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Task 3.2

Draft Modeling Protocol

Ozone Modeling of 2012 for Northeast Texas

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TEXAS COMMISSION ON ENVIRONMENTAL QUALITY

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LIST OF ACRONYMS AND ABBREVIATIONS

APCA	CAMx Anthropogenic Precursor Culpability Assessment
AQRP	Air Quality Research Program
BCs	Boundary Conditions
CAMS	Continuous Air Monitoring Station
CAMx	Comprehensive Air quality Model with extensions
CASTNET	Clean Air Status and Trends Network
CO	Carbon monoxide
CST	Central Standard Time
DSW	Downward Shortwave radiation
EAC	Early Action Compact
EBI	Euler Backward Iterative solver
ECMWF	European Centre for Medium-Range Weather Forecasts
EGU	Electric Generating Unit
EPA	Environmental Protection Agency
ETCOG	East Texas Council of Governments
FDDA	Four Dimensional Data Assimilation
GEOS	Goddard Earth Observing System
GOES	Geostationary Operational Environmental Satellite
HGB	Houston-Galveston-Brazoria Area
HNO_3	Nitric Acid
HYSPLIT	HYbrid Single-Particle Lagrangian Integrated Trajectory
ICs	Initial Conditions
IEH	Implicit-Explicit Hybrid solver
LCC	Lambert Conic Conformal
LSODE	Livermore Solver for Ordinary Differential Equations
MATS	Modeled Attainment Test Software
MDA1	Daily maximum 1-hour average
MDA8	Daily maximum 8-hour average
MDL	Meteorological Development Laboratory
MEGAN	Model of Emissions of Gases and Aerosols from Nature
NAM	North American Model
NASA	National Aeronautics and Space Administration
NCAR	National Center for Atmospheric Research
NMB	Normalized Mean Bias
NME	Normalized Mean Error
NAA	Non-Attainment Area (for the ozone NAAQS)
NAAQS	National Ambient Air Quality Standard
NETAC	Northeast Texas Air Care
NNA	Near Non-Attainment Area (for the ozone NAAQS)
NO	Nitric Oxide
NOAA	National Oceanic and Atmospheric Administration

NOx	Oxides of Nitrogen
OSAT	CAMx Ozone Source Apportionment Tool
PiG	Plume-in-Grid
PBL	Planetary boundary layer
PM	Particulate matter
ppb	Parts per billion
ppbC	Parts per billion carbon
PPM	Piecewise Parabolic Method
ppm	Parts per million
PRISM	Parameter-elevation Relationships on Independent Slopes Model
RMSE	Root mean square error
RPO	Regional Planning Organization
RRF	Relative reduction factor
SID	Sabine Industrial District
SIP	State Implementation Plan (for the ozone NAAQS)
SO_2	Sulfur dioxide
TCEQ	Texas Commission on Environmental Quality
TLM	Tyler-Longview-Marshall
TOMS	Total Ozone Mapping Spectrometer
Tpd	tons per day
TUV	Tropospheric visible Ultra-Violet model
UTC	Coordinated Universal Time
VOC	Volatile organic compound
WRF	Weather Research and Forecast model

1.0 INTRODUCTION

This Modeling Protocol describes the procedures that will be used in the development of a new ozone modeling database for the Tyler-Longview-Marshall (TLM) area in Northeast Texas. The requirements for a Modeling Protocol are described in the following U.S. Environmental Protection Agency (EPA) document:

"Draft Modeling Guidance for Demonstrating Attainment of Air Quality Goals for Ozone, $PM_{2.5}$, and Regional Haze"[1]. U.S. Environmental Protection Agency, Office of Air Quality Planning and Standards, Research Triangle Park, NC 27711. December, 2014.

The function of a Modeling Protocol is to set forth procedures to be used in conducting an ozone attainment demonstration, and EPA Guidance specifies that the Protocol must contain the following:

- overview of the air quality issue being considered including historical background,
- list of the planned participants in the analysis and their expected roles,
- schedule for completion of key steps in the analysis and final documentation,
- description of the conceptual model for the area,
- description of periods to be modeled, how they comport with the conceptual model, and why they are sufficient,
- models to be used in the demonstration and why they are appropriate,
- description of model inputs and their expected sources (e.g., emissions, meteorology, etc.),
- description of the domain to be modeled (expanse and resolution),
- process for evaluating base year model performance (meteorology, emissions, and air quality) and demonstrating that the model is an appropriate tool for the intended use,
- description of the future years to be modeled and how projection inputs will be prepared,
- description of the attainment test procedures and (if known) planned weight of evidence,
- expected diagnostic or supplemental analyses needed to develop weight of evidence analyses, and
- commitment to specific deliverables fully documenting the completed analysis.

In Section 1 of this Protocol, we describe the background and objectives of the Northeast Texas ozone modeling as well as the schedule, organizational structure and documentation. In Section 2, we discuss the conceptual model for ozone formation in Northeast Texas. Section 3 contains a description of episodes that are to be modeled or are under consideration. In Section 4, we describe the models to be used, and in Section 5, we discuss the domains over

[1] http://www3.epa.gov/scram001/guidance/guide/Draft_O3-PM-RH_Modeling_Guidance-2014.pdf.

which they will be applied. Section 6 gives additional detail about the meteorological modeling and its evaluation, and, in Section 7, we describe the air quality model configuration and the development of model inputs. Section 8 presents air quality model evaluation procedures, and Section 9 outlines methods for supplemental analyses.

1.1 Background

1.1.1 Northeast Texas Ozone Monitors and Attainment Status

The U.S. EPA sets a National Ambient Air Quality Standard (NAAQS) for ozone in order to protect public health and the environment. The 8-hour ozone NAAQS sets a maximum level for the three-year running average of the annual fourth-highest daily maximum 8-hour average (MDA8) concentration; this quantity is known as the design value. The Northeast Texas ozone monitoring data determine whether the area is in compliance with the NAAQS. The Northeast Texas (TLM) Near Non-Attainment Area (NNA) consists of Gregg, Upshur, Rusk, Smith, and Harrison Counties. The Texas Commission on Environmental Quality (TCEQ) operates three ozone monitors (Continuous Air Monitoring Station, CAMS) in the Northeast Texas NNA: CAMS 19 at Gregg County Airport in Longview, CAMS 82 at Smith County Airport in Tyler and CAMS 85 at Karnack in Harrison County. The locations of the monitoring stations are shown in Figure 1-1.

The Northeast Texas ozone monitors have seen large reductions in ozone during the last two decades as shown in Figure 1-2 and Figure 1-3, which report the monitors' annual 4th highest MDA8 ozone concentrations and design values, respectively. These ozone reductions have allowed the area to demonstrate compliance with increasingly stringent NAAQS. The 8-hour NAAQS are shown as red lines in Figure 1-2 and Figure 1-3. Northeast Texas successfully concluded its Early Action Compact (EAC) in 2007 with attainment of the 1997 0.08 parts per million (ppm) 8-hour ozone standard, and was designated in attainment of the 75 parts per billion (ppb) 2008 NAAQS in 2012.

EPA's most recent review of the ozone standard was finalized on October 1, 2015. On October 1, the EPA lowered the ozone NAAQS from the 75 ppb set in 2008 to a more stringent value of 70 ppb. The NAAQS is violated by a design value of 71 ppb or greater. The EPA expects to issue detailed guidance on the designation process in early 2016, but has indicated that attainment designations for the 2015 NAAQS will likely be based on 2014-2016 data[2]. State recommendations for designations of attainment and nonattainment areas are due to EPA by October 1, 2016 and EPA will finalize designations by October 1, 2017. Figure 1-3 shows that the Longview CAMS 19 monitor currently has a design value of 68 ppb, the Tyler CAMS 82 monitor has a design value of 67 ppb and the Karnack CAMS 85 monitor has a design value of 66 ppb; design values for all three monitors are less than the 2015 ozone NAAQS of 70 ppb. 2016 values of the 4th high MDA8 that are ≤ 78 ppb for Longview CAMS 19, ≤ 80 ppb for Tyler CAMS 82 and ≤ 84 ppb for Karnack CAMS 85 will produce 2016 design values that attain the 2015 NAAQS. If all three monitors attain the NAAQS at the end of the 2016 ozone season, an

Comment [HJ1]: This footnote is outdated, please update the link.

[2] http://www3.epa.gov/ozonepollution/pdfs/20151001designationsfs.pdf.

attainment demonstration of the 2015 NAAQS would not be necessary. However, if any of the monitors had a design value that exceeded 70 ppb at the end of 2016, the area could potentially be declared in nonattainment of the 2015 NAAQS, in which case an attainment demonstration might be necessary, depending on the area's designation.

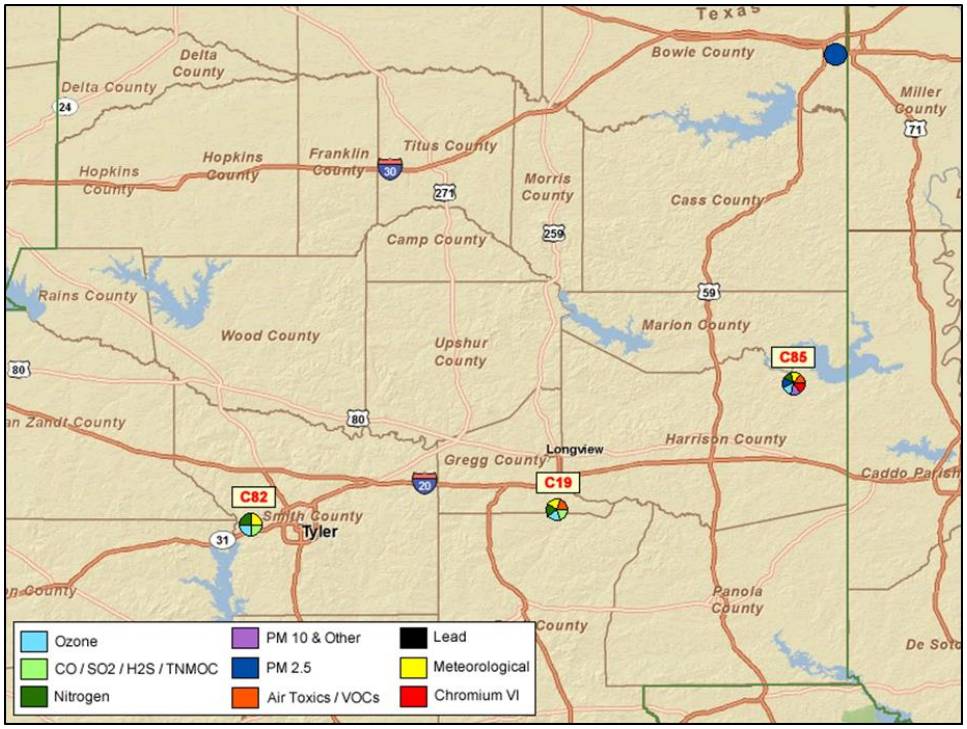

Figure 1-1. Map showing CAMS sites in Northeast Texas[3]. TCEQ figure.

1.1.2 TCEQ State Implementation Plan Ozone Modeling

The TCEQ is preparing for development of a State Implementation Plan (SIP) in response to the revised ozone standard. The SIP will describe the State of Texas' plan for bringing nonattainment areas within the State into compliance with the 2015 NAAQS and ensuring that NNAs continue to attain the NAAQS. The TCEQ plans to carry out photochemical modeling to demonstrate how areas of the State which do not attain the 2015 ozone standard will achieve attainment by a specified date; the attainment date will likely vary by area according to the severity of each area's ozone problem. As described in Section 2 of this Protocol, the TCEQ has enlisted the cooperation of the current NNAs in the SIP modeling effort. The TCEQ has developed the inputs for the State-wide ozone modeling effort and each NNA is carrying out photochemical modeling focused on its region.

[3] Map from TCEQ website at: http://www.tceq.state.tx.us/cgi-bin/compliance/monops/select_summary.pl?region05.gif.

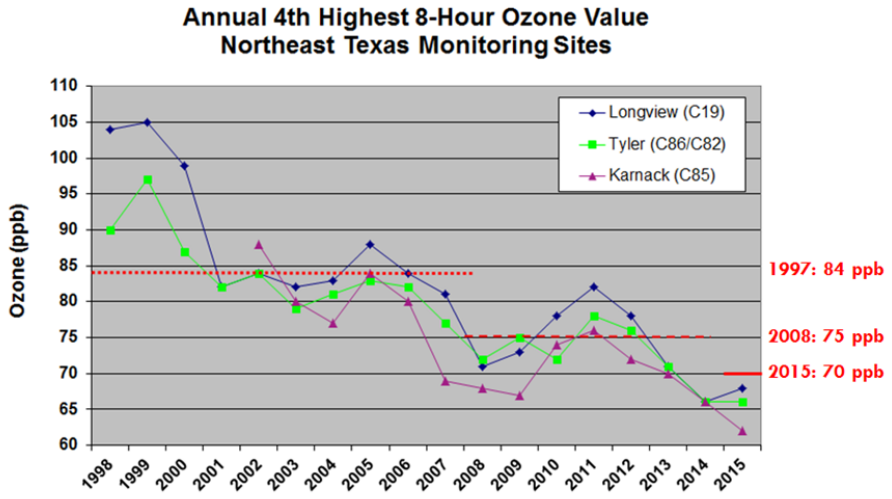

Figure 1-2. Trends in annual 4th highest 8-hour ozone values at the Longview (CAMS 19), Tyler (CAMS 82) and Karnack (CAMS 85) monitors in Northeast Texas. The red lines indicate the 1997 84 ppb, 2008 75 ppb and 2015 70 ppb ozone standards. All data have been validated by the TCEQ.

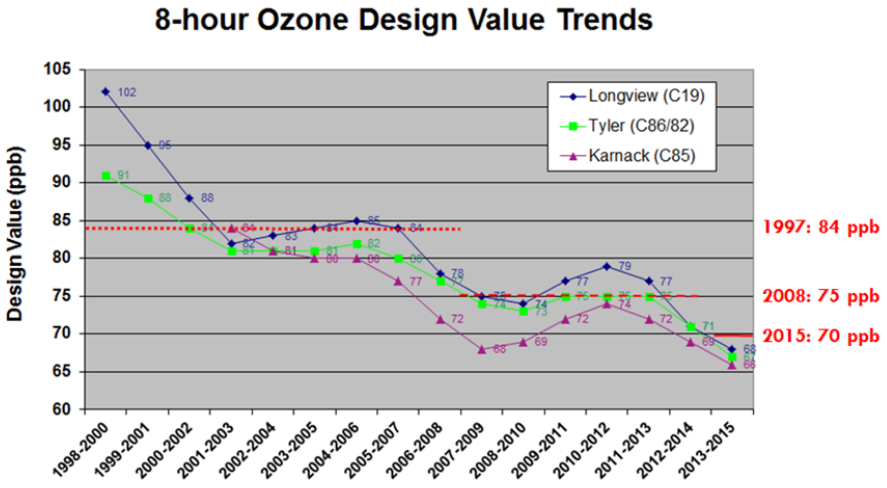

Figure 1-3. Trends in design values at the Longview (CAMS 19), Tyler (CAMS 82) and Karnack (CAMS 85) monitors in Northeast Texas. The red lines indicate the 1997 84 ppb, 2008 75 ppb and 2015 70 ppb ozone standards as in Figure 1-2. All data have been validated by the TCEQ.

1.2 Previous Northeast Texas Ozone Modeling Studies

In this section, we provide references to previous ozone modeling focused on Northeast Texas and a brief summary of the most recent modeling effort. Studies with modeled years prior to 2005 are described in the previous Northeast Texas Modeling/Analysis Protocol (ENVIRON, 2011). CAMx ozone modeling of the period May 31-July 2, 2006 was carried out by NETAC during the 2012-2013 biennium and is reported in ENVIRON (2013). During FY14-15, the TCEQ completed development of meteorological, emissions and other air quality modeling inputs for a June 2012 episode and made these inputs available to the NNAs. During FY14-15, NETAC developed a June 2012 CAMx ozone model from these inputs and evaluated model performance in reproducing meteorological and air quality measurements at surface monitoring stations in Northeast Texas and other areas of Texas (Johnson et al., 2015).

Overall, ozone model performance at the three Northeast Texas CAMS was characterized by a persistent positive bias. The model overestimated both the daytime maximum ozone values and the night time ozone minima. Model performance for sulfur dioxide (SO_2) and nitrogen oxides (NOx) was relatively poor; this occurred in part because the model misplaced plumes originating from power plants and other regional emissions sources relative to the three monitor locations. Analysis of the ozone model performance indicated that errors in the winds used by the CAMx model caused errors in the CAMx simulation of plumes of ozone and ozone precursors.

The main goal for Northeast Texas ozone modeling work during FY16-17 is to develop a 2012 ozone model that can be used for emission control strategy evaluation and for attainment demonstration modeling, should that become necessary. In order for the June 2012 model to be used for these purposes, the model's ability to simulate observed ozone and ozone precursors on high ozone days must be improved. Once model performance is improved, the model can be used to understand causes of high ozone in Northeast Texas as well as the potential impact of local emissions control strategies.

1.3 Study Objectives

1.3.1 Purpose and Method of the Northeast Texas Ozone Modeling Study

In partnership with the TCEQ, the East Texas Council of Governments (ETCOG) has undertaken the ozone modeling effort described in this Modeling Protocol in order to improve understanding of the processes that can cause high 8-hour ozone concentrations in Northeast Texas. Once these processes are better understood, targeted control measures may be proposed that will be aimed at reducing area ozone. As part of the modeling effort, the potential effectiveness of local emission reductions will be determined.

The method will be to develop and evaluate an ozone model for the Northeast Texas NNA by adapting the emissions inventories (for point, area, mobile, and biogenic sources), and meteorological database developed by the TCEQ, incorporating ambient monitoring data, and

bringing all the information together through the development and application of a photochemical ozone modeling system. This will:

- Provide a better understanding of conditions leading to elevated 8-hour ozone concentrations in Northeast Texas.
- Help evaluate the likelihood of future exceedances of the ozone NAAQS in the area.
- Develop emissions reduction strategies to ensure that the area does not exceed the ozone NAAQS in the future.

The first step in the development of a photochemical modeling database is the development of a Modeling Protocol (this document) that conforms to the requirements in the EPA guidance document (EPA, 2014). The key objectives in developing a photochemical modeling database for Northeast Texas are as follows:

- to incorporate the latest available emissions data for Northeast Texas as well as other areas within the regional-scale grid domain,
- to create accurate CAMx model simulations of the selected episodes, including diagnostic tests, performance evaluation, and sensitivity analyses,
- to estimate the effects of appropriate near-term emission control strategies, and
- to provide the CAMx air quality modeling databases and documentation to ETCOG, TCEQ and other interested parties.

1.4 Study Participants

1.4.1 Contractor

The modeling for this study is being performed by Ramboll Environ, formerly ENVIRON International Corporation (ENVIRON). The key personnel at Ramboll Environ who are directing and performing the study are identified below along with their contact information:

Dr. Greg Yarwood	Principal Investigator	415/899-0704	gyarwood@ramboll.com
Dr. Susan Kemball-Cook	Project Manager	415/899-0730	skemball-cook@ramboll.com
Mr. Jeremiah Johnson	Modeling Lead	415/899-0752	jjohnson@ramboll.com

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773 San Marin Drive, Suite 2115
Novato, California 94998
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www.camx.com

1.4.2 ETCOG

The contact at ETCOG is:

Julie Burnfield, Economic Development Lead
Email: Julie.Burnfield@etcog.org

East Texas Council of Governments
Kilgore, TX 75662
Phone (903) 218-6436
Fax (903) 983-1440

1.4.3 NETAC Policy Committee and Technical Advisory Committee

ETCOG will administer the contract with Ramboll Environ and act as a managing body for the project. Representatives from various local agencies, as well as from ETCOG, TCEQ and EPA, acting through the local stakeholder group NETAC, will provide technical information where needed and will oversee and review all work performed in this project.

In 1995, local elected officials and other leaders in local government, business and industry created NETAC in order to provide leadership and guidance in addressing ozone air quality issues in a five county area consisting of Gregg, Harrison, Rusk, Smith, and Upshur counties. A Policy Committee consisting of representatives of local government, business and industry, the general public and environmental interest groups governs NETAC.

