# Final Modeling Protocol

# Ozone Modeling of 2012 for the Killeen-Temple-Fort Hood Area

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## CONTENTS

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## TABLES

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## FIGURES

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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 |
| CTCOG | Central Texas Council of Governments |
| DSW | Downward Shortwave radiation |
| EBI | Euler Backward Iterative solver |
| ECMWF | European Centre for Medium-Range Weather Forecasts |
| EGU | Electric Generating Unit |
| EPA | Environmental Protection Agency |
| FDDA | Four Dimensional Data Assimilation |
| GEOS | Goddard Earth Observing System |
| GOES | Geostationary Operational Environmental Satellite |
| HGB | Houston-Galveston-Brazoria Area |
| $HNO_3$ | Nitric Acid |
| HOTCOG | Heart of Texas Council of Governments |
| HYSPLIT | HYbrid Single-Particle Lagrangian Integrated Trajectory |
| ICs | Initial Conditions |
| IEH | Implicit-Explicit Hybrid solver |
| KTF | Killeen-Temple-Fort Hood |
| 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 |
| 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 |
| SIP | State Implementation Plan (for the ozone NAAQS) |
| $SO_2$ | Sulfur dioxide |
| TCEQ | Texas Commission on Environmental Quality |
| 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 |

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# 1.0 INTRODUCTION

This Modeling Protocol describes the procedures that will be used in the development of a new ozone modeling database for the Killeen-Temple-Fort Hood (KTF) Area in Central Texas. The requirements for a Modeling Protocol are described in the following U.S. Environmental Protection Agency (EPA) Guidance 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. EPA (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 KTF Texas ozone modeling as well as the schedule, organizational structure and documentation. In Section 2, we discuss the conceptual model for ozone formation in the KTF Area. 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 which they will

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

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, including emissions. Section 8 presents air quality model evaluation procedures, and Section 9 outlines methods for supplemental analyses.

## 1.1   Background

### 1.1.1   KTF Area 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 KTF Area ozone monitoring data determine whether the area is in compliance with the NAAQS.  The KTF Near Non-Attainment Area (NNA) consists of San Saba, Coryell, Hamilton, Bell, Milam, Mills and Lampasas Counties. The TCEQ operates two Continuous Air Monitoring Station (CAMS) ozone monitors in the KTF Area that determine whether the Area is in compliance with the NAAQS: the Killeen Skylark monitor (CAMS 1047) and the Temple Georgia monitor (CAMS 1045), both located in Bell County.  The locations of the two active monitoring stations are shown in Figure 1-1. The Killeen CAMS 1047 monitor began operating on June 11, 2009, and the Temple Georgia CAMS 1045 monitor began data collection on October 4, 2013.
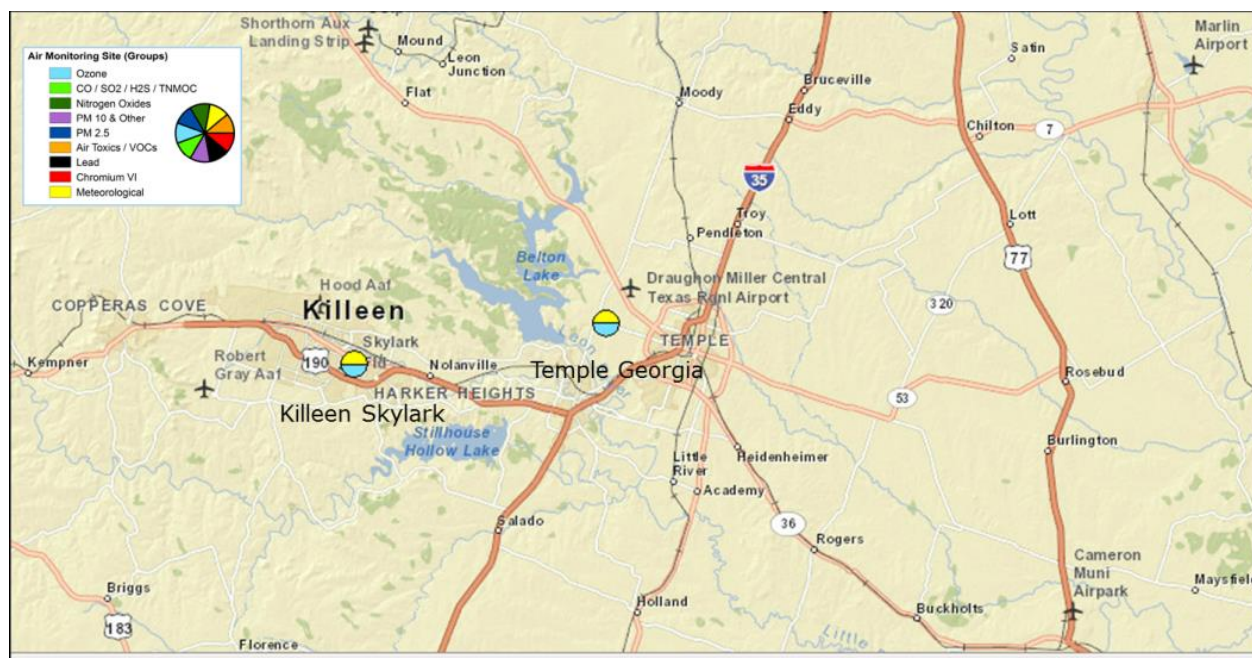


