < 10 km)
- the relationship between the amount of convective precipitation and flash rates or amount of NOx per flash is complex and not completely understood

The latest version of WRF contains a lightning parameterization which can be used to generate lightning flash rates (Wong et al., 2013). This approach has a significant advantage to other methods in that it has the ability to use simulated radar reflectivity from the microphysical scheme instead of convective precipitation, which allows it to be used for resolved convection, high resolution simulations. The downside to this approach is that it would require significant testing and analysis before it could be used operationally.

4.3 Website Recommendations

In addition to the suggestions listed above that could improve model performance, these are suggested recommendations to make the near real-time ozone modeling website better:

- Dynamic charting of “zoom-able” ozone time series updated hourly in near real-time. The benefit of this approach is that all runs can be displayed at once over the entire modeling period. Areas of interest can be examined in greater detail and data series for individual simulations can be turned on/off.
- Presenting ozone scatter plots at each CAMS site or Texas region with regression lines and correlation coefficients.
- Integrating Google maps for site selection.
- Improving the presentation of model performance statistics.

5.0 REFERENCES

Alapaty, K., J. A. Herwehe, T. L. Otte, C. G. Nolte, O. R. Bullock, M. S. Mallard, J. S. Kain, and J. Dudhia. 2012. Introducing subgrid-scale cloud feedbacks to radiation for regional meteorological and climate modeling, Geophys. Res. Lett., 39, L24809, doi:10.1029/2012GL054031.

Andrey, J., Cuevas, E., Parrondo, M. C., Alonso-Pérez, S., Redondas, A., & Gil-Ojeda, M. 2014. Quantification of ozone reductions within the Saharan air layer through a 13-year climatologic analysis of ozone profiles. Atmospheric Environment, 84, 28-34.

Astitha, M., & Kallos, G. 2009. Gas-phase and aerosol chemistry interactions in South Europe and the Mediterranean region. Environmental fluid mechanics, 9(1), 3-22.

Cuevas, E., González, Y., Rodríguez González, S., Guerra, J. C., Gómez Pélaez, A. J., Alonso Pérez, S., Bustos, J. & Milford, C. 2013. Assessment of atmospheric processes driving ozone variations in the subtropical North Atlantic free troposphere. Atmospheric Chemistry and Physics, 13, 1973-1998.

Darby, L., C. J. Senff, R.M. Banta, B. Orr, and J. George. 2002. Evaluation of Houston Sea Breeze and Circulation of Pollutants. National Oceanic and Atmospheric Administration report.

DiMego, G., and E. Rogers. 2011, "Q4FY11 NAM Upgrade Package Decision Brief", NCEP Director Briefing, Camp Springs, MD. 18 October 2011.

Emery, C., J. Jung, J. Johnson, G. Yarwood, S. Madronich, G.Grell. 2010. Improving the Characterization of Clouds and their Impact on Photolysis Rates within the CAMx Photochemical Grid Model. Prepared for the Texas Commission on Environmental Quality, Austin, TX. Prepared by ENVIRON International Corporation, Novato, CA (August 27, 2010).

Emmons, L. K., Walters, S., Hess, P. G., Lamarque, J.-F., Pfister, G. G., Fillmore, D., Granier, C., Guenther, A., Kinnison, D., Laepple, T., Orlando, J., Tie, X., Tyndall, G., Wiedinmyer, C., Baughcum, S. L., and Kloster, S. 2010. Description and evaluation of the Model for Ozone and Related chemical Tracers, version 4 (MOZART-4), Geosci. Model Dev., 3, 43-67, doi:10.5194/gmd-3-43-2010

ENVIRON, 2013. The Comprehensive Air quality Model with extensions (CAMx) homepage, http://www.CAMx.com.

ENVIRON and ERG. 2013. Technical Support Document: Photochemical Modeling for the Louisiana 8-Hour Ozone State Implementation Plan. Prepared for the Louisiana Department of Environmental Quality, Office of Environmental Services, Air Permits Division, Baton Rouge, LA. Prepared by ENVIRON International Corporation, Novato, CA and Eastern Research Group, Inc., Rancho Cordova, CA (in progress).

Environmental Modeling Center, 2003: The GFS Atmospheric Model. NCEP Office Note 442, Global Climate and Weather Modeling Branch, EMC, Camp Springs, Maryland.