From its inception, NETAC has emphasized the need to ensure that air quality planning activities are developed using scientifically sound techniques. In order to achieve this objective, NETAC created a Technical Advisory Committee to undertake, supervise, and guide technical studies such as emission inventory development, air quality modeling and control strategy development, and specialized monitoring studies. The Technical Advisory Committee reports to the Policy Committee. The Technical Advisory Committee consists of representatives from local government, local business and industry, EPA technical staff, TCEQ technical staff, Texas Department of Transportation planning staff, and the general public and environmental interest groups.

NETAC receives staff support for its activities from ETCOG, which receives and administers grant funds provided by the Texas Legislature for air quality planning activities.

NETAC and its subcommittees meet on an as-needed basis. All meetings are open to the public and are posted at the East Texas Council of Governments and on the NETAC website (www.netac.org) and advertised through the distribution of information packets to local media outlets. The individuals comprising the NETAC Technical and Policy Committees are shown below.

NETAC Policy Committee Members

- Gregg County
  - Judge Bill Stoudt, Co-Chair
- Harrison County
  - Judge Hugh Taylor
- Rusk County
  - Judge Joel Hale
- Smith County
  - Judge Joel Baker
  - Cary Nix
- Upshur County
  - Judge Dean Fowler
- City of Gilmer
  - Jeff Ellington, City Manager
- City of Henderson
  - Mayor Pat Brack
- City of Kilgore
  - Scott Sellers, City Manager
- City of Longview
  - Mayor Andy Mack
  - Councilman Gary Smith
- City of Marshall
  - Frank Johnson
- City of Tyler
  - Mayor Martin Heines, Co-Chair
  - Greg Morgan, Project Coordinator
- Marshall Economic Development Corporation (MEDCO)
  - Donna Maisel, Director,
- Longview Economic Development Corporation (LEDCO)
  - Susan Mazarakes-Gill
- Tyler Economic Development Corporation
  - Tom Mullins, Executive Director
- AEP/SWEPCO

- Keith Honey, General Manager
- Eastman Chemical Company
  - Tim Aldredge
- Luminant Energy
  - David Duncan, Environmental Regional Manager
- WE CAN
  - Tammy Campbell
- Westlake Chemical
  - Eddy Killingsworth

NETAC Technical Advisory Committee Members

- City of Longview
  - Robert Ray, Assistant City Attorney
- Longview MPO
  - Karen Owen, Longview MPO
- City of Marshall
  - Frank Johnson
- City of Tyler
  - Greg Morgan
- Tyler MPO
  - Heather Nick
  - Michael Howell
- EPA
  - Carrie Page
  - Erik Snyder
- TCEQ
  - Doug Boyer
  - Dan Robicheaux
  - Michelle Baetz
  - Leroy Biggers
- NETAC General Counsel
  - Jim Mathews, Mathews and Freeland
- TxDOT

- Brooke Droptini
- AEP/SWEPCO
  - Kelly Spencer
  - Kimberly Hughes
- CenterPoint Energy
  - Laura Guthrie
  - Patrick Coco
- Eastman Chemical Company
  - Shellie Dalby
- Luminant Energy
  - David Duncan
  - Jeremy Halland
  - ~~Donald Montgomery~~Troy Sellers
- Caddo Lake Institute, Inc.
  - Rick Lowerre, Lowerre & Frederick
- Westlake Chemical Corporation
  - Eddy Killingsworth
- Flint Hills Resources
  - Mark McMahon
- BP American Production Company
  - Dana Wood
- Environmental Defense Fund
  - Mr. Ramon Alvarez, Ph.D.
- Norit Americas
  - Amy Clyde

1.5 Schedule and Deliverables

The schedule of tasks currently planned for the Northeast Texas ozone modeling is shown in Table 1-1. This schedule is subject to revision, based on any changes that may occur in the technical direction from NETAC and/or TCEQ, including any revision of objectives or requirements for the study.

Table 1-1. Schedule for Northeast Texas ozone modeling activities.

Task	Completion Date
Draft Modeling Protocol Development	February 25, 2016
Final Modeling Protocol	March 25, 2016
Receipt of Modeling Inputs from the TCEQ	Ongoing
CAMx 2012 Ozone Modeling	March 15, 2017
Draft Report on 2012 Ozone Modeling	May 15, 2017
Final Report on 2012 Ozone Modeling	June 15, 2017

Comment [HJ2]: Should this still be Draft?

Reports and presentations describing the ozone modeling will be submitted to ETCOG, NETAC and the TCEQ. The reports will include the following:

- A draft Modeling Protocol (this document) will be submitted by Ramboll Environ to ETCOG. After NETAC and TCEQ comments on the draft Modeling Protocol are received, a final Modeling Protocol will be prepared and submitted. Note that the Modeling Protocol is a "living document' and may need to be updated from time to time as new information becomes available. Ramboll Environ will work closely with NETAC and TCEQ in cases where significant revisions to the Protocol are needed. For example, if monitored ozone in 2016 is high enough that the 2014-2016 design value for any Northeast Texas CAMS exceeds the 2015 NAAQS, Northeast Texas may be required to perform a modeled attainment demonstration. The Protocol would then be updated to describe the future year and attainment demonstration modeling. The activities undertaken after ~~March~~ May 2016 will be determined by NETAC and the TCEQ, and this Protocol will be updated to reflect the revised plan.
- The May, 2017 draft report describing the CAMx modeling will include methods, performance evaluation and a full description of all sensitivity/diagnostic applications, and will be submitted to ETCOG, NETAC and the TCEQ. After NETAC and TCEQ comments on the draft report are received, a final report will be prepared and submitted.

The CAMx modeling database will be made available to ETCOG, NETAC and the TCEQ.

2.0 CONCEPTUAL MODEL FOR OZONE IN NORTHEAST TEXAS

EPA's guidelines for modeled attainment demonstrations require formulation of a conceptual model for ozone formation in a region before selecting candidate modeling episodes. Stoeckenius and Yarwood (2004), Kemball-Cook and Yarwood (2008; 2010), ENVIRON (2012), Kemball-Cook et al. (2014a), and Parker et al. (2015) have developed a conceptual model of ozone formation in the TLM area, and this conceptual model provides the basis for evaluating the selection of ozone modeling episodes (Section 3). The conceptual model is summarized below.

2.1 Ozone and Air Quality Trends

The TCEQ CAMS monitoring stations determine whether Northeast Texas is in compliance with the NAAQS for ozone. For the three Northeast Texas CAMS monitors, annual 4th highest MDA8 ozone and 8-hour ozone design value trends are shown in Figure 1-2 and Figure 1-3, respectively. Figure 2-1 shows the number of days in each year from 2005 to 2015 in which the MDA8 ozone exceeded the 2008 75 ppb NAAQS and the 70 ppb 2015 NAAQS.

All three monitors show declining numbers of high ozone days from 2005 through 2015 at both the 70 ppb and 75 ppb thresholds. The Tyler CAMS 82 and Longview CAMS 19 monitors had more high ozone days in any given year than the Karnack CAMS 85 monitor at both threshold levels. The decrease in number of days exceeding 70 ppb and 75 ppb over the 2005-2015 period taken together with the declining annual 4th high MDA8 and design values during 2005-2015 (Figure 1-2 and Figure 1-3) indicate improvement in ozone air quality in the TLM area during this period.

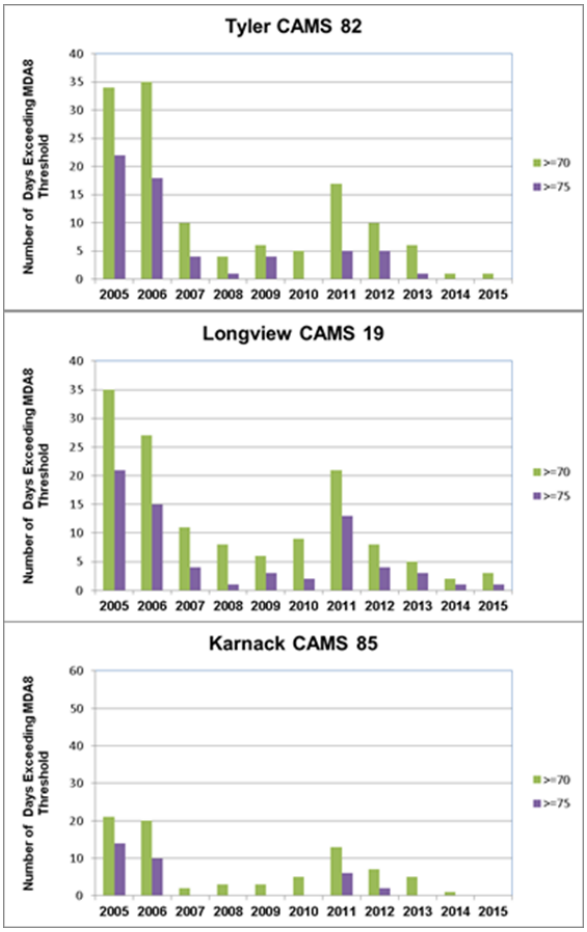


Figure 2-1. Number of days with MDA8 exceeding 70 ppb and 75 ppb in each year from 2005 – 2015. Top: Tyler (CAMS 82). Middle: Longview (CAMS 19). Bottom: Karnack (CAMS 85).

2.2 Summary of Emission Inventory and Trends

Emission inventories are used to assess the nature of an area's ozone problem and can help answer questions such as whether ozone formation in the region is limited by the amount of available NOx or VOC as well as which types of emissions sources are good candidates for emissions controls that would reduce the area's ozone levels. Emission inventories are also required for ozone modeling.

A detailed review of TCEQ's 2012 emission inventory for Northeast Texas was performed by Ramboll Environ in 2014 (Grant et al., 2013). This study provided a review of the most recent

2012 TCEQ anthropogenic emission inventories for the TLM area of Northeast Texas for off-road, area and point sources.

The TCEQ 2006 and 2012 emission inventories are summarized below to establish: (1) the relative importance of point, area, and off-road sources with respect to other emissions source categories (e.g. on-road mobile sources, biogenics) in the TLM area emission inventory and; (2) a comparison of 2012 to 2006 emissions. At the time this analysis was performed, 2012 was the most recent year for which a full TLM area emission inventory (i.e. anthropogenic and biogenic emissions) was available. Area source emissions presented in this section have been divided into two components, non-oil and gas area sources and oil and gas area sources, to facilitate understanding of contributions from oil and gas area sources; oil and gas sources comprise a larger fraction of the area source NOx and VOC inventories than any other single area emissions source category.

Figure 2-2 shows NOx emissions by source category in the TLM area for 2006 and 2012. TLM-~~wide~~ area NOx emissions decreased from 208 tons per day (tpd) in 2006 to 132 tpd in 2012 (or by 37%); emissions for point sources (24% decrease), on-road vehicles (43% decrease), oil and gas sources (45% decrease), off-road mobile sources (24% decrease) and area sources (80% decrease) all decreased. Decreases in NOx emissions from on-road vehicles were the result of fleet turnover to new vehicles between 2006 and 2012 rather than changes in vehicle activity, which were estimated to increase between 2006 and 2012 (Kemball-Cook et al., 2014a). Point sources are the largest contributor to NOx emissions, accounting for 65 tpd or 49% of the total NOx emissions in 2012. On-road mobile is the next largest contributor (30 tpd in 2012). Oil and gas sources (21 tpd in 2012) are the third largest contributor to NOx emissions. NOx emissions from off-road mobile sources are 13 tpd in 2012. NOx emissions from non-oil and gas area sources (3 tpd) and biogenics (<1 tpd) are relatively small compared to NOx emissions from the other categories.

Figure 2-3 presents the 2006 and 2012 TLM area anthropogenic VOC emissions and Figure 2-4 shows the total 2012 VOC emission inventory including both anthropogenic and biogenic sources. The 2012 VOC inventory is dominated by biogenics (i.e. natural sources) with 1,095 tpd (~90%). The same is true in 2006 (Grant et al., 2013). Abundant biogenic VOCs mean there is typically sufficient VOC to form ozone, so ozone formation is limited by the amount of available NOx. Oil and gas are the next largest source of VOC. Non-oil and gas area sources, on-road vehicles, and point sources are minor contributors to TLM area VOC emissions.

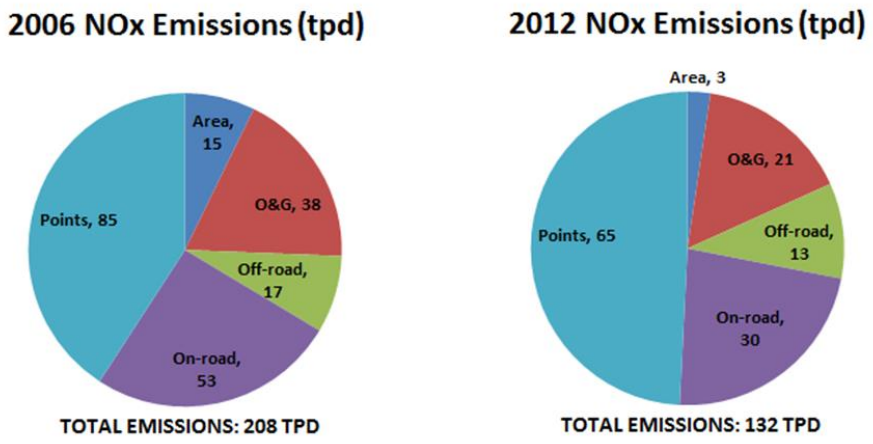


Figure 2-2. TLM Area anthropogenic NOx emissions (tpd) by source category for 2006 (left) and 2012 (right). (Note: oil and gas area source emissions are for calendar year 2011).

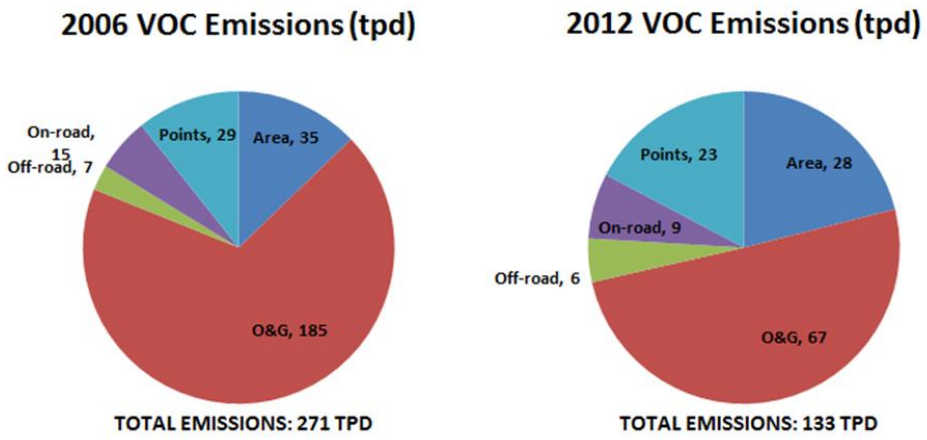


Figure 2-3. 5-county TLM area 2012 anthropogenic VOC emissions (tpd) by source category for 2006 (left) and 2012 (right). (Note: oil and gas area source emissions are for calendar year 2011).

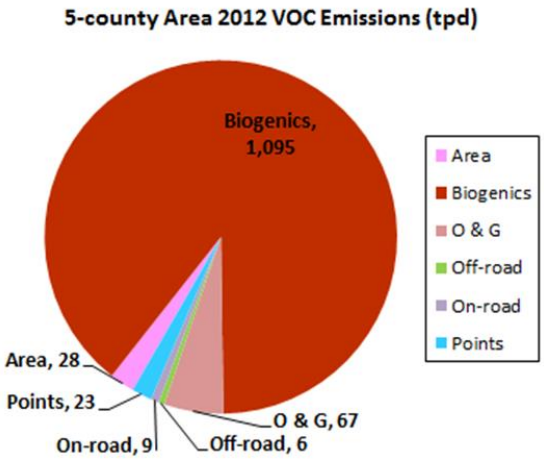


Figure 2-4. 5-county TLM area VOC emissions (tpd) by source category for 2012. Total = 1228 tpd.

In order to develop emission control strategies for Northeast Texas that will reduce the local contribution to ozone, it is necessary to understand how ozone formation in the area depends on the amount of available NOx and VOC. Northeast Texas is densely wooded so that there is sufficient biogenic VOC present during the ozone season for ozone formation to occur. The efficiency with which ozone forms depends on the ratio of VOC to NOx, where the ratio is taken in terms of ppbC/ppb, and ppbC stands for parts per billion of carbon. When the VOC/NOx ratio is higher than about 10, ozone formation is limited by the amount of available NOx and reducing NOx tends to decrease peak ozone concentrations. However, if the VOC/NOx ratio is less than about 7, reducing NOx tends to increase ozone levels, and the area is said to be VOC-limited. In this situation, which can occur in urban cores of large cities, ozone is suppressed in the urban area due to titration by large amounts of fresh nitrogen oxide (NO) emissions. When NOx emissions are reduced, the suppression of ozone by NO is lessened and ozone increases.

The VOC/NOx ratio in the June 2012 emission inventories for the 5-county area as a whole was calculated from the emissions in tons per year (tpy) and the molecular weights of NOx (assumed to be ~46 g/mol) and VOC (assumed to be ~14 g/mol). The 2012 VOC/NOx ratio is 29 ppbC/ppb. The VOC/NOx ratio based on 2006 emissions estimates was 28 ppbC/ppb. The VOC/NOx ratios for both 2006 and 2012 are far greater than 10, which indicates that the TLM 5-county area as a whole is a region where ozone formation is generally limited by the amount of available NOx. This finding is consistent with results of NETAC's ozone modeling, which also indicates that ozone formation in Northeast Texas is NOx-limited (ENVIRON, 2013; Kemball-Cook et al., 2014a, b). Under the right meteorological conditions, NOx from various sources, including several large power plants located within and upwind of the TLM area in addition to on- and off-road mobile sources, and oil and gas and other stationary sources, combine with VOCs to make significant amounts of ozone. While the VOC emissions in the TLM area are

mainly due to biogenic sources, anthropogenic VOC emissions can also contribute to ozone formation.

The Sabine Industrial District (SID) is a large chemical plant near Longview and includes facilities owned by Eastman Chemical Company, Westlake Chemical Corporation and Flint Hills Resources. The SID reports emissions of highly reactive VOCs (HRVOCs; i.e. alkenes such as ethene and propene) as well as NOx; HRVOCs have a strong tendency to form ozone. Rapid and efficient formation of ozone is possible downwind of a source that emits both HRVOCs and NOx (e.g. Kleinman et al., 2002). NETAC field studies and modeling efforts indicate that HRVOCs from the SID can play a role in high ozone events at the CAMS 19 monitor in Longview.

2.3 Meteorological Factors Associated with High Ozone Events

The conditions conducive to the transport, formation, and accumulation of ozone are highly dependent on the prevailing large-scale weather patterns. The TLM area is located on the Gulf Coastal Plain, where the lack of major geographic features means that upper level wind patterns are driven primarily by synoptic-scale meteorological influences. Episodes of high surface ozone concentrations in Northeast Texas occur most often between June and September when the area is under the influence of a semi-permanent subtropical high-pressure system, vertical mixing of pollutants in the atmosphere is restricted, skies are clear to partly cloudy, temperatures are high, and winds are light. Most episodes are associated with near-surface winds from either the east/northeast or south/southwest with the latter direction appearing less consistently on the highest days and with greater variability in direction. Episodes can be classified as either “stagnant”, with very little inflow of air from outside of Northeast Texas or “transport”, with pollutants usually arriving in Northeast Texas through northwestern Louisiana, southern Arkansas, or southeastern Texas.

Ozone exceedances at the Longview CAMS 19 monitoring site are often associated with daytime wind shifts that help keep locally-generated emissions within the area and cause plumes from major point sources to cross over the monitoring site. When these plume impacts occur in conjunction with already elevated regional ozone levels, exceedances of the ozone standard can result. Examination of Longview radar wind profiler data revealed the presence of moderately strong low-level southwesterly winds during the hours between midnight and sunrise on several days. Winds above this low-level flow varied from day to day but ranged from northeasterly to easterly on several of the high ozone days. By mid-day, convective mixing in response to surface heating breaks up the low-level southwest flow and brings the easterly component winds to the surface, causing a rotation of the surface winds from southwest to more easterly. The early morning southwest winds at Longview CAMS 19 may represent the northward intrusion of the previous afternoon’s sea breeze from the Gulf of Mexico. Shifts in surface winds on high ozone days are also observed at the Tyler CAMS 82 and Karnack CAMS 85 monitors.