**Figure 1-1. Map showing the Killeen Skylark CAMS 1047 and Temple Georgia CAMS 1045 active monitoring sites and monitored quantities in the KTF Area of Central Texas[2].**

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[2] Map from TCEQ website at:  https://gisweb.tceq.texas.gov/geotam3/.

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Figure 1-2 shows the 7-county KTF Area and the surrounding region. Urban areas are shaded according to population estimates for the year 2010. Major roadways such as Interstate I-35 are shown in blue and highways are shown in light brown. The locations of active and inactive KTF Area ozone monitors are also presented in Figure 1-2.

The KTF Area is located generally north of Austin and south to southwest of the Dallas-Fort Worth-Arlington (DFW) Metropolitan Statistical Area. Killeen is approximately 60 miles north of Austin, 45 miles southwest of Waco and 130 miles south of the DFW area. Austin had an estimated 2010 population of 810,759[3] and the DFW area had an estimated 2010 population of 6,371,773[4] and was the fourth largest metropolitan area in the U.S.[5]. Ozone precursor emissions from both Austin and the DFW area have been shown to influence ozone concentrations at the Killeen-Skylark CAMS 1047 monitor within the KTF Area (Parker et al., 2013; Kemball-Cook et al., 2015). In addition, ozone precursor emissions from other less populous urban areas that are located closer to the Bell County monitors can also influence ozone in the KTF Area. In particular, Killeen, Waco and Temple were estimated by the 2010 Census to have populations of 127,911[6], 124,810[7], and 66,312[8], respectively. Ozone precursor emissions from a variety of different emissions sources (e.g. cars, trucks and industrial facilities) in these urban areas can contribute to ozone concentrations in the KTF Area. Figure 1-2 displays the Interstate highway I-35 intersecting Bell County. I-35 is a major roadway that extends across Texas from Mexico to Oklahoma and passes through Austin and San Antonio as well as Waco and the DFW area.

Three air quality monitors are shown in Figure 1-2. The Killeen-Skylark monitor (CAMS 1047) and Temple Georgia (CAMS 1045) are the only currently active ozone air quality monitors in the KTF Area, and data from these monitors are used to calculate the ozone design values for the KTF Area. The Temple monitor (CAMS 651) operated during 2005-2006 only; however, data from this monitor is useful because it provides information on ozone concentrations in Bell County prior to 2009 when the Killeen CAMS 1047 monitor became active.

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[3] http://quickfacts.census.gov/qfd/states/48/4805000.html
[4] http://www.census.gov/population/www/cen2010/cph-t/CPH-T-2.pdf
[5] http://www.census.gov/compendia/statab/2012/tables/12s0020.pdf
[6] http://quickfacts.census.gov/qfd/states/48/4839148.html
[7] http://quickfacts.census.gov/qfd/states/48/4876000.html
[8] http://quickfacts.census.gov/qfd/states/48/4872176.html