Fairlie, T. D., Jacob, D. J., Dibb, J. E., Alexander, B., Avery, M. A., Donkelaar, A. V., & Zhang, L. 2010. Impact of mineral dust on nitrate, sulfate, and ozone in transpacific Asian pollution plumes. *Atmospheric Chemistry and Physics*, *10*(8), 3999-4012.

Guenther, A., Karl, T., Harley, P.,Wiedinmyer, C., Palmer, Geron, C. 2006. Estimates of global terrestrial isoprene emissions using MEGAN (Model of Emissions of Gases and Aerosols from Nature), Atmos. Chem Phys., 6, 3181-3210.

Johnson, J., E. Tai, P. Karamchandani, G. Wilson, and G. Yarwood. 2013. TCEQ Ozone Forecasting System. Prepared for Mark Estes, TCEQ. November.

Lee, P., H.-C. Kim, and F. Ngan, 2012. Investigation of nocturnal surface wind bias by the Weather Research and Forecasting (WRF)/ Advanced Research WRF (ARW) meteorological model for the Second Texas Air Quality Study (TexAQS-II) in 2006. Report prepared for TCEQ by NOAA-ARL, Silver Spring, MD.

McFiggans, G., J. M. C. Plane, B. J. Allan, L. J. Carpenter, H. Coe, and C. O'Dowd. 2000. A modeling study of iodine chemistry in the marine boundary layer, J. Geophys. Res., 105(D11), 14371–14385, doi:10.1029/1999JD901187.

Park, R. J., Hong, S. K., Kwon, H.-A., Kim, S., Guenther, A., Woo, J.-H., and Loughner, C. P.: An evaluation of ozone dry deposition simulations in East Asia, Atmos. Chem. Phys., 14, 7929-7940, doi:10.5194/acp-14-7929-2014, 2014.

Read, K. A., A. S. Mahajan, L. J. Carpenter, M. J. Evans, B. V. E. Faria, D. E. Heard, J. R. Hopkins, J. D. Lee, S. J. Moller, A. C. Lewis, L. Mendes, J. B. McQuaid, H. Oetjen, A. Saiz-Lopez, M. J. Pilling & J. M. C. Plane. 2008. Extensive halogen-mediated ozone destruction over the tropical Atlantic. Nature 453, 1232-1235.

Rodríguez, S., González, Y., Cuevas, E., Ramos, R., Romero, P. M., Abreu-Afonso, J., & Redondas, A. (2009). Atmospheric nanoparticle observations in the low free troposphere during upward orographic flows at Izaña Mountain Observatory. Atmospheric Chemistry and Physics, 9(17), 6319-6335.

Vizuete, W., H. E. Jeffries, T. W. Tesche, E. P. Olaguer, E. Couzo. 2011. Issues with ozone attainment methodology for Houston, TX. J. Air Waste Manag Assoc. 2011 Mar;61(3):238-53. Erratum in: J Air Waste Manag Assoc. 2011 Oct;61(10):1082.

Wesely, M. L.: Parameterization of surface resistances to gaseous dry deposition in regional-scale numerical models, Atmos. Environ., 23, 1293–1304, 1989.

Wiedinmyer, C., Akagi, S. K., Yokelson, R. J., Emmons, L. K., Al-Saadi, J. A., Orlando, J. J., and Soja, A. J.: The Fire INventory from NCAR (FINN): a high resolution global model to estimate the emissions from open burning, Geosci. Model Dev., 4, 625-641, doi:10.5194/gmd-4-625-2011, 2011.

Wong, J., Barth, M. C., and Noone, D. 2013. Evaluating a lightning parameterization based on cloud-top height for mesoscale numerical model simulations, Geosci. Model Dev., 6, 429-443, doi:10.5194/gmd-6-429-2013.

Yantosca, B., Long, M., Payer, M., Cooper, M. 2013. GEOS-Chem v9-01-03 Online User's Guide, http://acmg.seas.harvard.edu/geos/doc/man/.

Yarwood, G., H. Gookyoung, W.P.L. Carter, G.Z. Whitten. 2012. "Environmental Chamber Experiments to Evaluate NOx Sinks and Recycling in Atmospheric Chemical Mechanisms." Final Report prepared for the Texas Air Quality Research Program, University of Texas, Austin, Texas (AQRP Project 10-042, February 2012).