Comment [HJ3]: Is this current data or historical data? I suggest adding language identifying the time period of reference.

The lowering of the 8-hr ozone standard to 70 ppb alters the conceptual model by introducing ozone exceedance days with different meteorological characteristics. Analysis of recent high

ozone days shows that transport from the south plays a more important role for days with MDA8 in the 65-70 ppb range in Northeast Texas and at the Tyler CAMS 82 monitor in particular (Parker et al., 2015). High ozone days at Tyler CAMS 82 occurred most frequently when the flow was from the east, northeast or the south. The~~se~~ southerly trajectories frequently show the arrival in Tyler of air that had recently been in the vicinity of the Texas Gulf Coast. These trajectories typically show strong eastward curvature, arriving in Tyler from the southwest.

Comment [HJ4]: Do we have figures that need to be referenced to these two statements?

2.4 Regional Transport

EPA Guidance (EPA, 2014) recommends determining as part of the conceptual model for ozone formation whether regional transport of ozone/precursors is an important factor for the area to be modeled. Ozone formed within the TLM area is often augmented by transport of elevated ozone concentrations from outside the area, almost always from the east/northeast or south/southwest. NETAC's ambient data analyses of recent high ozone days in Northeast Texas show that background ozone upwards of 65 ppb can occasionally enter the TLM area from regions to the east/northeast or south (Kemball-Cook et al., 2014a; Parker et al., 2015). A relatively small amount of additional local ozone production is needed under such conditions to produce exceedances of the 8-hour NAAQS of 70 ppb. The lower threshold of the 2015 ozone standard is more easily exceeded by transported ozone before any local contribution. NETAC's modeling results, ambient data analyses and aircraft flight data all indicate that both local controls and regional emissions reduction strategies are required to reduce ozone levels in Northeast Texas.

Parker et al. (2015) reviewed trends in background ozone entering Northeast Texas. Analysis of ambient ozone data from Northeast Texas CAMS monitors showed that local contributions to the MDA8 ozone were much smaller than background contributions to MDA8 ozone on an average basis over the 2005 – 2015 ozone seasons. In addition, the analysis showed that reductions in 90th percentile highest background ozone MDA8 concentrations between 2005 and 2015 have occurred. This downward trend in transported background ozone entering Northeast Texas is consistent in sign with the reduction in transported ozone in the June 2006 ozone model using 2012 emissions compared to the same model using 2006 emissions (Kemball-Cook et al., 2014b). Both the modeling and the ambient analysis suggest a reduction in background ozone coming into Northeast Texas during the 2006-2012 period, which also saw a reduction in ozone design values in the TLM area. The ambient analysis also suggests that the local TLM area contribution to ozone at the Northeast Texas monitors has decreased during 2005-2015. This is consistent with the TCEQ 2006 and 2012 emission inventories for the TLM area that show a 75 tpd decrease in NOx emissions from 2006 to 2012 (Figure 2-2).

3.0 EPISODE SELECTION

3.1 EPA Guidance for Episode Selection

The modeling planned in this protocol follows the EPA episode selection requirements for 8-hour ozone attainment demonstrations (EPA, 2014). The overarching guideline for episode selection for preparing a demonstration of attainment of the 8-hour ozone NAAQS is:

"Choose time periods which reflect a variety of meteorological conditions that frequently correspond with observed 8-hour daily maxima concentrations greater than the level of the NAAQS at monitoring sites in the nonattainment area."

EPA's 8-hour ozone modeling guidance has four primary criteria for selecting meteorological episodes for 8-hour ozone attainment demonstration modeling. The four criteria below are taken directly from the EPA Modeling Guidance (EPA, 2014).

1. Model time periods that are close to the most recently compiled and quality assured NEI.
2. Model time periods in which observed concentrations are close to the appropriate base year design value or level of visibility impairment and ensure there are a sufficient number of days so that the modeled attainment test applied at each monitor violating the NAAQS is based on multiple days.
3. Model time periods both before and following elevated pollution concentration episodes to ensure the modeling system appropriately characterizes low pollution periods, development of elevated periods, and transition back to low pollution periods through synoptic cycles.
4. Simulate a variety of meteorological conditions conducive to elevated air quality.

Comment [HJ5]: I know we decided in the meeting to stick with the 2012 modeling episode. But, in August this will be a little harder to defend since the 2014 EI will be released.

3.2 June 2012 Modeling Episode

The TCEQ is carrying out photochemical modeling to demonstrate how areas of the State that do not attain the 2015 ozone standard will achieve attainment by a specified date which will vary by area. The current Texas nonattainment areas and near nonattainment areas will participate in modeling a common episode which will be used to understand each area's ozone problem and to evaluate emissions control strategies that will help each area formulate a plan to either attain or continue to attain the NAAQS. As part of the attainment demonstration modeling, the TCEQ has developed a June 2012 base case episode. Although 2011 is the year of the most-recently developed and quality-assured NEI, 2011 was an atypical year in Texas. 2011 was the hottest year on record[4] in Texas, and had an unusually active wildfire season. Therefore, the TCEQ has chosen to model 2012 rather than 2011. The choice of time period satisfies criterion 1 above in that 2012 was close to the most recently compiled and quality-assured NEI when episode development was begun.

[4] http://www.ncdc.noaa.gov/sotc/national/2011/8

The TCEQ has carried out meteorological modeling, emission inventory development and modeling for the June 2012 episode, and NETAC has performed CAMx modeling of June 2012 and model performance evaluation focused on Northeast Texas, as described in Section 1.2 and Johnson et al (2015). In the future, the TCEQ may expand this June 2012 episode so that the entire 2012 ozone season is modeled. NETAC is currently using the June 2012 modeling episode in its ozone air quality planning and will expand the episode to include the entire ozone season, should TCEQ decide to model the entire 2012 ozone season. In this section, we evaluate weather conditions during June 2012 and the whole of the 2012 ozone season with respect to the conceptual model of ozone formation in Northeast Texas and EPA Guidance on episode selection.

Figure 3-1 shows the MDA8 ozone at the three Northeast Texas monitors (see Figure 1-1 for monitor locations) during the 2012 ozone season, which extends from March-November in North Texas[5]. Ozone is generally higher during the summer months and lower during the spring and fall. There are many synoptic weather cycles within the 2012 ozone season. There are multiple periods when ozone is high with lower ozone periods preceding and following them. Therefore, Criterion 3 is met for the 2012 ozone season. Table 3-1 lists all days during 2012 when the MDA8 ozone exceeded 70 ppb at any monitor in Northeast Texas. There are two multi-day episodes during which the MDA8 exceeded 70 ppb: June 26-28 and August 7-14. The 2012 ozone season had 12 distinct days with MDA8 > 70 ppb at any Northeast Texas monitor. There were five days with MDA8 ozone > 70 ppb at the Longview CAMS 19 monitor, seven days at the Tyler CAMS 82 monitor, and six days at the Karnack CAMS 85 monitor (Table 3-1).

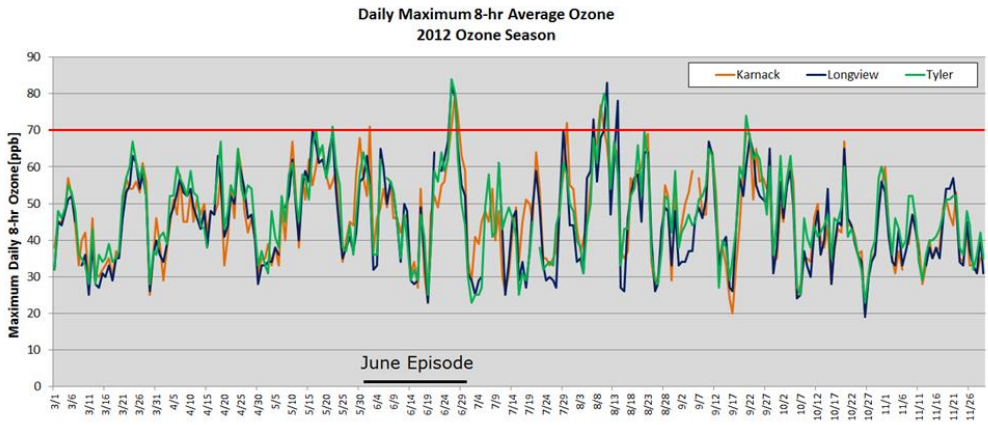


Figure 3-1. Daily maximum 8-hour average ozone at the Northeast Texas monitors during the 2012 ozone season. Duration of the June 2012 episode is indicated by the black bar and the

[5] http://www3.epa.gov/ozonepollution/pdfs/20151021webinar.pdf

red bar shows the level of the 70 ppb 2015 NAAQS for ozone. Breaks in the time series indicate periods of missing data. All data have been validated by the TCEQ.

Table 3-1. List of 2012 days with MDA8 ozone greater than 70 ppb at the Northeast Texas monitors.

Location	CAMS	Date	Time of MDA8 Ozone	MDA8 Ozone
Longview C19/A127/C644	19	June 26 2012	9:00	82
Longview C19/A127/C644	19	June 27 2012	10:00	79
Longview C19/A127/C644	19	August 7 2012	10:00	73
Longview C19/A127/C644	19	August 11 2012	10:00	83
Longview C19/A127/C644	19	August 14 2012	11:00	78
Tyler Airport Relocated C82	82	May 22 2012	10:00	71
Tyler Airport Relocated C82	82	June 26 2012	11:00	84
Tyler Airport Relocated C82	82	June 27 2012	8:00	80
Tyler Airport Relocated C82	82	August 9 2012	12:00	75
Tyler Airport Relocated C82	82	August 10 2012	11:00	80
Tyler Airport Relocated C82	82	August 11 2012	10:00	76
Tyler Airport Relocated C82	82	September 21 2012	10:00	74
Karnack C85/AFHP303	85	June 2 2012	10:00	71
Karnack C85/AFHP303	85	June 26 2012	9:00	71
Karnack C85/AFHP303	85	June 27 2012	10:00	80
Karnack C85/AFHP303	85	June 28 2012	9:00	74
Karnack C85/AFHP303	85	July 30 2012	10:00	72
Karnack C85/AFHP303	85	August 9 2012	12:00	77

Figure 3-2 shows time series of the MDA8 ozone at the three Northeast Texas monitors for the June 2012 episode, which corresponds to the black bar in Figure 3-1. There is one episode of MDA8 ozone > 70 ppb at all monitors (June 26-28); the high ozone period is preceded by a multi-week low ozone period and followed by a two-day transition to lower ozone on June 29-30. Therefore, the June 2012 episode satisfies Criterion 3.

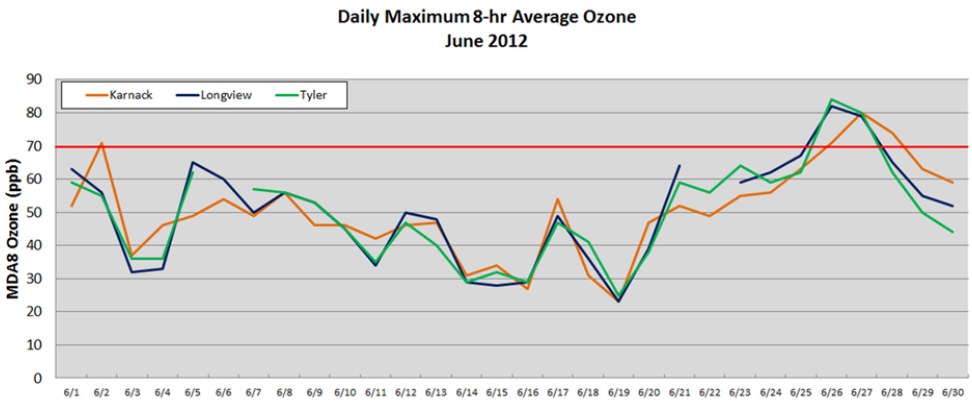


Figure 3-2. Daily maximum 8-hour average ozone at the Northeast Texas monitors during June 2012 TCEQ modeling. Red bar shows the level of the 70 ppb 2015 NAAQS for ozone.

Criterion 2 requires that observed concentrations be close to the base year design value and that there are a sufficient number of days so that the modeled attainment test applied at each monitor violating the NAAQS is based on multiple days. EPA Guidance recommends calculating the modeled relative response factor (RRF) used in the attainment demonstration based on the highest 10 modeled days in the simulated period at each monitoring site as long as the MDA8 for each day is ≥ 60 ppb.

A ranked list of the ten days with the highest MDA8 ozone at the three Northeast Texas monitors during the 2012 ozone season is shown in Table 3-2, and Table 3-3 shows the corresponding list for the month of June 2012.

Table 3-2. Ranked list of 10 days with highest MDA8 during 2012 for each Northeast Texas CAMS. June days are shaded in pink.

	Longview CAMS 19		Tyler CAMS 82		Karnack CAMS 85	
Rank	Date	MDA8	Date	MDA8	Date	MDA8
1	11-Aug	83	26-Jun	84	27-Jun	80
2	26-Jun	82	27-Jun	80	9-Aug	77
3	27-Jun	79	10-Aug	80	28-Jun	74
4	14-Aug	78	11-Aug	76	30-Jul	72
5	7-Aug	73	9-Aug	75	2-Jun	71
6	16-May	70	21-Sep	74	26-Jun	71
7	29-Jul	70	22-May	71	10-Aug	70
8	10-Aug	70	17-May	70	23-Aug	69
9	22-May	69	22-Aug	70	21-Sep	69
10	9-Aug	68	7-Aug	68	22-Sep	69

Table 3-3. Ranked list of 10 days with highest MDA8 during June 2012 for each Northeast Texas CAMS. Days with MDA8 < 60 ppb are shaded in green.

	Longview CAMS 19		Tyler CAMS 82		Karnack CAMS 85	
Rank	Date	MDA8	Date	MDA8	Date	MDA8
1	26-Jun	82	26-Jun	84	27-Jun	80
2	27-Jun	79	27-Jun	80	28-Jun	74
3	25-Jun	67	23-Jun	64	2-Jun	71
4	5-Jun	65	5-Jun	62	26-Jun	71
5	28-Jun	65	25-Jun	62	25-Jun	63
6	21-Jun	64	28-Jun	62	29-Jun	63
7	1-Jun	63	1-Jun	59	30-Jun	59
8	24-Jun	62	21-Jun	59	8-Jun	56
9	6-Jun	60	24-Jun	59	24-Jun	56
10	23-Jun	59	7-Jun	57	23-Jun	55

Table 3-2 indicates that the 2012 ozone season has 10 days with MDA8 ≥ 60 ppb for all three monitors. Therefore, there are enough days meeting the 60 ppb threshold that an RRF can be calculated for each Northeast Texas monitor. At Longview CAMS 19, the MDA8 on the 10 highest days ranges from 68-83 ppb, which brackets the 78 ppb three year average of design values centered on 2012. At Tyler CAMS 82, the MDA8 on the 10 highest days ranges from 68-84 ppb, while the three year average of design values centered on 2012 is 75 ppb. For Karnack CAMS 85, the three year average is 73 ppb, and the 10 highest values range from 69-80 ppb. Based on the values of the 10 highest MDA8 days at the Northeast Texas monitors, Criterion 2 is met if the 2012 ozone season is used as a modeling episode.

Table 3-2 and Figure 3-1 show that June 2012 had some of the highest MDA8 values during the 2012 ozone season at all three Northeast Texas monitors. All of the days with MDA8 > 70 ppb occurred during the June 26-28 high ozone episode except for June 2, which had MDA8 of 71 ppb at Karnack CAMS 85. Ozone during the remainder of June was lower. None of the three Northeast Texas monitors had 10 days with MDA8 ≥ 60 ppb during June 2012. June days with MDA8 < 60 ppb are shaded green in Table 3-3. EPA notes in the Modeling Guidance that days with higher values of ozone are more likely to have a contribution from local sources that would be the focus of local emissions controls, while days with lower ozone are more likely to be dominated by background ozone. Days with higher ozone in the base year are more likely to be representative of days that contributed to the base year design value. Because June 2012 does not have a sufficient number of high ozone days to form an RRF that is consistent with EPA Guidance, it is preferable to use the entire 2012 ozone season if an attainment demonstration is needed for Northeast Texas.

Below, we review the two multi-day high ozone episodes during the 2012 ozone season in order to determine whether Criterion 4 is satisfied in that a variety of meteorological conditions

conducive to elevated air quality are represented during June 2012 and during the entire 2012 ozone season.

3.2.1 June 26-28 Episode

June 24-27, 2012 was a high ozone episode throughout much of East Texas. During this episode, temperatures in Texas and the rest of the central U.S. were very high; there were many large fires active in the central and western U.S. and much of the region was affected by smoke (Kemball-Cook et al., 2014c).

The highest 8-hour ozone reading in 2012 in Northeast Texas was 84 ppb at Tyler CAMS 82 on June 26. On this day, Longview CAMS 19 also recorded high ozone with MDA8 of 82 ppb. On June 27, 2012, the MDA8 ozone exceeded 70 ppb at all three Northeast Texas monitors, and then on June 28, MDA8 ozone dropped below 70 ppb at Longview CAMS 19 and Tyler CAMS 82, but remained over 70 ppb at Karnack CAMS 85. During this 3-day episode, transported background ozone was high; the background 8-hour ozone value was ~65 ppb on June 26 (Figure 3-3), ~75 ppb on June 27 (Figure 3-4) and 65 ppb on June 28 (Figure 3-5). Thus, all monitors were brought close to an exceedance of the NAAQS by transported ozone alone. Emissions from wildfires burning in the Midwest may have contributed to the high background ozone during these days as described in Kemball-Cook et al. (2014c); however, local sources also played an important role in high ozone at Tyler CAMS 82 and Longview CAMS 19.

The late afternoon peak at Tyler CAMS 82 on June 26 was likely due to the Tyler urban plume. Figure 3-3 shows AQplot back trajectories for the time of peak 1-hour ozone at Tyler CAMS 82. The back trajectories show that air arriving at the monitor at the time of peak 1-hour ozone had recently transited the Tyler urban area, suggesting that the Tyler urban plume enhanced ozone at the monitor. On June 27, the Longview CAMS 19 monitor was affected by a plume from a coal-fired power plant. An SO_2 reading of over 40 ppb that coincided with an enhancement in Longview CAMS 19 ozone is shown in Figure 3-4. It is not clear what source(s) caused high ozone in the morning (7-10 am) at Tyler CAMS 82, when Tyler CAMS 82 ozone was up to ~10 ppb higher than ozone at Longview CAMS 19 and Karnack CAMS 85.

June 26 and June 27 illustrate how high background ozone taken together with impacts from local sources (Tyler urban plume on June 26, local power plant impact on June 27) can combine to produce high ozone at Northeast Texas monitors. These days are typical of high ozone days in Northeast Texas in recent years, in which high ozone occurred at Tyler CAMS 82 in the late afternoon during easterly winds, and power plant emissions enhanced ozone at Longview CAMS 19. On June 28, unknown local source(s) enhanced ozone at Karnack CAMS 85 relative to Longview CAMS 19 and Tyler CAMS 82. The high values of $PM_{2.5}$ and the presence of both local and regional fires suggest that fire emissions may have contributed to high ozone at Karnack CAMS 85. The back trajectories extending southward pass over the Panola and Harrison County gas fields as well as the vicinity of two large power plants. Because there is no SO_2 monitor at Karnack CAMS 85, it is not possible to distinguish impacts among these sources.