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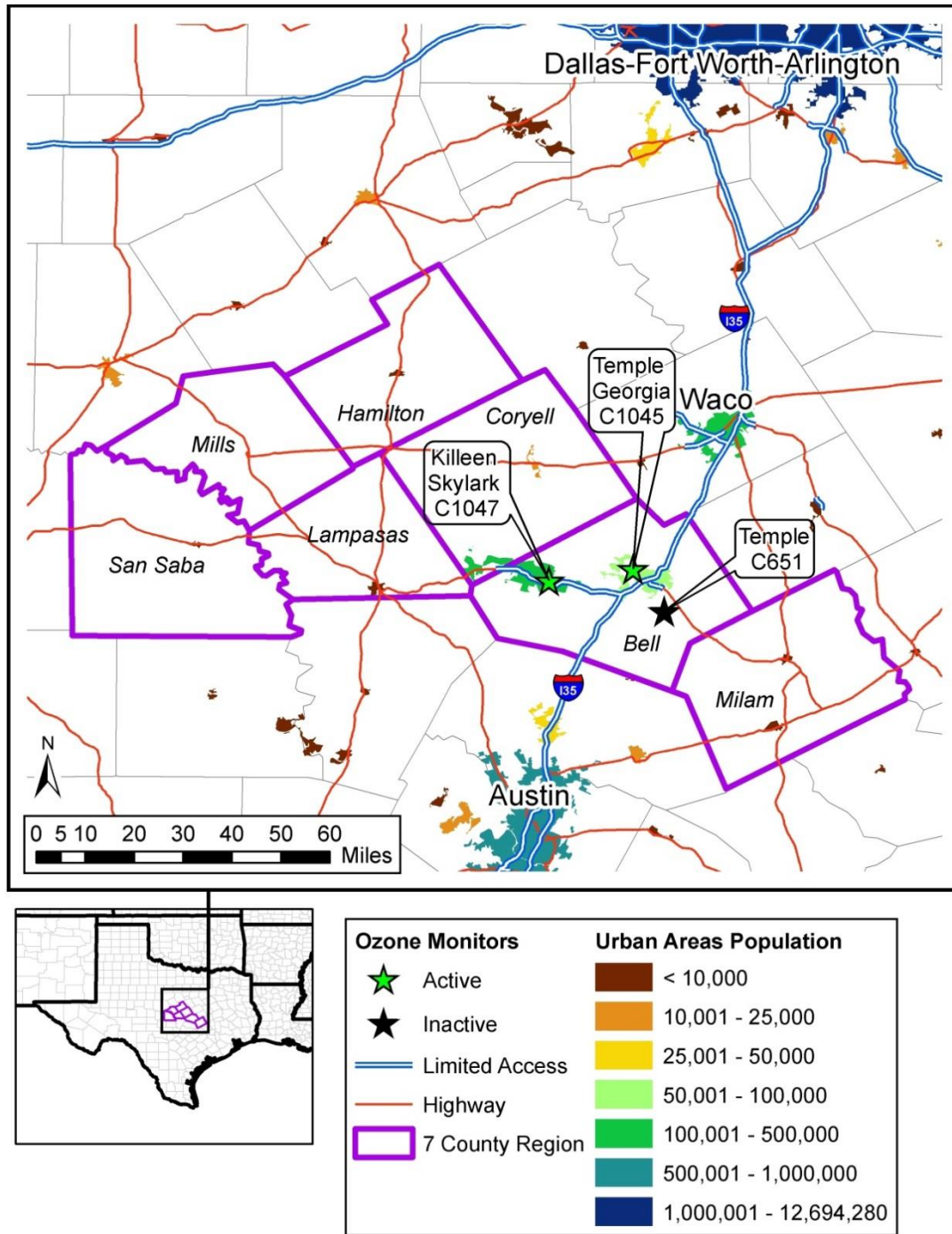


**Figure 1-2. The seven county KTF Area, location of active and inactive CAMS in Bell County, population distributions and major roadways in the surrounding region.**

Recent trends in KTF Area ozone are shown in Figure 1-3 and Figure 1-4, which report the monitors' annual 4th highest MDA8 ozone concentrations and 8-hour ozone design values, respectively.  The 8-hour NAAQS are shown as red lines in Figure 1-3 and Figure 1-4. The KTF Area was designated in attainment of the 75 parts per billion (ppb) 2008 NAAQS in 2012 based on the 2008-2010 readings from the Killeen Skylark CAMS 1047 monitor.

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 level set in 2008 to a more stringent value of 70 ppb[9].  The 2015 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 be based on 2014-2016 data[10].  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 1-4 shows that the Killeen CAMS 1047 monitor had a design value of 69 ppb at the end of the 2015 ozone season. The TCEQ ozone compliance website[11] reports a 2015 design value of 64 ppb for the Temple Georgia CAMS 1045 monitor but notes that this is not a regulatory design value because the monitor does not yet have three complete years of data.  By the end of the 2016 ozone season, the Temple Georgia monitor will have three complete years of data and a design value will be calculated for comparison with the 2015 ozone NAAQS.

2016 values of the 4th high MDA8 that are ≤ 76 ppb for Killeen CAMS 1047 monitor and ≤ 73 ppb for Temple Georgia CAMS 1045 monitor will produce 2016 design values that attain the 70 ppb 2015 NAAQS.  If both monitors attain the NAAQS at the end of the 2016 ozone season, an attainment demonstration of the 2015 NAAQS would not be necessary.  However, if either monitor 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 a modeled attainment demonstration might be necessary, depending on the area's designation.

### 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.

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[9] https://www.epa.gov/ozonepollution/2015-national-ambient-air-quality-standards-naaqs-ozone
[10] http://www3.epa.gov/ozonepollution/pdfs/20151001designationsfs.pdf.

[11] http://www.tceq.state.tx.us/cgi-bin/compliance/monops/8hr_attainment.pl
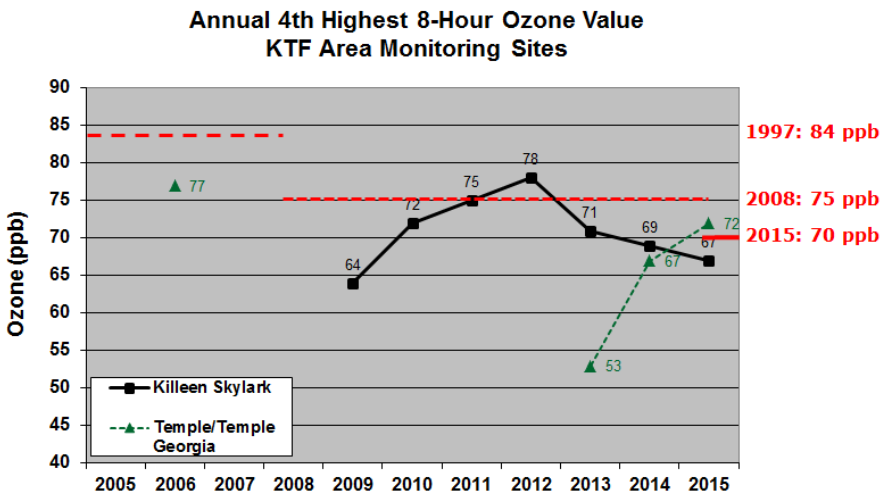
**Figure 1-3. Trends in annual 4th highest 8-hour ozone values at the Killeen Skylark (CAMS 1047), Temple Georgia (CAMS 1045) and Temple (CAMS 651) monitors in Central Texas. The red lines indicate the 1997 84 ppb, 2008 75 ppb and 2015 70 ppb ozone NAAQS. All data have been validated by the TCEQ. Temple Georgia CAMS 1045 data for 2013 is for a partial year.**
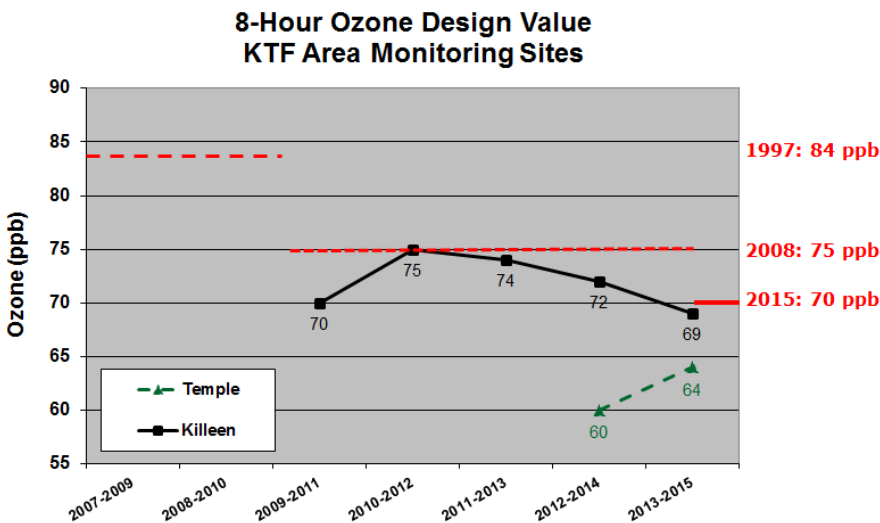


**Figure 1-4. Trends in design values at the Killeen Skylark (CAMS 1047) monitor and Temple Georgia (CAMS 1045) monitors in Central Texas. The red lines indicate the 1997 84 ppb, 2008 75 ppb and 2015 70 ppb ozone NAAQS. All data have been validated by the TCEQ. Temple Georgia CAMS 1045 design values are reported as they appear on the TCEQ's website[12] but do not yet have the three full years of data needed for a regulatory design value.**

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[12] http://www.tceq.state.tx.us/cgi-bin/compliance/monops/8hr_attainment.pl

## 1.2   Previous KTF Area Ozone Modeling Studies

In this section, we describe recent ozone modeling focused on the KTF Area of Central Texas. Modeling of June 2006 and June 2012 has been carried out for the KTF Area.