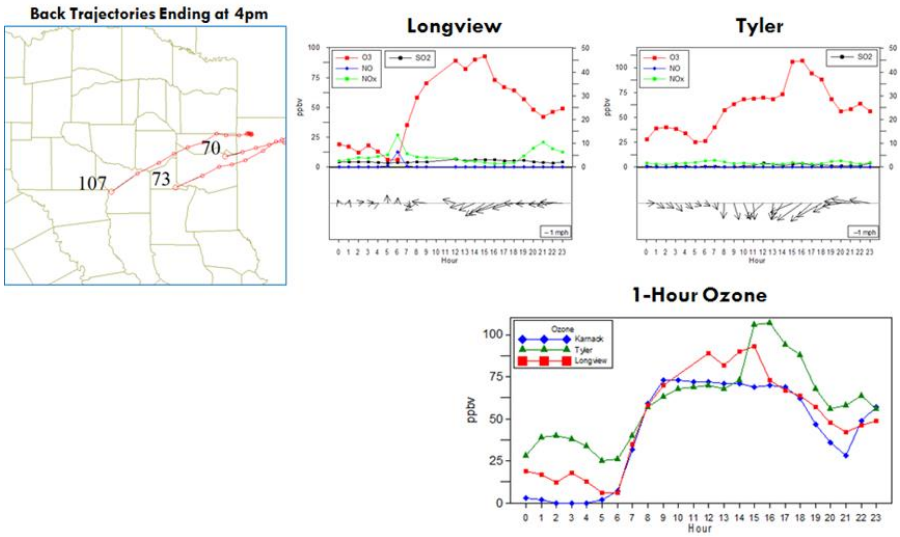


Figure 3-3. June 26, 2012 high ozone day at Tyler CAMS 82. Upper left panel: AQplot back trajectories for the Northeast Texas monitors for June 26 at the time of peak 1-hour ozone at the monitor with highest MDA8 (Tyler CAMS 82). Upper center and right panels: time series of 1-hour ozone, NO, NOx and wind vectors at the Longview CAMS 19 and Tyler CAMS 82 monitors on June 26. Lower right panel: 1-hour average ozone time series for the Northeast Texas monitors.

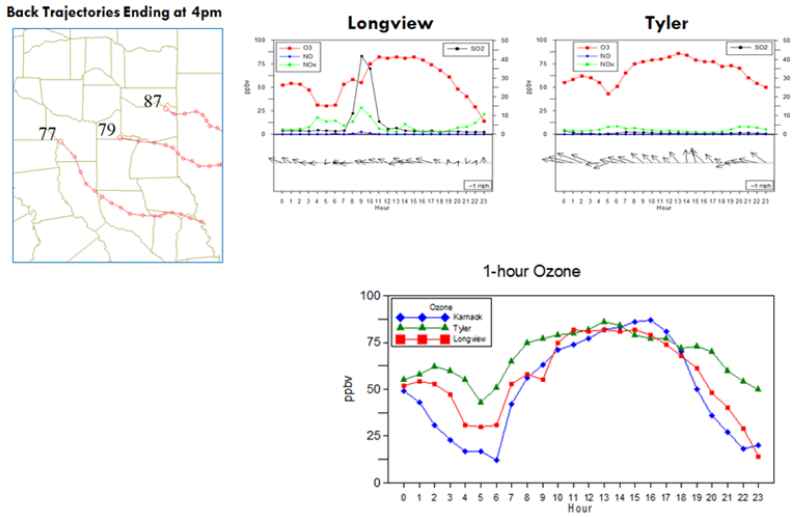


Figure 3-4. As in Figure 3-3, for June 27, 2012.

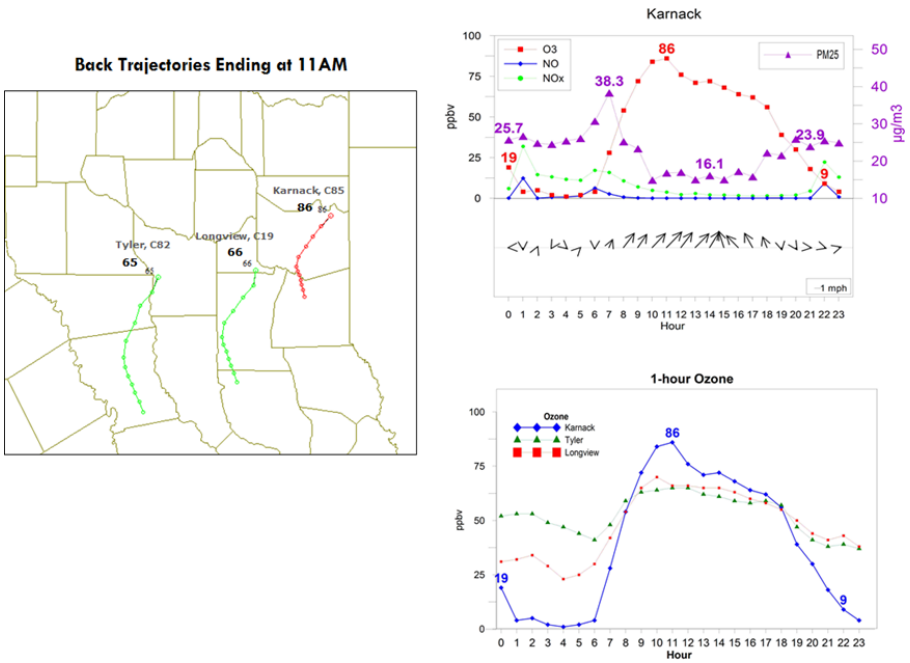


Figure 3-5. As in Figure 3-3, for June 28, 2012.

3.2.2 August 7–14 Episode

The second multi-day high ozone episode in 2012 occurred in the middle of August and included a total of five high ozone days at Northeast Texas monitors (Table 3-4~~Table 3-4~~). These days are shown in Figure 3-6 through Figure 3-10 and are described in Kemball-Cook et al. (2013). Similar to the June episode, transported background ozone was high, with background ozone contributing 60 ppb or more to Northeast Texas ozone on all five days. On August 9, winds were from the southwest and were unusually strong for a high ozone day. The causes of the local contribution to high ozone at Longview CAMS 19 and Tyler CAMS 82 on August 9 are not clear. Small amounts of SO_2 were present at Longview CAMS 19and Tyler CAMS 82 and indicate that power plants contributed but were not the primary cause of high ozone. By August 10, winds had shifted to northerly, but remained strong. Both the Longview CAMS 19 and Tyler CAMS 82 monitors had late afternoon ozone maxima. The northerly wind direction indicates that the late afternoon Longview CAMS 19 peak may be due to an HRVOC plume impact from the Sabine Industrial District. The cause of the late afternoon peak at Tyler CAMS 82 is not clear. August 11 and 14 were characterized by light winds, with very slow recirculating surface wind patterns observed on August 11. On both days, the SO_2 time series at Longview CAMS 19 indicate a late afternoon impact from a coal-fired power plant plume associated with enhanced ozone at the monitor.

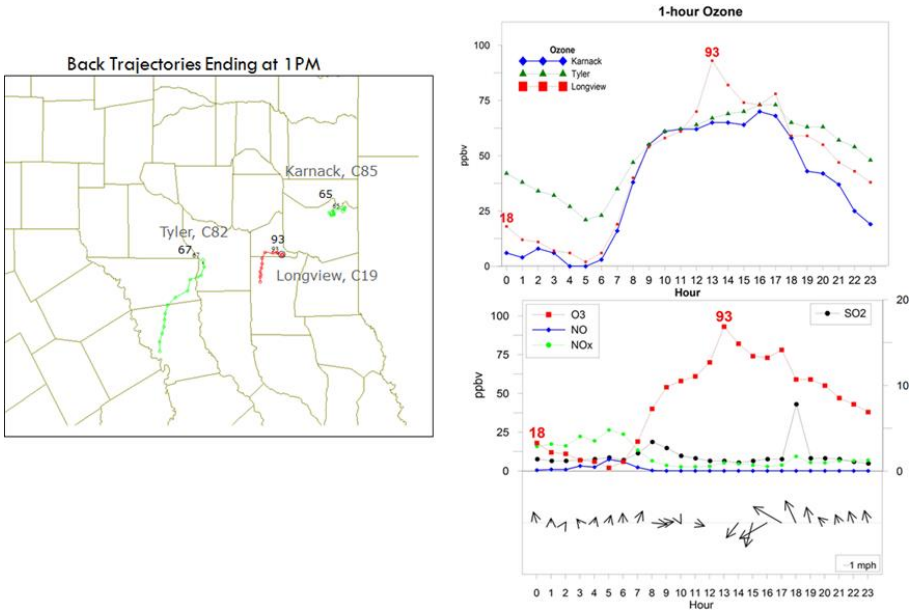


Figure 3-6. As in Figure 3-3, for August 7, 2012.

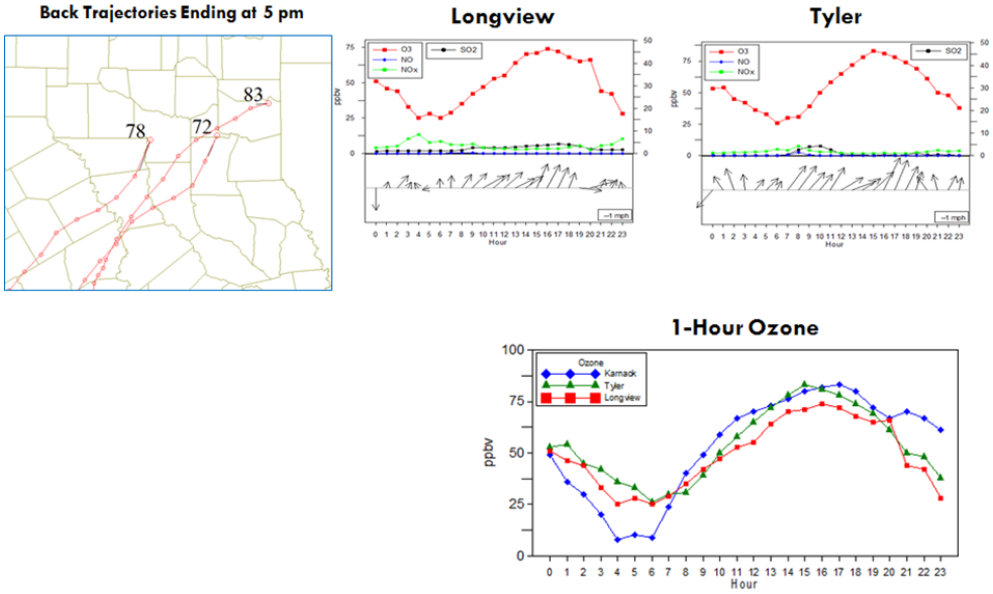


Figure 3-7. As in Figure 3-3, for August 9, 2012.

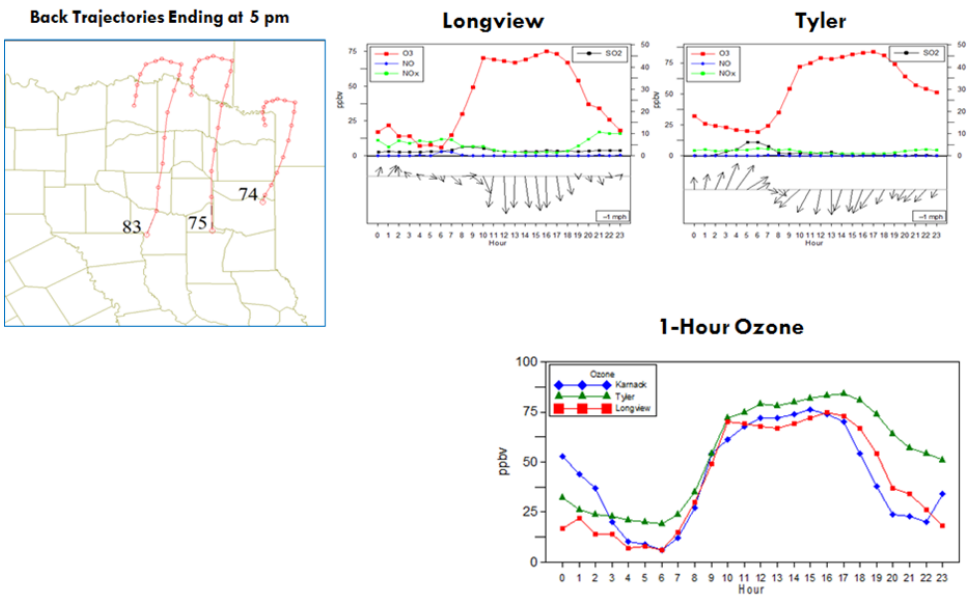


Figure 3-8. As in Figure 3-3, for August 10, 2012.

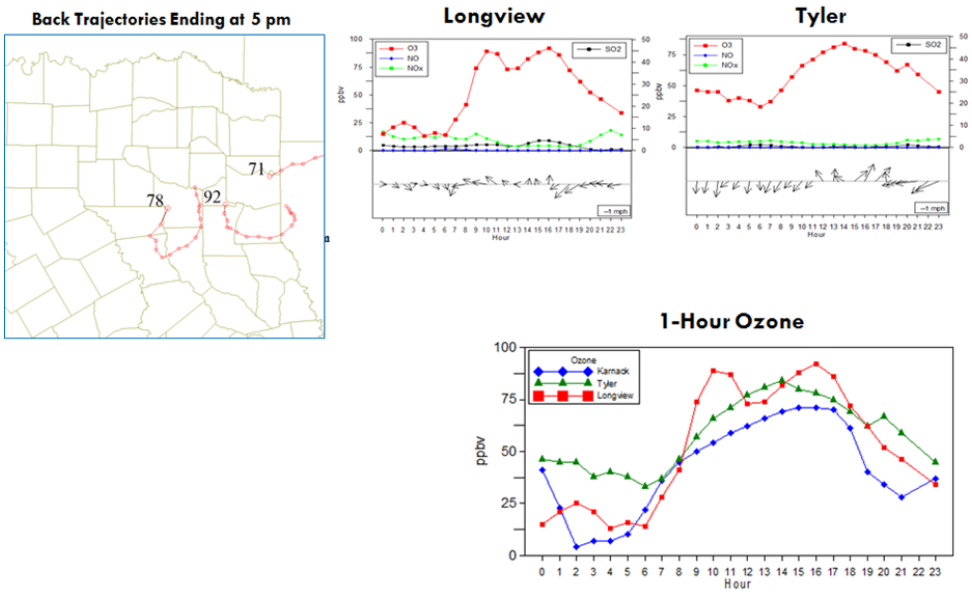


Figure 3-9. As in Figure 3-3, for August 11, 2012.

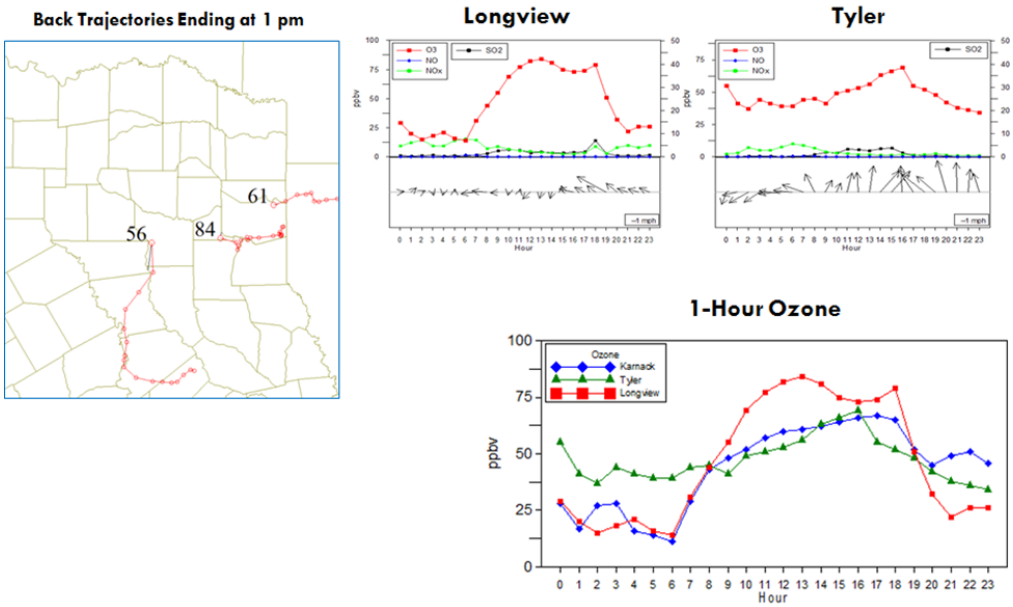


Figure 3-10. As in Figure 3-3, for August 14, 2012.

Summary of 2012 Multi-Day Episodes

The August days are similar to the June episode in that they conform to the typical pattern of Northeast Texas exceedances occurring on days with high background ozone with an additional contribution from local source(s) (Table 3-4~~Table 3-4~~). The August and June days taken together contain days with a variety of wind directions and source-receptor relationships that are typical of high ozone days in Northeast Texas.

Table 3-4. Summary of factors contributing to high ozone days in 2012.

Day	Monitors with MDA8>70 ppb	Power Plant Impact	≥ 60 ppb regional contribution	Possible HRVOC Contribution	Comments
June 26	Longview, Tyler	small	x		Regional background ~70 ppb, Tyler urban plume impact at Tyler
June 27	Longview, Tyler, Karnack	x	x		Regional background ~75 ppb, Power plant impact at Longview
June 28	Karnack		x		Regional background ~65 ppb, possible fire impact at Karnack
August 7	Longview	small	x	x	Regional background ~65 ppb, possible HRVOC impact at Longview
August 9	Tyler, Karnack	small	x		Regional background ~70 ppb
August 10	Tyler		x	x	Regional background ~65 ppb, possible HRVOC impact at Longview
August 11	Longview, Tyler	x	x		Regional background ~65 ppb
August 14	Longview,	x	x		Regional background ~60 ppb

For example, the June 2012 episode contains an episode of moderate ozone in the first week followed by a period of cleaner air associated with strong southerly winds, and concluding with a more stagnant period of high ozone late in the month. Figure 3-11 shows back trajectories ending at the Longview CAMS 19 monitor during June 23-26, 2012. 72-hour back trajectories were prepared using NOAA's HYSPLIT model (Draxler et al., 2013) driven by the NAM 12 km Analysis (upper panels) and the modeled winds used as inputs to the CAMx air quality model (lower panels). Note that back trajectories are a qualitative tool subject to theoretical and data limitations and can only provide approximate information regarding possible source regions for pollutants transported to a monitor.

Figure 3-11 shows the period leading up to the June 26-28 high ozone episode. Figure 3-11 indicates that the back trajectories developed with CAMx model input winds and NAM analysis winds are relatively short and sinuous for all of the days from June 23-26; this is consistent with a regional stagnation event. By contrast, Figure 3-12 (June 7-10) shows an episode when back trajectories were far longer and less sinuous; this corresponds to an episode when the CAMx winds and the NAM analysis are consistent in suggesting that transported ozone played a role in controlling ozone levels in Northeast Texas. For all days, HYSPLIT back trajectories prepared

with the CAMx input winds agree well with HYSPLIT trajectories prepared with the NAM 12 km Analysis.

Comment [HJ6]: I agree they are similar, but believe that "agree well" is overstating the similarities while disregarding the differences.

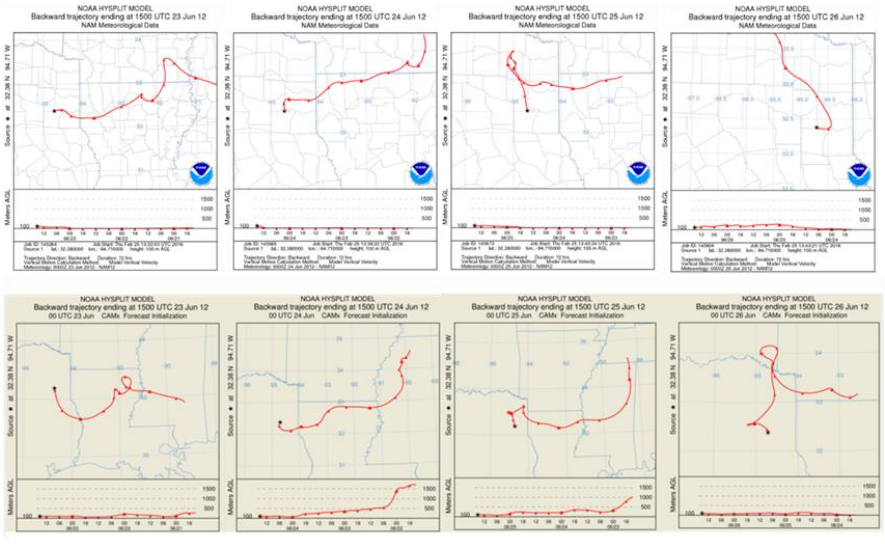


Figure 3-11. HYSPLIT 72-hour back trajectories using NAM 12 km Analysis (upper panels) and CAMx model winds (lower panel) ending at 100 m above the Longview CAMS 19 monitor during June 23-26, 2012.

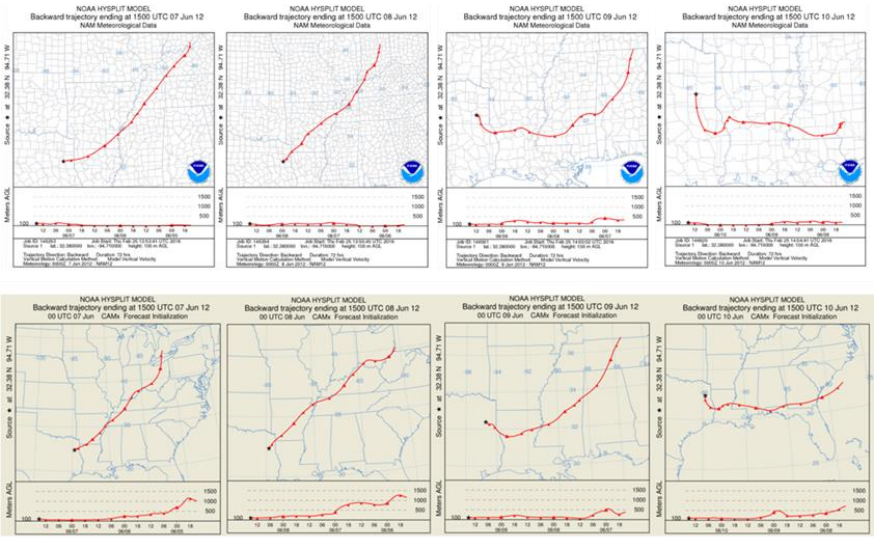


Figure 3-12. HYSPLIT 72-hour back trajectories using NAM 12 km Analysis (upper panels) and CAMx model winds (lower panel) ending at 100 m above the Longview CAMS 19 monitor during June 7-10, 2012.

Comment [HJ7]: The scale of the figures is different, which is a little misleading. If it is not possible to have both graphics on the same scale, please include a statement making that more obvious.

3.3 Episode Selection Summary

In summary, the 2012 ozone season satisfies all four EPA criteria for an ozone episode to be used in an attainment demonstration. The June 2012 modeling episode satisfies Criteria 1, 3 and 4, but not Criterion 2, because none of the Northeast Texas monitors had 10 days with MDA8 ozone ≥ 60 ppb during June 2012. While the June 2012 episode is useful for air quality planning and analysis for Northeast Texas, expanding the episode to encompass the entire 2012 ozone season would provide days with additional wind directions and source-receptor relationships not present during June and would allow a sufficient number of high ozone days for an attainment demonstration, if that were to become necessary for Northeast Texas.

4.0 MODEL SELECTION

EPA (2014) recommends that models used in ozone attainment demonstrations be selected on a case-by-case basis with appropriate consideration being given to the candidate model's

- technical formulation, capabilities and features,
- pertinent peer-review and performance evaluation history,
- public availability and capability for user to modify the model source code
- applicability for the intended modeling
- availability of databases sufficient to support the model's application
- availability of a User's Guide
- availability of probing/diagnostic tools, and
- demonstrated success in similar regulatory applications.

All of these considerations should be examined for each class of models to be used (e.g., emissions, meteorological, and photochemical) in part because EPA no longer recommends a specific model or suite of photochemical models for regulatory application as it did previously (EPA, 1991).

The models selected by the TCEQ for modeling of 2012 are:

- the Weather Research and Forecasting Model meteorological model (WRF; Skamarock et al., 2005) ,
- Version 3 of the Emissions Processing System (EPS3) for anthropogenic emissions,
- the MEGAN biogenic emissions model (Guenther et al., 2012), and
- the CAMx photochemical grid model (Ramboll Environ, 2016).

A brief description of each model is provided below, and the TCEQ's rationale for model selection is provided in the TCEQ's Dallas-Fort Worth Modeling Protocol[6].

4.1 WRF Meteorological Model

The CAMx model requires as an input gridded weather data that is provided by an off-line meteorological model. The TCEQ has elected to use WRF for the meteorological modeling for the June 2012 ozone episode. WRF is the successor to the MM5 model (Dudhia et al., 1993) that the TCEQ has used for previous SIP modeling. MM5 was developed at the Pennsylvania State University over 20 years ago, and was supported and updated thereafter through collaboration between PSU and the National Center for Atmospheric Research (NCAR) as well as other users; however, following the release of its successor, WRF, MM5 is no ~~being~~ longer

[6] https://www.tceq.texas.gov/assets/public/implementation/air/sip/dfw/dfw_ad_sip_2016/DFW_SIP_Appendix_E_pro.pdf

being maintained or developed. WRF is now widely used for preparing inputs to urban- and regional-scale photochemical air quality models.

WRF's development was led by NCAR and the National Oceanographic and Atmospheric Administration (NOAA) in collaborations with universities and other government agencies within the U.S. and overseas. WRF is a public-domain model that is freely available. WRF is based on the full set of non-hydrostatic primitive equations. Optional parameterizations exist for boundary layer schemes; cloud and precipitation physics; heat budgets for multiple soil layers; the kinematic effects of terrain; and cumulus convection. One- or two-way interactive grid nesting is allowed. WRF contains a four-dimensional data assimilation (FDDA) capability that allows the "nudging" of the model solution toward gridded analyses and individual observations, either separately or in combination.

The model equations are solved horizontally on an Arakawa-C grid structure defined on a number of available map projections. The Lambert Conic Conformal projection was selected by the TCEQ. The WRF vertical coordinate is a terrain-following hydrostatic pressure representation. The vertical layer structure used in the June 2012 modeling and the grid nesting strategy are described in Section 6.2.

4.2 EPS3 Emissions Modeling System

Raw emission inventory databases provide annual or seasonal emission estimates of "criteria" pollutants (CO, NO_x, VOC, SO_x, PM) by county or geodetic grid square and by source category. The detail in source category stratification varies greatly among the datasets. To use these emission estimates in an air quality model, emission rates from all sources need to be adjusted to season, day-of-week (if applicable), and hour, speciated into NO, NO_2, and model VOC species, and spatially allocated to the higher resolution CAMx air quality modeling grid using various land type or human activity surrogates. The processing of raw emission datasets to model-ready inputs is accomplished through the use of an emissions model. The TCEQ used the Emissions Processing System (EPS3) emissions modeling system to generate model-ready anthropogenic emissions for the June 2012 episode. EPS3 is an emissions modeling system that generates hourly gridded speciated emission inputs of mobile, nonroad, area, point, fire and biogenic emission sources for photochemical grid models. It is the emissions modeling system used by the State of Texas for SIP modeling. It is FORTRAN-based, and incorporates a strong quality assurance and reporting capability. EPS3 is a mature, thoroughly-tested emissions modeling system that has been employed by a wide variety of governmental, commercial, academic, and private users in numerous regions throughout the U.S. and abroad.

Biogenic emissions must be developed outside of EPS3. Biogenic emissions sources are naturally-occurring (i.e., not from human activities) and are emitted by vegetation such as trees and agricultural crops as well as by microbial activity in soils or water. Some biogenic VOC such as isoprene and pinenes are highly reactive, which means they are especially likely to contribute to ozone formation. The 2012 biogenic emission inventory was developed by the TCEQ using the Model of Emissions of Gases and Aerosols from Nature (MEGAN; Guenther et al., 2012)

version 2.10. MEGAN calculates hourly, day-specific emissions that depend on photosynthetically active solar radiation and temperature as well as other inputs such as land cover and plant type.

4.3 CAMx Air Quality Model

Several photochemical air quality models have been developed for ozone modeling and applied to different areas in the U.S. EPA's latest guidance document (EPA, 2014) notes that EPA has no "preferred model," but lists the following *prerequisites* for a photochemical model to be accepted:

- The model should meet requirements for "alternative models" in 40CFR Part 51 Appendix W.
- The model must not be proprietary and its source code must be made available to users at low or no cost.
- User must be able to revise the code to perform diagnostic analyses and/or improve the model's ability to reproduce observations.
- A user's guide should be available.
- It should have received a scientific peer review.
- It should be applicable to the specific problem on a theoretical basis.
- It should be used with a database that is adequate to support the application.
- It should have performed in past applications in such a way that estimates are not likely to be biased low.
- It should have probing tools such as a source apportionment capability.
- It should be applied consistently with a protocol on methods and procedures.

The TCEQ has selected the CAMx model (Ramboll Environ, 2016) for the June 2012 modeling. The TCEQ's rationale for the selection of CAMx is documented in the Dallas-Fort Worth Modeling Protocol (TCEQ, 2014), but some aspects of CAMx relevant to model selection are presented below.

CAMx was developed by Ramboll Environ and is publicly available at www.camx.com. CAMx is a "one-atmosphere" model for ozone, PM, visibility and air toxics. CAMx has been used by the State of Texas for the Houston-Galveston, Beaumont-Port Arthur, and Dallas-Fort Worth ozone attainment demonstration modeling for the Texas SIP. CAMx has also been used by other states for their 8-hour ozone planning and by the EPA for the NOx SIP Call, Clean Air Transport Rule, and other rulemakings.

In selecting an air quality model for Northeast Texas ozone, the following technical capabilities are considered important:

- Two-way grid nesting is essential for regional scale modeling in order to accurately depict local ozone formation in Northeast Texas and to characterize ozone transport from

upwind regions. One-way grid nesting is considered inadequate because emissions are not treated consistently between the coarse and fine grids.

- A plume-in-grid algorithm is required to adequately represent the near source impacts of major NOx sources.
- An updated chemical mechanism is required, and CAMx has as an option the CB6r2 chemical mechanism (Yarwood et al., 2012), which is a state-of-the-science mechanism.
- Updated transport algorithms with low numerical diffusion are highly desirable to accurately represent plume impacts of major sources.
- Free public access and availability without any restrictions on use.
- CAMx has numerous "probing" tools (e.g., source apportionment, process analysis and the direct decoupled sensitivity analysis).
- The State of Texas uses CAMx for other SIP modeling in Texas.
- CAMx is a full-scale one-atmosphere model that can account for all atmospheric processes up to ~100 mb as recommended by (EPA, 2014).

In summary, all of the models selected by the TCEQ for the June 2012 ozone modeling are appropriate for the Northeast Texas ozone modeling.

5.0 MODELING DOMAINS FOR THE JUNE 2012 EPISODE

The TCEQ has specified a set of 3 nested modeling grids (36/12/4 km) designed to be suitable for use by all of the NNAs. The TCEQ has supplied emissions and meteorological and air quality model inputs for the June 2012 episode on these grids. In this section, we describe the TCEQ grids.

5.1 Lambert Conformal Projection Definition

The modeling grids specified by the TCEQ are defined on a Lambert Conformal Projection (LCP). Several parameters define an LCP horizontal grid coordinate system, namely a latitude/longitude "center" (0 km, 0 km) point, two true latitude parallels, and a grid origin offset from the "center" and the east-west and north-south extent of the modeling domain. The modeling grids are defined on the national Regional Planning Organization (RPO) LCP mapping projection used by most other states, as well as EPA, for continental-scale air quality modeling. The RPO grid has a center point of 97° W longitude and 40° N latitude with true latitudes of 33° N and 45° N. The main advantage of using the national projection criteria is direct compatibility of modeling files between the TCEQ and other regulatory modeling efforts. All TCEQ meteorological and air quality modeling grids in the June 2012 modeling effort use the RPO projection and all TCEQ CAMx-ready meteorology and emissions files were prepared on the RPO projection.

5.2 TCEQ CAMx Modeling Domains

For the June 2012 episode, the modeling domain for WRF meteorological modeling and the domain for the CAMx ozone model were defined by the TCEQ. There is necessarily a close relationship between CAMx and WRF grids to ensure that meteorological information is transferred accurately from WRF to CAMx. To minimize interpolation of meteorological variables from WRF to CAMx and the resulting potential for disruption of mass consistency, CAMx used the same coordinate system as WRF. The TCEQ defined CAMx modeling grids to use the same LCP projection as the WRF modeling.

EPA's guidance on applying models for 8-hour ozone (EPA, 2014) states that the most important factors that determine the horizontal extent of the domain are the nature of the ozone problem and the spatial scale of emissions which affect the region of interest. The overall strategy in defining a nested modeling grid system is that a fine grid provides higher resolution in the area of interest while a coarse grid provides computational efficiency over a larger modeling region. The TCEQ nested grid air quality modeling system for the June 2012 episode is shown in Figure 5-1. In accordance with EPA (2014) guidance, the outer 36 km CAMx domain shown in black in Figure 5-1 was designed to be large enough to encompass all important upwind sources of emissions and to allow use of clean or relatively clean boundary conditions. Backward trajectory analyses performed by the TCEQ have suggested that air mass transport from the Ohio Valley/Midwest to Texas occurs frequently. The 36 km modeling domain is consistent with EPA's guidance that all major upwind source areas that influence the downwind area are included in the modeling domain (EPA, 2014).

The 12 km CAMx grid (shown in light blue in Figure 5-1) includes all areas in eastern Texas that are conducting ozone modeling so that a consistent 12 km grid can be used in all studies. In addition the 12 km grid includes a substantial area that would typically be upwind of Texas during an ozone episode with easterly or northeasterly winds. This is important to accurately represent any influence of ozone formation that may be modeled more accurately by a 12 km grid than a 36 km grid, provided higher resolution model inputs are available on the 12 km grid. The intention is to accurately model potential transport of ozone from areas at a distance upwind from Texas of about the breadth of one state.

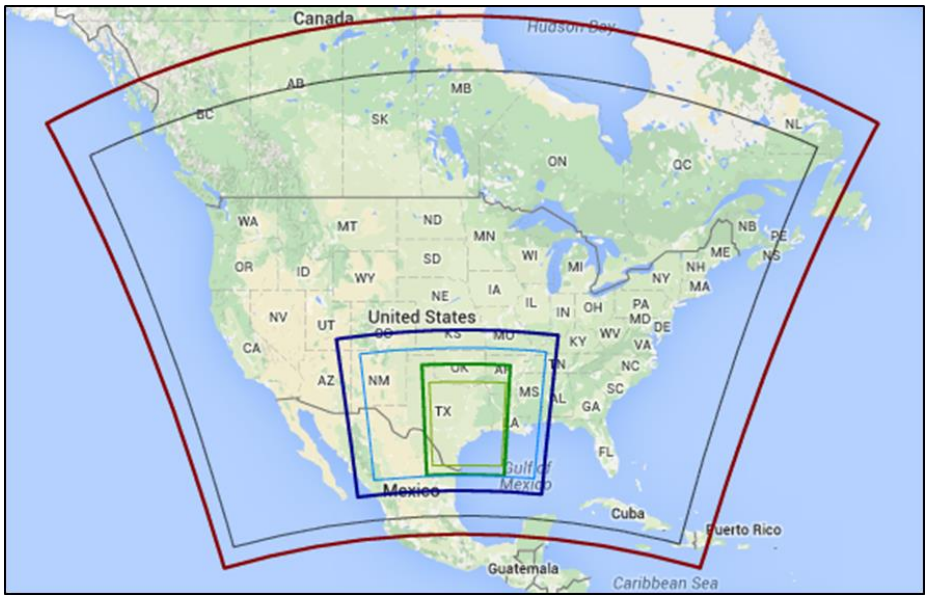


Figure 5-1. TCEQ 36/12/4 km CAMx nested modeling grids for the Texas ozone modeling of June 2012. 36 km CAMx grid extent is outlined in black. 12 km CAMx grid is outlined in light blue and the 4 km CAMx grid is outlined in light green. Each CAMx modeling grid lies just within the corresponding WRF grid.

The TCEQ's 4 km CAMx grid (shown in light green in Figure 5-1) encompasses all of the TLM 5-county area, and includes nearby electric generating units (EGUs), as well as conventional oil and gas development and the Haynesville Shale, including its Louisiana parishes. The Northeast Texas Conceptual Model (Kemball-Cook et al., 2014a; Parker et al., 2015) also indicates that transport from the south may play an important role in determining ozone levels in Northeast Texas. The Houston-Galveston-Brazoria-Port Arthur nonattainment area is the largest urban area to the south. The TCEQ's previous Houston modeling (e.g. TCEQ, 2010) has shown that accurate simulation of ozone formation in the area requires high-resolution 4 km modeling in order to reproduce the effects of the sea breeze circulation, as well as the effects of numerous point sources of emissions on ozone production and transport. In order to accurately model

ozone formation in the Houston area and its possible transport into Northeast Texas, it is necessary to model the Houston area at 4 km resolution in this study. Running CAMx on the nested grid system in Figure 5-1 allows the best balance of computational efficiency and accuracy in simulating processes that determine ozone levels in Northeast Texas.

5.3 WRF Domain

WRF coarse and nested grids defined by the TCEQ are shown in Figure 5-1. Modeling domains are defined on a Lambert Conformal Conic (LCC) map projection identical to that used in the Regional Planning Organization (RPO) modeling[7]. The RPO projection is defined to have true latitudes of 33°N and 45°N and central latitude and longitude point (97°W, 40°N). The 36 km WRF modeling domain encompasses the continental U.S. and parts of Canada and Mexico. The 12 km grid includes Texas and adjacent states and the 4 km grid is centered on East Texas. WRF 36, 12 and 4 km grids are slightly larger than the corresponding CAMx grids to remove any artifacts (i.e., numerical noise) that can arise in WRF adjacent to fine grid boundaries.

5.4 Vertical Layer Structure in CAMx AND WRF

EPA's current guidance on applying models for 8-hr ozone (EPA, 2014) includes the following information on vertical layer structure:

- There is no current recommended number of vertical layers, however, EPA notes that recent applications have used 14-35 vertical layers within the troposphere.
- The surface layer should be no thicker than ~40 m.
- There should be a close correspondence between the meteorological model and air quality model layers.
- Excessively thick layers within the PBL are to be avoided.
- The top of the modeling domain should be set at approximately 50-100 mb (~16,000 meters).

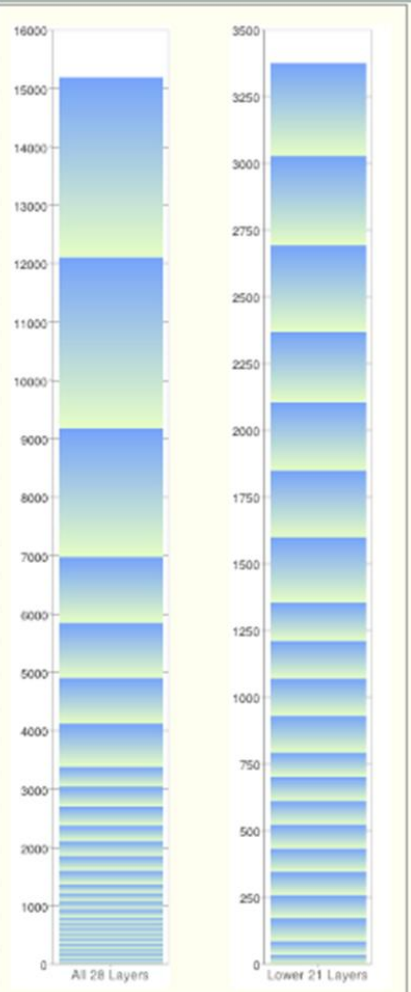
The vertical layer configuration selected by the TCEQ (Table 5-1) meets all of these requirements.

[7] http://www.epa.gov/visibility/regional.html

Table 5-1. WRF and CAMx model layer structure. TCEQ figure[8].

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.

[8] http://www.tceq.texas.gov/airquality/airmod/rider8/modeling/domain

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6.0 METEOROLOGICAL MODELING

EPA Modeling Guidance (EPA, 2014) requires that the meteorological data developed to support air quality modeling be extensively evaluated because of the sensitivity of the air quality modeling results to the input weather data.