### 1.2.1   June 2006 Modeling

In 2013, the Heart of Texas Council of Governments (HOTCOG) carried out a study to assess whether the Waco and Killeen areas should be considered to lie within the same airshed (Parker et al., 2013).  Ozone modeling of the period May 31-July 2, 2006 was performed for all of East Texas based on input data provided by the TCEQ to the Texas NNAs. The Comprehensive Air Quality Model with Extensions (CAMx; Ramboll Environ, 2016) photochemical grid model was used in this study,

Ozone source apportionment modeling of the June 2006 episode showed that the Killeen CAMS 1047 and Waco CAMS 1037 monitors were generally influenced by emissions from different Texas source regions on high ozone days. The Killeen CAMS 1047 monitor was frequently affected by the Austin urban plume; over the course of the entire episode, the Austin area's influence at the Killeen CAMS 1047 monitor was greater than that of the local emissions from Bell County. The Austin area did not affect the Waco CAMS 1037 monitor with the same frequency and intensity as the Killeen CAMS 1047 monitor, and impacts from the DFW area were more frequent at Waco than at Killeen.

### 1.2.2   June 2012 Modeling

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. In 2015, Ramboll Environ 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 the KTF Area and other areas of Texas (Johnson et al., 2015).

Overall, the evaluation of photochemical model performance at the Killeen CAMS 1047 monitor showed that the model captures much of the observed ozone variability but has an overall high bias and a low bias on days when the MDA8 ozone exceeds 70 ppb. These biases may result from emissions sources that are not well-characterized in the local KTF emissions inventory, errors in modeled winds and/or other factors that are yet to be determined.

The main goal for the KTF Area 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; in particular, modeled ozone at the Killeen CAMS 1047 monitor must be brought into closer agreement with observations.  Once model performance is improved, the model can be used with greater confidence to understand causes of high ozone in the KTF Area as well as the potential impact of local emissions control strategies.

## 1.3 Study Objectives

### 1.3.1 Purpose and Method of the Central Texas Ozone Modeling Study

In partnership with the TCEQ, the Central Texas Council of Governments (CTCOG) 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 values at KTF Area monitors. Once these processes are better understood, targeted control measures may be proposed that will be aimed at reducing ozone concentrations at area monitors. 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 Central 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 the KTF Area.
- 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 the KTF Area are as follows:

- to incorporate the latest available emissions data for the KTF Area as well as other areas within the regional-scale modeling 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 CTCOG, 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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### 1.4.2 CTCOG

The contact at CTCOG is:

Jennifer Lawyer, Environmental Planner
Email: Jennifer.Lawyer@ctcog.org

Central Texas Council of Governments

Belton, TX 76513

Phone (254) 770-2379

### 1.4.3 CTCOG Air Quality Advisory Committee

CTCOG 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 CTCOG, TCEQ and EPA, acting through the CTCOG Air Quality Advisory Committee, will provide technical information where needed and will oversee and review all work performed in this project.

The membership of the CTCOG Air Quality Advisory Committee had not yet been determined at the time this document was written. This Protocol will be updated to include the Committee roster once this information becomes available.

## 1.5 Schedule and Deliverables

The schedule of tasks currently planned for the CTCOG 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 CTCOG Air Quality Advisory Committee and/or TCEQ, including any revision of objectives or requirements for the study.

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**Table 1-1. Schedule for the CTCOG ozone modeling activities.**

| Task | Completion Date |
|---|---|
| Draft Modeling Protocol Development | April 1, 2016 |
| Final Modeling Protocol | May 1, 2016 |
| Receipt of Modeling Inputs from the TCEQ | Ongoing |
| CAMx 2012  Ozone Modeling | January 15, 2017 |
| Draft Report on 2012 Ozone Modeling | March 15, 2017 |
| Final Report on 2012 Ozone Modeling | April 15, 2017 |

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

- A draft Modeling Protocol (this document) will be submitted by Ramboll Environ to CTCOG.  After CTCOG 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 CTCOG, the Air Quality Advisory Committee, and the 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 either KTF Area CAMS exceeds the 2015 NAAQS, Central 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 May 2016 will be determined by CTCOG and the TCEQ, and this Protocol will be updated to reflect the revised plan.
- The March, 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 CTCOG, the Air Quality Advisory Committee and the TCEQ. After all comments on the draft report are received, a final report will be prepared and submitted.

The CAMx modeling database will be made available to CTCOG, the Air Quality Advisory Committee and the TCEQ.

## 2.0 CONCEPTUAL MODEL FOR OZONE IN THE KTF AREA OF CENTRAL 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.  Kemball-Cook et al. (2015) developed a conceptual model of ozone formation in the KTF Area, and this conceptual model provides the basis for evaluating the selection of ozone modeling episodes (Section 3).  The conceptual model is summarized in Section 2 below.

### 2.1   Ozone and Air Quality Trends

Data collected at the TCEQ CAMS determine whether the KTF Area of Central Texas is in compliance with the NAAQS for ozone.  The two active KTF Area CAMS are located in Bell County, and their annual 4th highest MDA8 ozone and 8-hour ozone design value trends are shown in Figure 1-3 and Figure 1-4, respectively.  Figure 2-1 and Figure 2-2 show the number of days in each year from 2009 to 2015 (Killeen CAMS 1047) and 2006 to 2015 (Temple CAMS 651 and CAMS 1045) in which the observed MDA8 ozone exceeded the 2008 75 ppb NAAQS and the 70 ppb 2015 NAAQS.

KTF monitors show an overall decline in numbers of high ozone days over the period of record at both the 70 ppb and 75 ppb thresholds. 2011 and 2012 were years with unusually high summer temperatures and extended periods of high ozone in East Texas[13,14]  and had a relatively large number of days exceeding the threshold.  Between 2012 and 2015, the Killeen CAMS 1047 monitor saw a steady  decrease in the number of days with MDA8> 70 ppb and no days with MDA8 > 75 ppb. This is significant because the NAAQS is framed in terms of the 4th highest MDA8 value in each year.  As the number of days exceeding the 70 ppb threshold is reduced, the likelihood of a violation of the NAAQS at either KTF Area CAMS declines. The decrease in the number of days exceeding the 70 ppb and 75 ppb thresholds over the last decade at KTF Area monitors taken together with the declining annual 4th high MDA8 and design values (Figure 1-3 and Figure 1-4) indicate improvement in ozone air quality in the KTF Area during this period.

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[13] https://www.ncdc.noaa.gov/sotc/national/201113
[14] https://www.ncdc.noaa.gov/sotc/national/201213#analysis
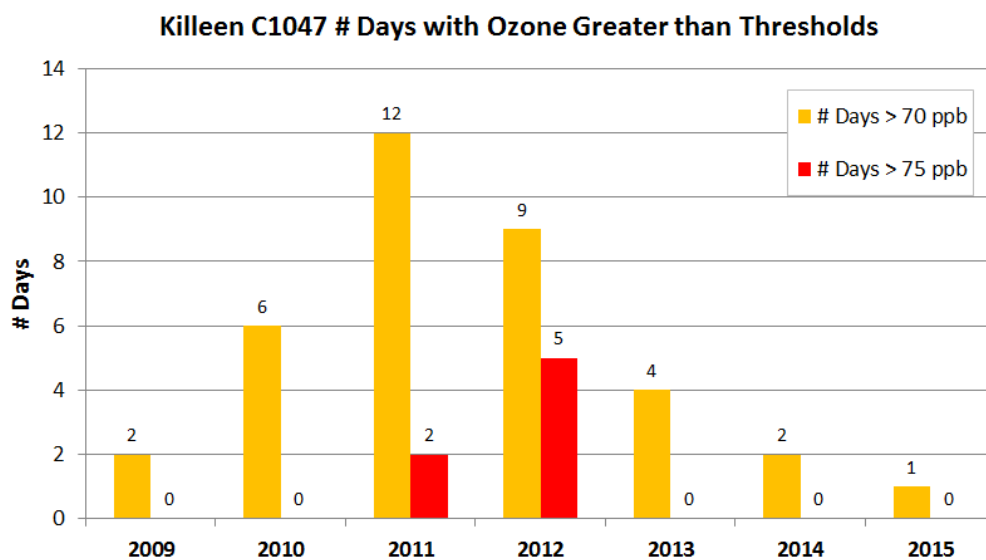
**Figure 2-1. Number of days with MDA8 exceeding 70 ppb and 75 ppb in each year from 2009 – 2015 for Killeen Skylark CAMS 1047**
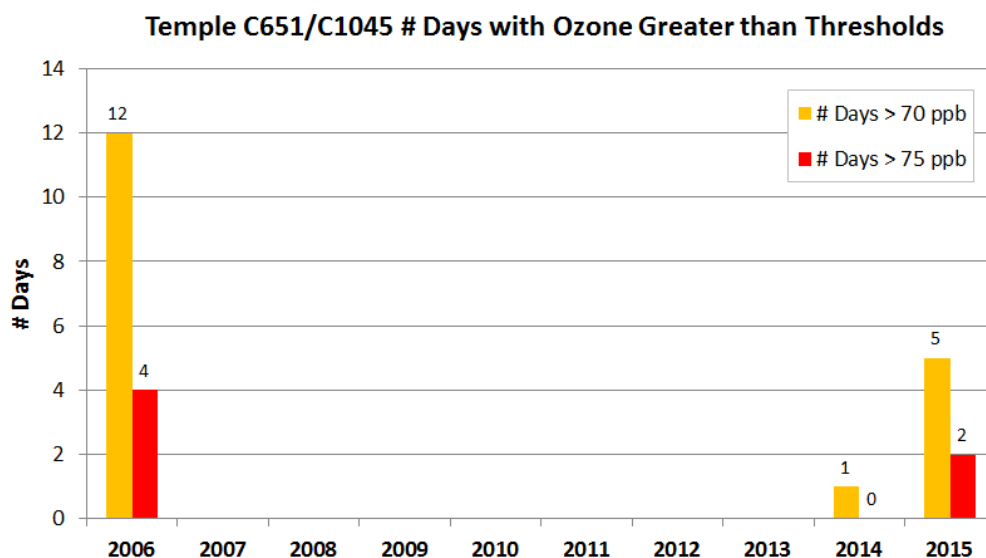