CAMx requires meteorological input data for the parameters shown in Table 6-1. For the June 2012 episode, the TCEQ developed meteorological input data for CAMx using the WRF meteorological model version 3.6.1 (Skamarock et al., 2005) and then processed WRF outputs using the WRFCAMx preprocessor to generate model-ready meteorological files containing each field in Table 6-1. In this section, we describe the configuration used by the TCEQ for the June 2012 meteorological modeling that has already been conducted. Two additional, differently-configured WRF runs were conducted by Ramboll Environ in FY14-15 to improve model performance for winds over Northeast Texas, but did not result in a substantially more accurate simulation (Johnson et al., 2015). Because additional WRF modeling may be necessary in FY16-17 to refine WRF model performance, we outline the model performance evaluation strategy for any WRF modeling that is performed by Ramboll Environ during the Northeast Texas Ozone Modeling Study.

Table 6-1. CAMx meteorological input data requirements.

Input Parameter	Description
Layer interface height (m)	3-D gridded time-varying layer heights for the start and end of each hour
Winds (m/s)	3-D gridded wind vectors (u,v) for the start and end of each hour
Temperature (K)	3-D gridded temperature and 2-D gridded surface temperature for the start and end of each hour
Pressure (mb)	3-D gridded pressure for the start and end of each hour
Vertical Diffusivity (m^2/s)	3-D gridded vertical exchange coefficients for each hour
Water Vapor (ppm)	3-D gridded water vapor mixing ratio for each hour
Clouds and Rainfall (g/m^3)	3-D gridded cloud and rain liquid water content for each hour

6.1 WRF Application

The WRF model provides a wealth of options to configure the model for various parameterizations and physics packages. Model physics options selected by the TCEQ for the June 2012 WRF simulation are shown in Table 6-2.

Consistent with recommendations in EPA (2014), TCEQ has applied WRF using the model's FDDA capability. WRF is a predictive (i.e. forecasting) model; the WRF solution is therefore subject to increasing error over the course of an extended simulation due to uncertainties in initial/boundary conditions, limits in spatial and temporal resolution, and simplification and discretization in the governing equations. In retrospective simulations of historical episodes (as opposed to forecasting), FDDA is used to "nudge" model predictions toward observational analyses and/or discrete measurements to control model "drift" from conditions that actually occurred. ~~The WRF model's FDDA capability can be used to nudge model predictions toward observational analyses and/or discrete measurements to control model "drift" from conditions~~

~~that actually occurred.~~ This approach has consistently been shown to provide advantages in running mesoscale models for multiday episodes, and has become the standard for retrospective photochemical applications. WRF may be nudged toward gridded analyses ("analysis nudging") or toward individual observations ("observation nudging"). TCEQ supplied the WRF FDDA system with gridded meteorological analyses derived from observations from a combination of several systems (routine measurements from surface and upper air sites, radar networks, and wind profilers). The model solution was then "nudged" toward the analysis throughout the 2012 run. The nudging options used are shown in Table 6-2.

Comment [HJ8]: This seems redundant, consider deleting this sentence.

Table 6-2. Physics parameterizations used in the TCEQ WRF simulation.

	TCEQ June 2012 WRF Base Case Run Configuration
WRF version	3.6.1
Horizontal Resolution	36/12/4 km
Microphysics	36/12 km: WSM5 4 km: WSM6
Longwave Radiation	RRTM
Shortwave Radiation	Dudhia
Surface Layer Physics	Revised MM5 similarity
LSM	Pleim-Xiu
PBL scheme	Yonsei University (YSU)
Cumulus parameterization	Kain-Fritsch on 36/12 km grids; None on 4 km grid
Boundary and Initial Conditons Data Source	40 km NAM analysis
Analysis Nudging Coefficients (s^{-1})	36/12 km: 3-D 4 km: 3-D and surface
Winds	$3x10^{-4}$
Temperature	3x10-4 (above planetary boundary layer only)
Mixing Ratio	3x10-4 (above planetary boundary layer only)
Observation Nudging Coefficients (s^{-1})	4 km only
Winds	$6x10^{-4}$
Temperature	None
Mixing Ratio	None
Miscellaneous Notes	Run as two simulations (4/30/2012 0Z - 6/2/2012 0Z and 5/31/2012 0Z - 7/2/2012 0Z) 4 km simulation run separately; IC/BCs from ndown

6.2 Grid Nesting

Two-way nesting refers to the transfer of large-scale information down to nested grids, and the feedback of smaller scale influences up to larger grids. The TCEQ ran the 36/12 km grids in two-way nested mode. TCEQ then ran the 4 km simulation separately, using information from the 12 km grid to supply initial and boundary conditions. Because the information from the 4 km grid does not get transferred to the 36/12 km grids, this is called "one-way" nesting.

6.3 Meteorological Model Evaluation

EPA modeling guidance (EPA, 2014) recommends operational and phenomenological evaluation of the meteorological fields to be used in the photochemical modeling. Operational evaluation focuses on comparisons between observed and modeled data paired in time and space, while phenomenological evaluation determines whether specific phenomena that can influence the air quality modeling are reproduced accurately in the model. Examples of these are transport patterns that influence source-receptor relationships, sea breeze circulations, etc.

To provide a reasonable meteorological characterization to CAMx, WRF must represent with good accuracy the large-scale and mesoscale wind, temperature, humidity and precipitation fields. If errors in the meteorological fields are too large, the ability of the air quality model to replicate regional pollutant levels over the June 2012 period will be hampered and the predicted ozone results will be unreliable. Accurate simulation of winds is critical to model transport of pollutants from emissions sources to receptors within the domain. Any new WRF runs performed for the Northeast Texas ozone modeling will be evaluated in accordance with EPA Guidance. Depending on the focus of the WRF run, graphical and/or statistical evaluation of model performance will be carried out for modeled fields such as winds, temperature, solar radiation and precipitation.

Output from WRF will be compared against meteorological observations from the various networks operating in Texas such as the CAMS stations and the airport meteorological sites shown in Figure 6-1. A graphical and statistical evaluation of model performance will be carried out for winds, temperatures, humidity and boundary layer heights (if observed data become available), and the placement, intensity, and evolution of key weather phenomena. The focus of this evaluation will be on model performance in Northeast Texas and areas that are often upwind on high ozone days in Northeast Texas. Examples of graphical products are shown in Figure 6-2. To place the WRF performance in context of other Texas air quality modeling efforts, the performance of any new June 2012 WRF runs will be compared with that of previous Texas meteorological modeling applications. An example of such a comparison is shown in Figure 6-3. The Taylor Diagram in Figure 6-3 summarizes WRF performance in three different simulations with respect to observations in terms of correlation coefficient, standard deviation, normalized mean bias and centered root mean squared error (RMSE). Taylor Diagrams are described in Taylor et al. (2001).

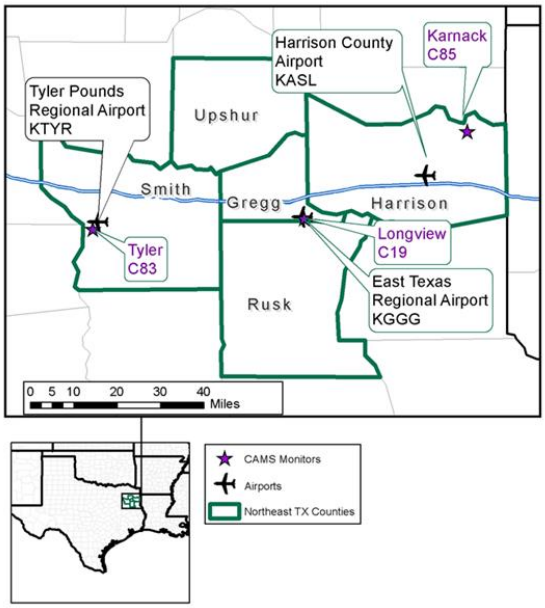

Figure 6-1. Map of Northeast Texas showing ds472.0 airport locations and CAMS monitoring sites.

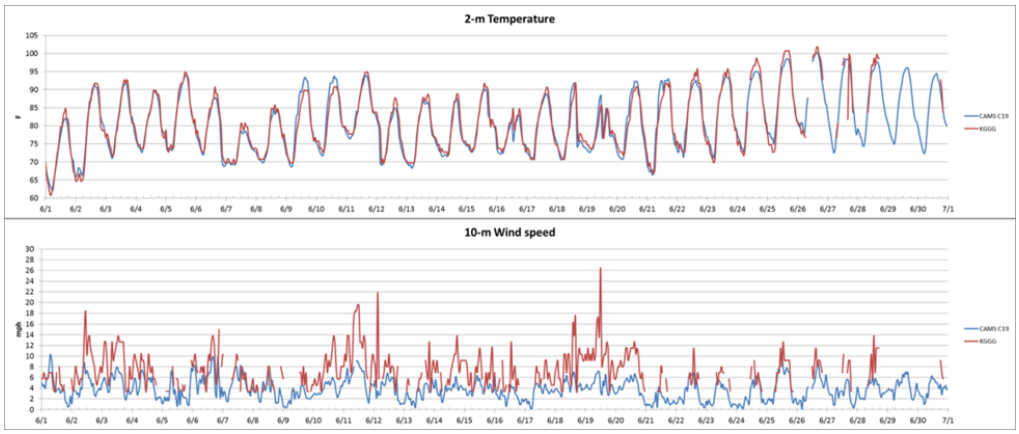

Figure 6-2. Time series of observed 2-m temperature (top) and 10-m wind speed (bottom) at the Longview CAMS 19 (blue) and East Texas Regional Airport (red) monitoring sites.

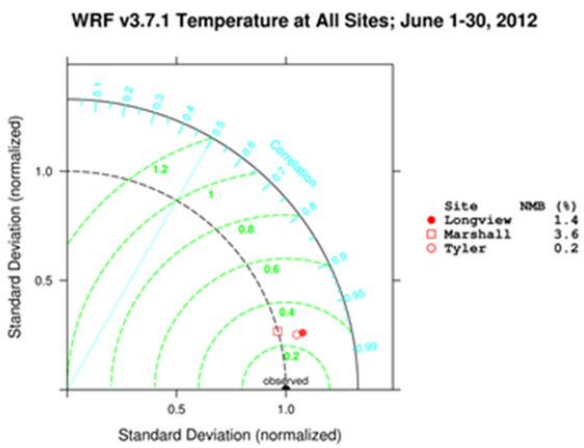

Figure 6-3. Example of statistical evaluation comparing multiple WRF simulations. June 2012 Taylor diagrams for the W0 (filled circle), W4 (square) and W5 (open circle) WRF simulations for near-surface wind speed at the KGGG (left), KTYR (middle) and KASL (right). Figure from Johnson et al. (2015).

WRF daily precipitation totals can be evaluated by comparing them with daily PRISM (Parameter-elevation Relationships on Independent Slopes Model[9]) precipitation analysis fields. The PRISM analysis fields are based on precipitation observations from U.S. monitoring sites and cover the continental United States and do not extend into Canada or over the ocean. The WRF precipitation fields, on the other hand, cover the entire domain, but we will show WRF precipitation over land only for model performance evaluation. Because precipitation monitoring sites tend to be located at lower elevations (e.g., airports), the PRISM observation fields may not fully capture the enhanced precipitation at high elevations due to orographic effects that could be present in the WRF simulations. Therefore, PRISM includes an elevation effect to account for orographic effects that increase precipitation over high terrain. While there is no high terrain in Northeast Texas, accounting for the effects of mountains is important in evaluating precipitation patterns within the 36 km continental-scale modeling domain (Figure 5-1). An example of a WRF precipitation evaluation on the 4 km modeling grid from Johnson et al. (2015) is shown in Figure 6-4.

[9] ftp://rattus.nacse.org/pub/prism/docs/appclim97-prismapproach-daly.pdf

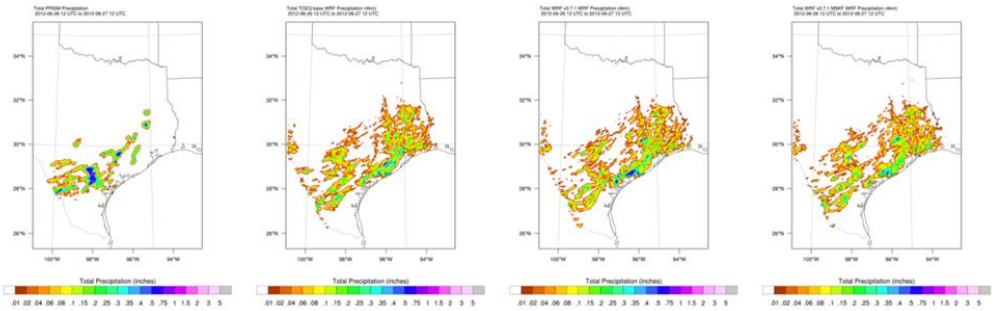

Figure 6-4. Example of precipitation evaluation. June 26, 2012 precipitation comparison. From left to right: PRISM daily precipitation total and WRF daily precipitation totals for the W0, W4 and W5 simulations.

To evaluate the WRF model's simulation of observed cloudiness, WRF downward shortwave radiation (DSW) at the surface can be compared with visible light images from the geostationary satellite GOES 13 (GOES 13 4 km Ch1 VIS). The colors in the WRF DSW plots are scaled so that areas where skies are clear (high DSW values) are dark and areas where clouds are present (low DSW) are gray. This convention is chosen so that cloudy areas show up as gray in both the satellite and the WRF panels. Afternoon hours for the comparison are most relevant because they to coincide with the hours of most frequent high ozone values at the Northeast Texas monitors. An example of comparison of observed and modeled cloud fields is shown in Figure 6-5.

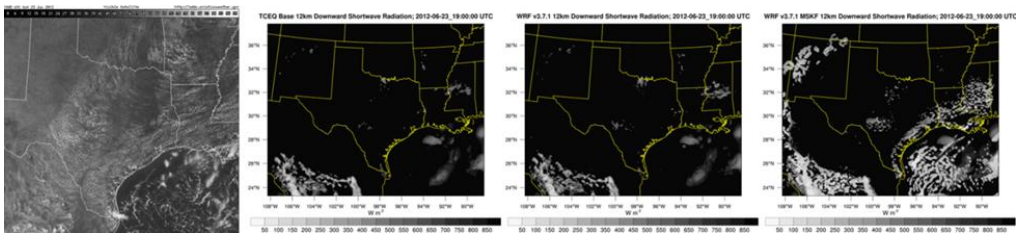

Figure 6-5. GOES visible satellite image (left panel) and WRF 12 km grid DSW for the W0, W4 and W5 (right panels) simulations for June 23, 2012, 19 UTC.

Each new WRF run will be compared to observations and previous model runs for the episode (i.e. the initial TCEQ run and the runs performed by Ramboll Environ as documented in Johnson et al., 2015). The best-performing run will be used in subsequent CAMx air quality modeling. Depending on the outcome of the model performance evaluation, the NETAC may elect to refine WRF model options or input data and perform additional runs in order to improve model performance over Northeast Texas. Results from the local and regional evaluations may suggest any necessary modifications needed in the WRF configuration.

Comment [HJ9]: Do we have any additional language to state how this procedure will be implemented?

7.0 CAMX AIR QUALITY MODELING

In this section, we describe air quality model configuration and inputs for the Northeast Texas ozone modeling study.

7.1 Version of CAMx

The current publicly available version of CAMx is Version 6.20. This is the version of the model that will be used for the Northeast Texas ozone modeling of the June 2012 episode. If a new version of CAMx is released during the Northeast Texas Ozone Modeling Study, we will consider using it if there is reason to believe that use of the updated model version may improve model performance in Northeast Texas or regions that may influence Northeast Texas.

7.2 Emissions

CAMx requires two types of emission input files:

1. Surface emissions from area, mobile, non-road, low-level point and biogenic sources are gridded to the CAMx nested model grids. This means that separate surface emissions files must be prepared for the 36 km, 12 km and 4 km grids. The surface emissions are injected into the lowest layer of the model.

2. Elevated emissions from major point sources are injected into CAMx at the coordinates of each source. The plume rise for each source is calculated by CAMx from stack parameters and local meteorology so that the emissions are injected into the appropriate vertical layer. Emissions from major NOx emitters selected by the TCEQ are treated with the CAMx Plume-in-Grid module, GREASD PiG (Greatly Reduced Execution and Simplified Dynamics Plume-in-Grid).

The emission files for the June 2012 episode were prepared by the TCEQ on the RPO LCP projection using the EPS3 system. The emissions model performs several tasks:

Temporal adjustments: Adjust emission rates for seasonal, day-of-week and hour-of-day effects.

Chemical speciation: Emission estimates for total VOC must be converted to the more detailed chemical speciation used by the CB6r2 Carbon Bond chemical mechanism in CAMx. Total unspeciated NOx emissions must be allocated to NO and NO_2 components.

Gridding: The spatial resolution of the emissions must be matched to the CAMx grid(s). Area sources are often estimated at the county level, and are allocated to the grid cells within each county based on spatial surrogates (e.g., population and economic activity). Mobile source emissions may be link specific (from transportation models), so links must be allocated to grid cells.

Growth and Controls: Emissions estimated for one year may need to be adjusted for use in a different year. In this database, for example, portions of TCEQ's 2011 NEI emissions database were adapted by the TCEQ for the 2012 modeling year.

Quality Assurance: The emissions model must have QA and reporting features to keep track of the adjustments at each processing stage and ensure that data integrity is not compromised.

The outputs from the emissions model are called the "model-ready" emissions, and they are day-specific, gridded, speciated and temporally (hourly) allocated. EPS3 performs all of the processing steps for the anthropogenic emissions. The biogenic emissions are prepared using a different model (MEGAN) because they are based on different input data and have specialized processing requirements (e.g., dependence on temperature, solar radiation and drought conditions).

7.2.1 Quality Assurance

Thorough quality assurance of the emissions processing is essential for this study to provide meaningful results. The TCEQ has performed quality assurance and evaluation of all emissions inputs for the 2012 modeling. This effort will be described in forthcoming documentation of TCEQ's 2012 modeling.

7.3 Meteorology

CAMx requires meteorological input data for the parameters described in Table 6-1. For the 2012 modeling, all of these input data will be derived from the results of WRF meteorological modeling for the 2012 episode as described in Section 6. WRF output fields are translated to CAMx-ready inputs using Ramboll Environ's WRFCAMx translation software (available at www.camx.com). This program performs several functions:

1. Extracts data from WRF grids and adjusts as appropriate to the corresponding CAMx grid.

2. Performs mass-weighted vertical aggregation of data for CAMx layers that span multiple WRF layers.

3. Diagnoses key variables that are not directly output by WRF (e.g., vertical diffusion coefficients and cloud information).

The WRFCAMx program has been written to preserve the consistency of the predicted wind, temperature and pressure fields output by WRF. This is the key to preparing mass-consistent inputs for CAMx, and therefore for obtaining high quality performance from CAMx.

The WRFCAMx data are directly input to CAMx with the exception of the vertical diffusivity coefficients (K_v). Vertical diffusivities determine the rate and depth of mixing in the PBL and above. In general, diffusivities from meteorological models require careful examination before they are used in air quality modeling. This may be because the photochemical model results

are much more sensitive to diffusivities than the meteorological model results. Typical adjustments depend upon landuse (e.g., urban, forest, agricultural, water, etc.) to represent different impacts of mechanical mixing and surface heat input (e.g., urban heat island effect).

In preparing the inputs for the June 2012 modeling, the TCEQ used the WRFCAMx v4.2 preprocessor to convert raw WRF output files into model-ready input files formatted for CAMx. WRFCAMx was used to calculate the Kv, which were derived from meteorological data supplied to CAMx by the WRF meteorological model. The CMAQ Kv method was used. The CAMx pre-processor KVPATCH was then used to adjust Kv to improve turbulent coupling between the surface and lower boundary layer. The Kv 100 patch was applied to Kv calculated within WRFCAMx. In the Kv 100 patch the minimum Kv for all layers within the lowest 100 m (defined to be the stable boundary layer) is set to the maximum Kv value found within the lowest 100 m. Ramboll Environ will evaluate the need for different/additional adjustments to the Kv to improve model performance in simulating ozone and precursors at Northeast Texas monitors.