**Figure 2-2. Number of days with MDA8 exceeding 70 ppb and 75 ppb in each year from 2006 – 2015 for Temple CAMS 651 (2006 data) and Temple Georgia CAMS 1047 (2014-2015 data) monitors.**

## 2.2   Summary of Emission Inventory and Trends

Ozone is not emitted directly into the atmosphere, but forms from nitrogen oxides (NOx) and volatile organic compounds (VOCs) in the presence of sunlight. NOx and VOCs are emitted by both natural processes and human activities. Emission inventories of ozone precursors 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 the KTF Area was performed by Ramboll Environ in 2015 (Grant et al., 2015). The TCEQ 2012 emission inventory is summarized below to outline the relative importance of point, area, on-road, and off-road sector emissions in the KTF Area emission inventory. At the time this analysis was performed, 2012 was the most recent year for which a full KTF Area emission inventory (i.e. anthropogenic and biogenic emissions) was available.

Figure 2-3 shows NOx and VOC emissions by source category in the KTF Area for 2012. KTF-wide 2012 total emission estimates are 62 tpd NOx and 1,026 tpd VOC. The largest three emissions source categories, on-road vehicles (23 tpd, 37%), off-road sources (16 tpd, 26%), and biogenic sources (12 tpd, 19%), account for 82% of KTF Area NOx emissions. Point sources (9.2 tpd, 15%) and area sources (2.2 tpd, 4%) sources together account for less than 20% of KTF Area total NOx emissions. Biogenic sources are the largest VOC category comprising 95% (978 tpd) of KTF Area total VOC emissions. Anthropogenic sources account for 5% of VOC emissions with contributions from: area sources (3%, 32 tpd), on-road vehicles (1%, 8.1 tpd), off-road sources (1%, 6.0 tpd), and points sources (<1%, 2.2 tpd).

Biogenic emission estimates for 2012 were developed by the TCEQ using the Model of Emissions of Gases and Aerosols from Nature (MEGAN; Guenther et al., 2012) version 2.10. MEGAN emissions provide 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. Episode average biogenic emissions were calculated from the TCEQ 2012 biogenic emission inventory for the KTF Area[15].

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[15] http://www.tceq.texas.gov/airquality/airmod/data/tx2012
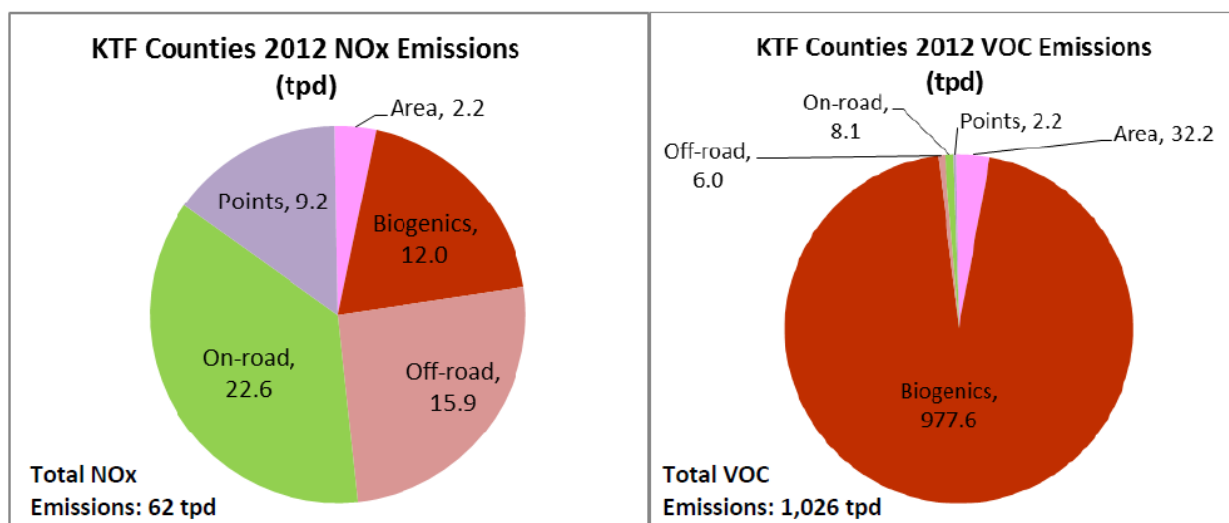
**Figure 2-3. KTF Area 2012 NOx emissions (tpd) (left) and VOC emissions (tpd) (right) by source category. (Note: oil and gas area source emissions are for calendar year 2011).**