7.4 Other Input Data

7.4.1 Initial and Boundary Conditions

The initial conditions (ICs) are the pollutant concentrations specified throughout the modeling domain at the start of the simulation. Boundary conditions (BCs) are the pollutant concentrations specified at the perimeter of the 36 km modeling domain. The TCEQ has supplied initial and boundary condition files for the June 2012 episode. The boundary conditions were prepared by application of the GEOS-Chem global chemistry-transport model (Bey et al., 2001; Yantosca et al., 2014). In FY14-15, Ramboll Environ determined that ozone overestimates in the boundary conditions are unlikely to be the cause of the CAMx model's overall high bias for ozone in Northeast Texas in June 2012 (Johnson et al., 2015).

7.4.2 Surface Characteristics (Land Use)

CAMx requires gridded land use data to characterize surface boundary conditions, such as surface roughness, deposition parameters, vegetative distribution, and water/land boundaries. CAMx land use files provide the fractional contribution (range 0 to 1) of land use categories. TCEQ has supplied the land use files used on each model grid for the June 2012 episode.

7.4.3 Chemistry Data

The CAMx chemistry parameters file determines which photochemical mechanism is used to model ozone formation. The modeling will use the Carbon Bond mechanism (CB6r2; Yarwood et al., 2012). The CAMx chemistry parameters file specifies the rates for all of the thermochemical reactions in the C6r2 chemical mechanism. The CB6r2 mechanism also includes photolysis reactions that depend upon the presence of sunlight. The photolysis rates input file determines the rates for photolysis reactions in the mechanism. Photolysis rates for the June 2012 episode were developed by the TCEQ using the Tropospheric visible Ultra-Violet (TUV) model developed by the National Center for Atmospheric Research (NCAR, 2011). TUV is a state-of-the-science solar radiation model that is designed for photolysis rate calculations.

TUV accounts for environmental parameters that influence photolysis rates including solar zenith angle, altitude above the ground, surface UV albedo, aerosols (haze), and stratospheric ozone column. The TCEQ used episode-specific satellite ozone column data from the Total Ozone Mapping Spectrometer (TOMS) as an input for the calculation of the photolysis rates.

7.5 CAMx Model Options

CAMx has several user-selectable options that are specified for each simulation. Most of these options follow naturally from other choices about model inputs. There are three main optional inputs that must be decided: the advection scheme, the plume-in-grid scheme, and the chemistry solver.

Advection scheme: CAMx has two optional methods for calculating horizontal advection (the movement of pollutants due to horizontal winds) called the Bott method and the Piecewise Parabolic Method (PPM). The Piecewise Parabolic Method was used by the TCEQ in the initial June 2012 modeling and will be used for the remainder of this study since it has provided reasonable results in previous Texas modeling work.

Plume-in-Grid: CAMx includes an optional sub-grid scale plume model that can be used to represent the dispersion and chemistry of major NOx point source plumes close to the source. In the June 2012 modeling, the GREASD Plume-in-Grid (PIG) sub-model was used by the TCEQ for selected major NOx sources.

Chemistry Solver: CAMx has three options for the numerical solution scheme for the gas phase chemistry. They are the Euler Backwards Iterative (EBI) solver, the Implicit-Explicit Hybrid (IEH), and the Livermore Solver for Ordinary Differential Equations (LSODE). The fully explicit Gear-type LSODE solver is highly accurate and can be used to "benchmark" a simulation to evaluate the performance of EBI or IEH, but is too slow for use in this application. The IEH solver is comparable to reference methods such as LSODE but is several times slower than EBI. The EBI chemistry solver was used by the TCEQ in the initial June 2012 modeling and will be used in this application because it offers the best combination of speed and accuracy.

7.6 The Archiving and Documentation of Modeling and Other Analyses

All components of the modeling system (emission and meteorology, air quality modeling outputs, supplemental analyses, etc.) will be backed up on external hard drives and made available to ETCOG, NETAC, TCEQ, EPA and other interested parties upon request. All aspects of the modeling will be documented as described in Section 1.

8.0 2012 BASE CASE OZONE MODEL PERFORMANCE EVALUATION

All CAMx runs made during the Northeast Texas ozone modeling will be evaluated against available air quality data. The purpose of the evaluation is to determine the model's reliability as an ozone prediction tool. The proposed evaluation plan follows the procedures recommended in the EPA guidance (EPA, 2014). The initial modeling of June 2012 model has been evaluated by the TCEQ as well as by NETAC. NETAC's evaluation focused on Northeast Texas and is documented in Johnson et al. (2015). New CAMx runs aimed at improving model performance over Northeast Texas will be made in FY16-17. If the TCEQ develops inputs for a 2012 ozone season episode model, Ramboll Environ will run CAMx for the 2012 ozone season. All new CAMx runs will be evaluated in accordance with EPA (2014) modeling guidance. The approach to CAMx model performance evaluation is outlined in this section.

8.1 Approach to Ozone Model Performance Evaluation

It is important to first establish a framework for assessing whether the 2012 photochemical modeling system performs with sufficient reliability to justify its use in developing ozone control strategies for Northeast Texas. The framework for assessing the model's reliability consists of the following principles, which are based on EPA's 8-hour modeling guidance:

- **The Model Should be Viewed as a System.** When we refer to evaluating a "model" we include not only the CAMx photochemical model but its various companion preprocessor models (e.g., meteorological and emissions models), the supporting aerometric and emissions database, and all other related analytical and numerical procedures used to produce modeling results.
- **Model Acceptance is a Continuing Process of Non-Rejection.** Over-reliance on explicit or implied model "acceptance" criteria should be avoided, including EPA's performance goals (EPA, 1991). Models should be accepted gradually as a consequence of successive non-rejections, and confidence builds as the model undergoes a number of different applications (hopefully involving stressful performance testing) without encountering major or fatal flaws that cause the model to be rejected.
- **Criteria for Judging Model Performance Must Remain Flexible.** This approach recognizes that the model can give the right answers for various combinations of wrong inputs. Statistical tests are a first step in the performance evaluation, but not in themselves final or definitive. The model output must also be compared to time series and geographical plots as well as precursor data when it is available. Performance may even be degraded as new information and procedures are inserted into the model, because new elements may illustrate the presence of compensating errors that were previously unknown.
- **Previous Experience is Used as a Guide for Judging Model Acceptability.** Interpretation of the CAMx modeling results for the episode, considered against the backdrop of the quality of the meteorological and emissions inputs and previous modeling experience (e.g. Simon et al., 2012) will aid in identifying potential performance problems and suggest whether the model should be modified, tested further, or rejected.

8.1.1 Model Performance Metrics

EPA recommends (EPA, 2014) that, at a minimum, the following statistical measures be calculated: mean observed value, mean modeled value, mean bias, mean error and/or root mean square error, normalized mean bias and/or fractional bias, normalized mean error and/or fractional error, and the correlation coefficient. These metrics will be used in evaluating all CAMx modeling performed in FY16-17. The statistical metrics to be computed for surface monitoring locations are defined in Table 8-1~~Table 8-1~~.

Table 8-1. Definition of statistical metrics to be used in model performance evaluation.

Statistical Measure	Mathematical Expression	Notes
Coefficient of determination (r2)	$\frac{\left[\sum_{i=1}^{N}(P_i-\overline{P})(O_i-\overline{O})\right]^2}{\sum_{i=1}^{N}(P_i-\overline{P})^2\sum_{i=1}^{N}(O_i-\overline{O})^2}$	Pi = prediction at time and location i; Oi = observation at time and location i; $\overline{P}$ = arithmetic average of Pi, i=1,2,…, N; $\overline{O}$ = arithmetic average of Oi, i=1,2,…,N
Normalized Mean Error (NME)	$\frac{\sum_{i=1}^{N}\lvert P_i-O_i\rvert}{\sum_{i=1}^{N}O_i}$	Reported as %
Root Mean Square Error (RMSE)	$\left[\frac{1}{N}\sum_{i=1}^{N}(P_i-O_i)^2\right]^{1/2}$	Reported as %
Mean Error (ME)	$\frac{1}{N}\sum_{i=1}^{N}\lvert P_i-O_i\rvert$	Reported as concentration (e.g., ppb)
Mean Bias (MB)	$\frac{1}{N}\sum_{i=1}^{N}(P_i-O_i)$	Reported as concentration (e.g., ppb)
Normalized Mean Bias (NMB)	$\frac{\sum_{i=1}^{N}(P_i-O_i)}{\sum_{i=1}^{N}O_i}$	Reported as %

The NMB shows whether a modeled quantity such as ozone is under- or overpredicted on average compared to observations. The NME is similar to NMB, but calculates the absolute value of the difference between the observed and modeled values. It is useful to compare the magnitudes of the NMB and NME statistics together to determine the nature of the biases. For example, if the NMB equals +10% and the NME equals 10%, then the model error is completely explained by positive biases. RMSE is a general purpose statistical metric used to measure model performance in meteorological and air quality studies. Because the difference between the observed and modeled values is squared, occasional large errors are penalized more than

with other metrics. A threshold of 60 ppb will be applied for calculation of ozone statistical metrics, so that the metrics are calculated using only data pairs where the observed value exceeds 60 ppb. This methodology focuses the model performance evaluation on high ozone periods which are more important for attainment demonstration modeling and is consistent with EPA Guidance (EPA, 2014). Consistent with EPA recommendation, the grid cell value in which the monitor resides will be used for statistical comparisons between observed and modeled ozone.

Comment [HJ10]: This approach seems to avoid the known model issue of not titrating ozone from NOX emissions in the evening hours. The monitored ozone values go to near zero while the model is still showing 40-50 ppb (see Figure 8-1).

Or, is this due to the winds being incorrect during the evening hours and the plume not being misplaced?

8.1.2 Graphical and Statistical Evaluation Methods

The evaluation of performance for new CAMx runs for the June 2012 modeling episode will be carried out in two sequential phases, beginning with the simplest comparisons of modeled and observed ground-level 1-hour and 8-hour ozone concentrations, and progressing to potentially more detailed analyses if necessary (e.g., examination of precursor and product species, comparisons of pollutant ratios and groupings). The proposed evaluation methods are listed below and example figures from previous Northeast Texas modeling of 2012 are provided:

- Inspection of computer generated graphics, images and animations.
  - Time series plots of predicted and observed ozone and available precursors (Figure 8-1)
  - Statistical metrics for ozone (Figure 8-1)
  - Scatter plots of predicted and observed ozone (Figure 8-2)
  - Hourly tile plots of predicted ozone and precursors across the modeling domain (Figure 8-4, Figure 8-5, and Figure 8-6)
  - Animations of predicted ozone and precursor concentrations for periods of interest (not shown)
- Comparison of observed and predicted precursor emissions or species concentrations (Figure 8-3).
- Comparison of model performance among different runs using statistical metrics displayed in Taylor Diagrams (Figure 6-3).

Comment [HJ11]: These plots are for ozone, NOX, and SO2, to identify a connection between emissions sources and ozone formation. But, each figure is for different date/time and does not show any direct correlation.

I suggest using the same date/time for each plot to prevent any misinterpretation of the data.

The following principles will govern the model performance improvement process:

- Any significant changes to the model or its inputs must be documented;
- Any significant changes to the model or its inputs must be supported by scientific evidence, analysis of new data, or by re-analysis of the existing data where errors or misjudgements may have occurred.

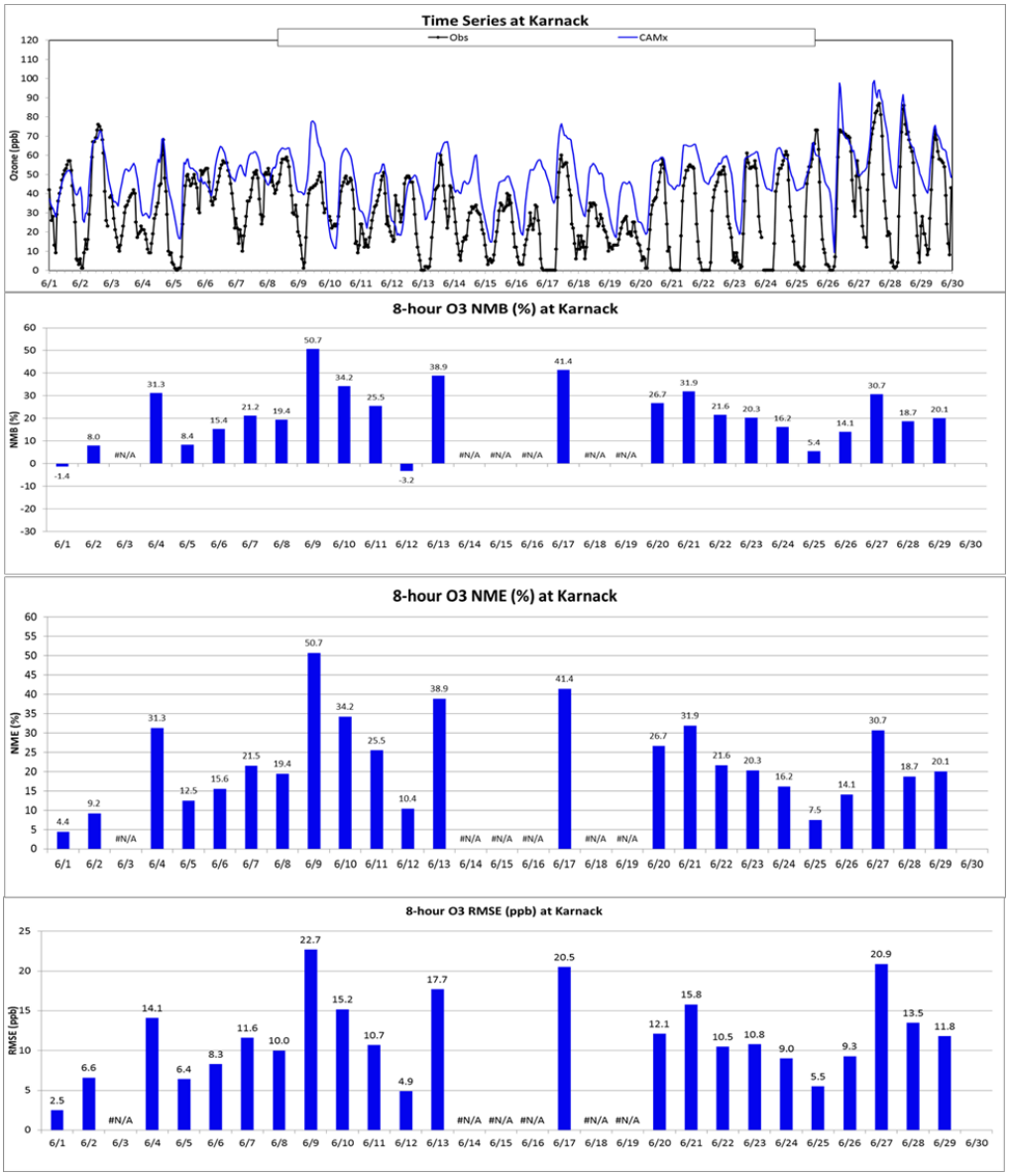

Figure 8-1. Top panel: observed 1-hour ozone (black) at the Karnack CAMS 85 monitor versus modeled 1-hour average surface layer ozone during the June 1-29, 2012 period. Lower three panels: normalized mean bias (NMB), normalized mean error (NME) and root mean squared error (RMSE) for 8-hour ozone at the Karnack CAMS 85 monitor.

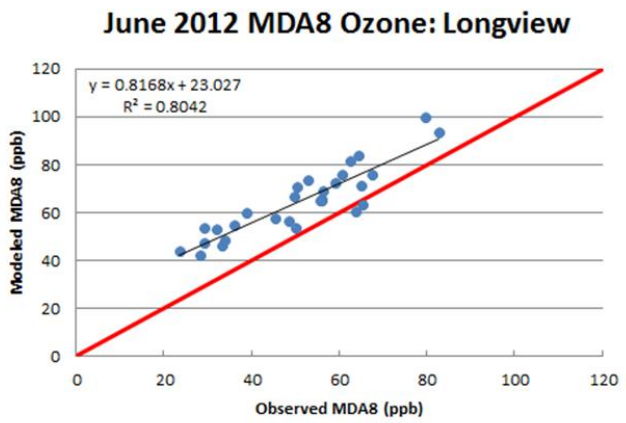

Figure 8-2. Scatter plot comparison of predicted and observed daily maximum 8-hour ozone concentrations during June 2012 at the Longview CAMS 19 monitor.

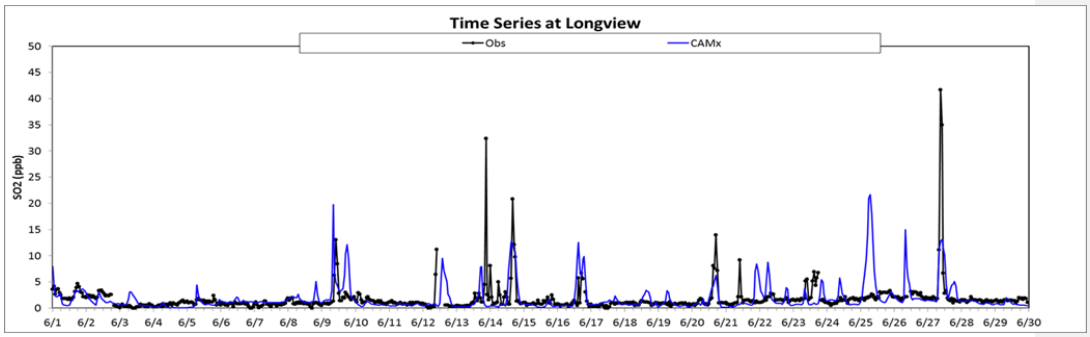

Figure 8-3. Observed 1-hour SO_2 (black) at the Longview CAMS 19 monitor versus modeled 1-hour average surface layer SO_2 during the June 1-29, 2012 period.

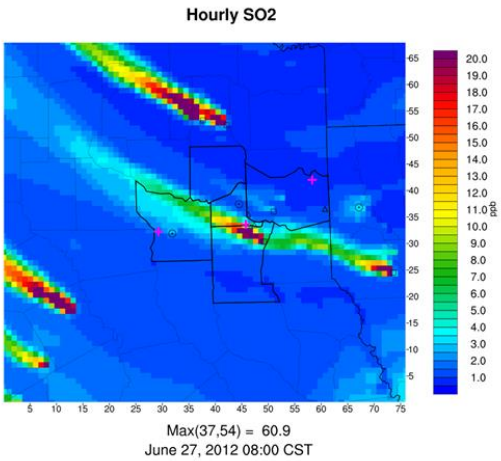

Figure 8-4. CAMx SO_2 concentrations for June 27, 2012 at 08:00 CST. Northeast Texas CAMS monitors are shown as cross symbols, coal-fired power plants (HW Pirkey, Martin Lake, Dolet Hills, Monticello and Welsh) are shown as squares, other selected point sources (Knox Lee, Eastman Cogeneration Facility, Waskom Gas Plant and Stateline Generation Station) are shown as triangles, and selected city centers (Tyler, Longview and Shreveport) are shown as bull's-eye symbols..

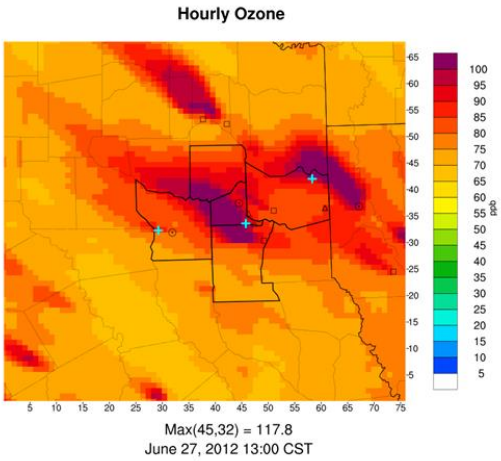

Figure 8-5. CAMx ozone concentrations for June 27, 2012 at 13:00 CST. Symbols are described in Figure 8-4.

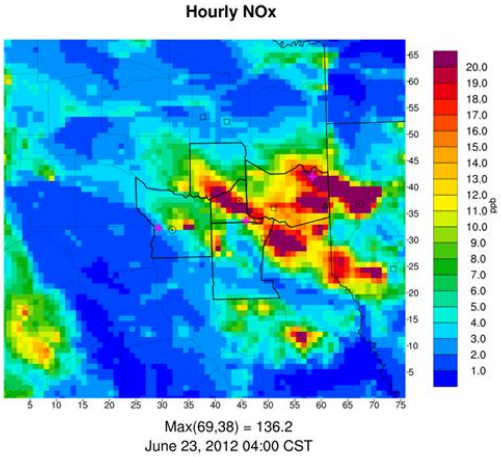

Figure 8-6. CAMx NOx concentrations for June 23, 2012 at 4:00 CST. Symbols are described in Figure 8-4.

8.2 Monitors to be Used in Model Performance Evaluation

CAMx model performance will be evaluated throughout the 36/12/4 km modeling domains. Figure 8-7 shows TCEQ CAMS within the 4 km CAMx grid. All sites within the 4 km grid that have data available for the 2012 episode will be used in the evaluation. We will focus the detailed model performance evaluation on the three Northeast Texas monitors.

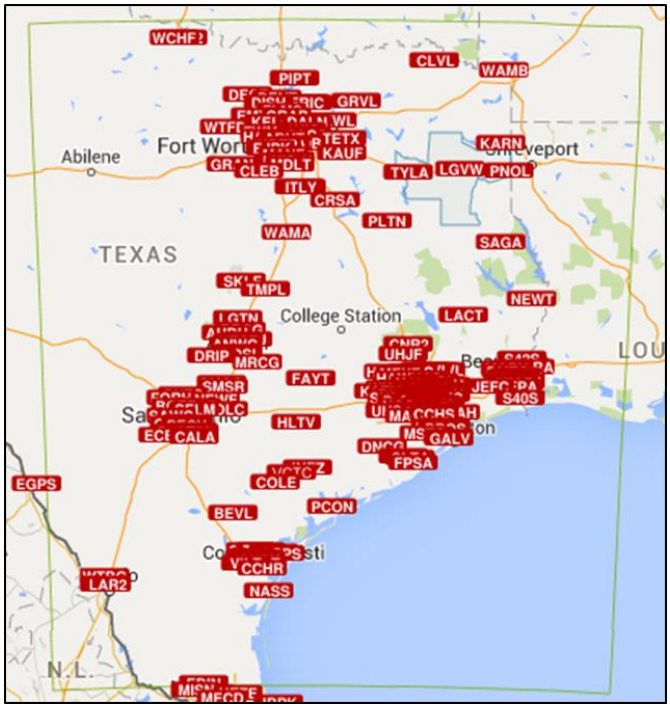

Figure 8-7. TCEQ CAMS on 4 km grid, which is outlined in light green. Note that not all monitors shown have data available for June 2012. Blue outline shows the 5-county TLM area of Northeast Texas. TCEQ figure[10].

We will evaluate the model's simulation of ozone transport into Northeast Texas by assessing model performance in areas upwind of Northeast Texas prior to high ozone episodes. Rural/suburban sites will be used to evaluate performance on the 36 km grid, which cannot be expected to accurately simulate variations in ozone within urban areas. We will evaluate CAMx against ground level observations from Clean Air Status and Trends Network (CASTNET) sites within the 36 km grid (Figure 8-8) and rural/suburban sites in the EPA AQS network (not shown).

[10] https://www.tceq.texas.gov/airquality/airmod/data/site

Figure 8-8. CASTNet Sites. EPA figure.[11]

8.3 Diagnostic and Sensitivity Simulations

8.3.1 Objectives

A limited number of diagnostic simulations will be performed to help understand and possibly improve base case model performance. In addition, sensitivity tests can be performed to diagnose model sensitivity to changes in key inputs. These tests are an important component of the base case model evaluation process. In general, diagnostic and sensitivity analyses serve to:

- reveal model responses that are inconsistent with expectations or other model responses,
- identify what parameters (or inputs) dominate (or do not dominate) model results,
- examine the relationship between uncertainties in model inputs and model outputs (error propagation through the model), and
- provide guidance for model refinement and data collection programs.

8.3.2 Potential Sensitivity Tests

Sensitivity experiments will be considered as part of the performance evaluation analysis as appropriate. The potential need for and nature of these simulations will be discussed with NETAC and TCEQ staff in periodic telephone conferences and briefed to the NETAC Technical and Policy Committees as required.

[11] http://epa.gov/castnet/javaweb/docs/CASTNET_Factsheet_2013.pdf

Potential diagnostic evaluation runs include changes to:

- boundary conditions, sensitivity of local background concentrations to more or less polluted boundary conditions,
- biogenic emissions, to evaluate sensitivity to uncertainties in biogenic emissions due to model algorithms and/or input data,
- dry deposition algorithms, and
- meteorology, specific diagnostic tests identified during the preparation of the meteorological modeling such as: alternate vertical diffusion coefficients to adjust daytime and night time mixing heights toward observed data; impacts of clouds on photolysis rates; and impacts of nudging to observations and analyses.

Potential sensitivity runs include:

- sensitivity to reductions/increases in total anthropogenic VOC and/or NOx emissions,
- sensitivity to reductions/increases in anthropogenic VOC and/or NOx emissions from specific source categories such as point, area, and mobile. An example of results from such a sensitivity run is shown in Figure 8-9.
- sensitivity to reductions/increases in anthropogenic VOC and/or NOx emissions from specific urban areas and source regions (e.g., distant or local).

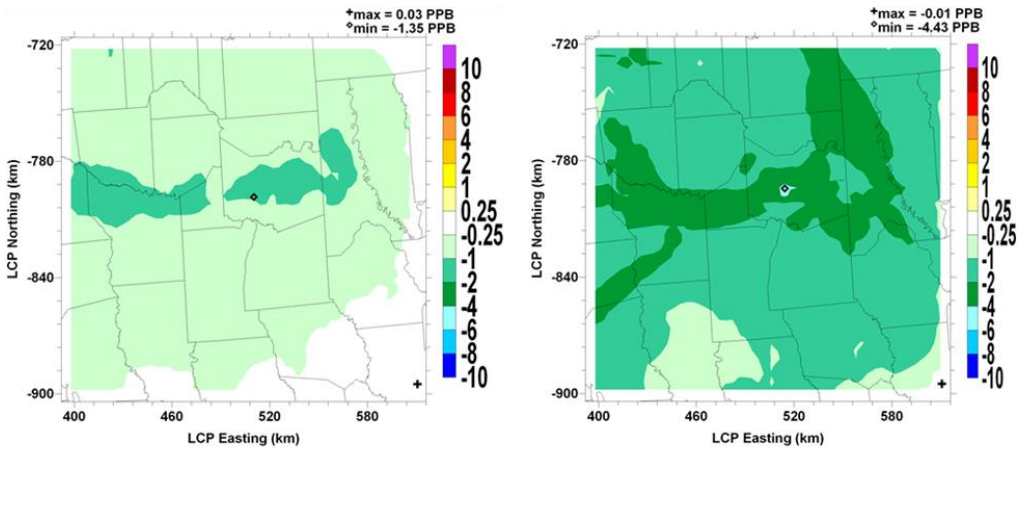

Figure 8-9. Change in 8-hour average surface layer ozone for 30% reduction in on-road mobile source NOx emissions. Left hand panel: Average change in 8-hour ozone. Right hand panel: Maximum change in 8-hour ozone. Differences calculated only for times when the surface layer ozone concentration was > 60 ppb.

9.0 SUPPLEMENTAL ANALYSES

9.1 Introduction

Once the June 2012 modeling episode has been evaluated and performance has been found to be satisfactory, the model will be used to investigate ozone formation in Northeast Texas as well as the transport of ozone and precursors into the area. The model will be used to carry out supplemental analyses. The goal of the supplemental analyses is to provide NETAC and the TCEQ with information regarding emissions control strategies that will reduce ozone levels in Northeast Texas and help the NNA continue to comply with the NAAQS for ozone.

9.2 CAMx APCA Source Apportionment Analysis

Ozone source apportionment can be used to determine which source regions and emissions categories contribute to ozone at a particular time and location. In this section, we describe the CAMx source apportionment capability and outline its potential application for the Northeast Texas ozone modeling.

9.2.1 Description of the CAMx APCA Source Apportionment Tool

The CAMx Anthropogenic Precursor Culpability Assessment (APCA) tool uses multiple tracer species to track the fate of ozone precursor emissions (VOC and NOx) and the ozone formation caused by these emissions within a simulation. The tracers operate as spectators to the normal CAMx calculations so that the underlying CAMx-predicted relationships between emission groups (sources) and ozone concentrations at specific locations (receptors) are not perturbed. Tracers of this type are conventionally referred to as “passive tracers,” however it is important to realize that the tracers in the APCA tool track the effects of chemical reaction, transport, diffusion, emissions and deposition within CAMx. In recognition of this, they are described as “ozone reaction tracers.” The ozone reaction tracers allow ozone formation from multiple “source groupings” to be tracked simultaneously within a single simulation. A source grouping can be defined in terms of geographical area and/or emission category. So that all sources of ozone precursors are accounted for, the CAMx boundary conditions and initial conditions are always tracked as separate source groupings. This will allow an assessment of the role of transported ozone and precursors in contributing to high ozone episodes within Northeast Texas.

The methodology is designed so that all ozone and precursor concentrations are attributed among the selected source groupings at all times. Thus, for all receptor locations and times, the ozone (or ozone precursor concentrations) predicted by CAMx is attributed among the source groupings. The methodology also estimates the fractions of ozone arriving at the receptor that were formed en-route under VOC- or NOx-limited conditions. This information suggests whether ozone concentrations at the receptor may be responsive to reductions in VOC and NOx precursor emissions and can guide the development of additional sensitivity analyses.

APCA differs from the standard CAMx Ozone Source Apportionment Tool (OSAT) in recognizing that certain emission groups are not controllable (e.g., biogenic emissions) and that

apportioning ozone production to these groups does not provide information that is relevant to development of control strategies. To address this, in situations where OSAT would attribute ozone production to non-controllable (i.e., biogenic) emissions, APCA re-allocates that ozone production to the controllable portion of precursors that participated in ozone formation with the non-controllable precursor. For example, when ozone formation is due to biogenic VOC and anthropogenic NOx under VOC-limited conditions (a situation in which OSAT would attribute ozone production to biogenic VOC), APCA re-directs that attribution to the anthropogenic NOx precursors present. The use of APCA instead of OSAT results in more ozone formation attributed to anthropogenic NOx sources and less ozone formation attributed to biogenic VOC sources, but generally does not change the partitioning of ozone attributed to local sources and the transported background for a given receptor.

9.2.2 Application of the APCA Tool in Northeast Texas Ozone Modeling Study

APCA will be used to determine source regions and emissions source categories that contribute to high modeled ozone at Northeast Texas ozone monitors during the June 2012 simulation. (This type of analysis was carried out for the May-June 2005 and June 2006 episodes.) The Northeast Texas ozone modeling will use an updated version of the APCA tool (Yarwood and Koo, 2015). The updated APCA scheme replaces the existing APCA NOx tracer family with a more comprehensive set of reactive nitrogen tracer families and adds two more tracer families to track odd-oxygen in NO_2 formed from ozone, resulting in a total of 10 tracer families. This update produces an additional improvement in the accuracy of the APCA scheme by keeping track of NOx recycling where NOx is converted to a different form of oxidized nitrogen, such as HNO_3, and later converted back to NOx. Another important change to the APCA scheme is the attribution of transported ozone. When ozone is transported into NOx-rich areas, such as portions of Northeast Texas with substantial NOx emissions, it can be converted to NO_2 by reaction with locally emitted NO and later returned as ozone. The new APCA scheme can correctly attribute this returned ozone to the more distant source region (where the ozone was originally formed), whereas the old scheme would most likely attribute the returned ozone to a local source (Yarwood and Koo, 2015).

Comment [HJ12]: Consider some additional explanation on this new tool which could have new implications on NOX sources.

The APCA tool can be used to address the following questions:

- Is high ozone at a monitor on a particular day due to local sources or transport or both?
- What are the relative contributions of different regions and emissions source types to high ozone at a given monitor on a given day?

An example of APCA source apportionment results from previous CAMx modeling of June 2006 is shown in Figure 9-1. The green bar shows the contribution to the Longview CAMS 19 MDA8 from emissions sources within the 5-county area of Northeast Texas. This is the ozone contribution from local sources that can be reduced through local emission controls. The contribution from emissions sources within Texas but outside the 5-county area is shown in gray. The contribution from regions outside Texas but within the 36 km modeling domain shown in Figure 9-1 are shown in light blue. The contribution of the boundary conditions is

shown in dark blue. The boundary conditions represent the contributions from emissions sources outside the U.S. and the contribution from the stratosphere.

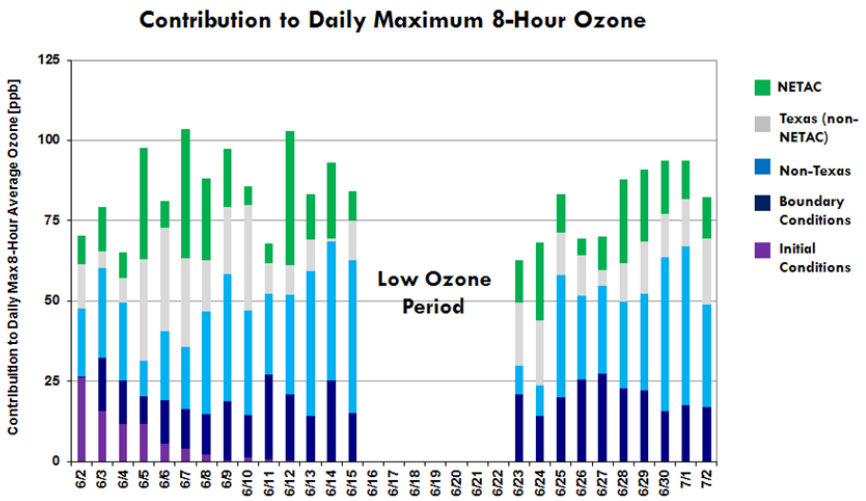

Figure 9-1. Example of CAMx APCA results for the June 2006 episode.

A tool that generates HYSPLIT back trajectories based on the horizontal wind fields input to CAMx and the CAMx vertical velocity algorithm can be used to assess the accuracy of the model winds during the ozone episode (e.g., Figure 3-11 and Figure 3-12). Together with the APCA results, this tool can help to develop a more detailed picture of modeled transport on a given day. By comparing HYSPLIT back trajectories made using North American Model (NAM) 12 km resolution observational meteorological analysis inputs to otherwise identical HYSPLIT back trajectories made with CAMx meteorological inputs, potential problems with ozone transport due to errors in modeled winds may be diagnosed. Using multiple analysis tools in this manner allows evaluation of the reliability of the model results.

Comment [HJ13]: The NAM 12km data is the input to WRF, which is the input to CAMx. Therefore, the refinements made in the 4 km wind field are not necessarily "errors", but may be better resolution. Should we consider comparing the winds at NWS stations which are "real" instead of comparing WRF winds to "estimated" winds by the NAM model? If the NAM is wrong, the WRF will also be equally incorrect.

9.3 CAMx HDDM Sensitivity Analysis

9.3.1 Description of the HDDM Tool

The CAMx APCA and Higher Order Decoupled Direct Method (HDDM; Dunker et al., 2002) analysis tools will provide complementary information for the Northeast Texas ozone modeling. APCA is used to quantify contributions by source region and emissions source category to ozone at a given receptor and time. However, APCA does not give information about how such a contribution may change if source region emissions change. HDDM can be used to derive estimates of model response to changes in emissions. For example, the HDDM probing tool can

calculate sensitivity coefficients that indicate how ozone at a given location would change in response to a change in emissions in a particular source region.

The CAMx implementation of HDDM calculates both first and second order sensitivity coefficients of all gas concentrations to changes in emissions, initial conditions and boundary conditions. In the Northeast Texas analysis, if the effect of an emissions change on ozone at the Temple monitor were to be investigated, the first and second order sensitivity coefficients, $S^{(1)}$ and $S^{(2)}$, would have the form:

$$S^{(1)} = \frac{\partial O_3}{\partial(\text{emissions})}, \qquad S^{(2)} = \frac{\partial^2 O_3}{\partial(\text{emissions})^2}.$$

Through calculation of such HDDM sensitivity coefficients, it is possible to determine whether VOC and/or NOx reduction strategies in a given source region are a more effective method to reduce ozone. The CAMx HDDM tool permits the evaluation of sensitivity coefficients with respect to parameters related to emissions, boundary conditions, initial conditions, or rate constants.

Figure 9-2 shows an example of the use of HDDM in a simulation of the June 2006 episode. The left panel of the figure shows the change in MDA8 ozone at several rural Texas receptors that would result from reducing point source NOx emissions in the Ohio and Tennessee Valley regions. The HDDM results indicate that all of the Texas rural monitors would see a reduction in MDA8 ozone during this episode if elevated point source NOx emissions were decreased in the source region.

The right hand panel for Figure 9-2 shows the sensitivity (i.e. the first order sensitivity coefficient $S^{(1)}$) of domain-wide 8-hour ozone to changes in elevated point source NOx emissions in the Ohio and Tennessee Valley regions. A positive value means that ozone increases if elevated point source NOx emissions in the source region increases. The sensitivity of ozone to the NOx emissions is largest in the source region. The results indicate that ozone in East Texas is sensitive to changes in NOx emissions in the Ohio and Tennessee Valley source regions and that ozone levels would be reduced if these emissions were controlled.

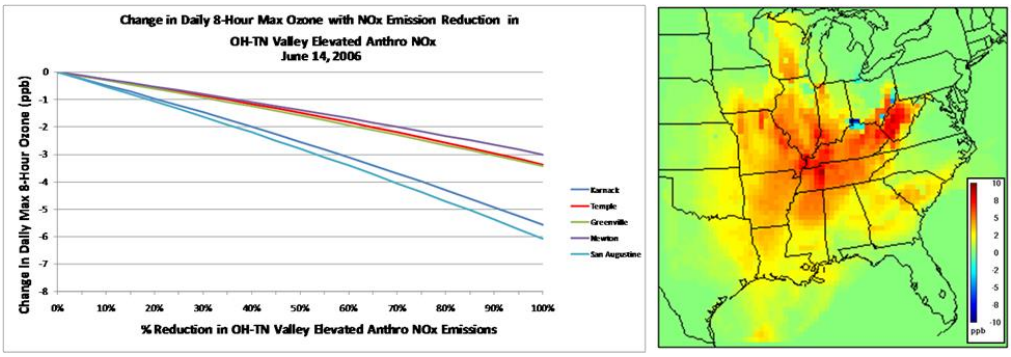

Figure 9-2. Left panel: Change in daily max 8-hour ozone at rural Texas monitors with NOx emissions reductions from point sources in the Ohio and Tennessee Valleys. Right panel: June 13-15, 2006 average model ozone sensitivity to point source NOx emissions in the Ohio and Tennessee Valleys. Positive (negative) values indicate ozone increases (decreases) if NOx emissions increase (decrease).

9.3.2 Application of the HDDM Tool in the Northeast Texas Ozone Modeling Study

In the Northeast Texas CAMx ozone modeling study, HDDM can be used to answer the following question:

If certain sources are controlled, how is ozone at local monitors affected?

HDDM can be used to investigate model sensitivity to broad changes in precursor emissions as well as to evaluate potential local voluntary or mandatory control strategies.

NETAC will analyze and model control strategies that meet the following criteria:

1. The geographic applicability is limited to the 5-county NETAC area; and
2. The control strategy is either voluntary or can be implemented under a political subdivision's existing legal authority.

9.4 Future Analyses

The development and use of a 2012 CAMx modeling episode has been outlined in this Protocol. If Northeast Texas is required by EPA to demonstrate attainment of the NAAQS to be promulgated in 2015, a demonstration that the selected ozone control plan will attain the 8-hour ozone standard by a future year will also be performed. The future year would be determined as part of EPA's designation process. If such a modeling effort is required, this Protocol will be updated to include a description of the methods to be used in carrying out the modeled attainment demonstration and supporting analyses.

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