Biogenic NOx emissions contributions in the KTF Area are higher than in other areas of East Texas for which Ramboll Environ has conducted emission inventory reviews (e.g. Grant et al. 2015a; Grant et al., 2015b). This is due, at least in part to intensive agricultural activity in the KTF Area. The nitrogen cycle is the process by which nitrogen is transformed from one form to another through processes such as fixation, ammonification, nitrification, and denitrification. Denitrification is the process by which microorganisms in soil convert nitrate or nitrite molecules into gaseous forms of nitrogen (such as nitrogen oxide; NO). Fertilizer application and the presence of abundant organic material in soil increase the rate of nitrogen cycling in a soil system while soil properties and water content determine the amount of nitrogen released into the atmosphere. Higher temperatures, anaerobic conditions, and water saturation are all factors that increase nitrogen emissions to the atmosphere from soils (Sakulyanontvittaya et al., 2012). Therefore, we expect that agricultural areas where nitrogen-based fertilizers are applied to the soil to have biogenic NOx emissions and that these emissions would increase during periods of hot weather or following heavy rains. In 2012 there were 723,979 planted acres in the KTF Area with three crop types accounting for over 75% of the planted acres:  grass (52%), wheat (13%), and corn (11%)[16].

In order to develop emission control strategies for the KTF Area 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. Ozone formation depends on the presence of sufficient NOx and VOC.  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

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[16] United States Department of Agriculture (USDA) Farm Services Agency (FSA) Crop Acreage Data. 2012 acreage data as of January 2013. http://www.fsa.usda.gov/FSA/webapp?area=newsroom&subject=landing&topic=foi-er-fri-cad

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 7-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).  For the KTF Area, the emission inventory VOC/NOx ratio is 54 ppbC/ppb, which is well within the NOx-limited regime. The presence of abundant biogenic VOC emissions ensures that there are sufficient VOCs to allow ozone formation and that ozone formation is limited by the amount of available NOx. This means local emissions control strategies should focus on reducing NOx emissions.

## 2.3  Meteorological Factors Associated with High Ozone Events

Meteorological factors are known to play a critical role in ozone formation. Ozone formation is driven by solar ultraviolet radiation through a series of photochemical reactions. Ozone is more likely to form on clear summer days when abundant sunlight reaches the lower atmosphere and daytime temperatures are high.  Another local meteorological condition conducive to ozone formation is slow wind speeds since slow winds tend to limit the dispersion of pollutants.  Slow or stagnant wind conditions may be due to a surface level high pressure system affecting the region. The location of a monitor in relation to large sources of ozone precursor emissions will be a factor that determines which wind directions may be likely to transport polluted air to a monitor, thus wind direction at some monitors may be an important factor associated with high ozone.  A conceptual model for ozone in the KTF Area was developed during 2015 (Kemball-Cook et al., 2015).  The conceptual model was developed prior to October 2015, when the EPA lowered the NAAQS for ozone from 75 ppb to 70 ppb.  Therefore, the conceptual model developed in 2015 treated 75 ppb as the threshold for high ozone concentrations.  Below, we summarize the conceptual model.

The KTF Area is located on the eastern edge of the Edwards Plateau in Central Texas, where the lack of major topographical features means that wind patterns are driven primarily by synoptic-scale meteorological influences. Episodes of high ground level ozone (> 75 ppb) in the KTF Area 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.  These conditions, which are conducive to ozone formation, can also be produced by passage of a cold front or the presence of a stationary front (e.g. McGaughey et al., 2010; 2012). Most ozone episodes are associated with light near-surface winds from the north/east/south/southwest, with southerly directions appearing less frequently on days with highest ozone.  Days during the ozone season with low ozone (< 60 ppb) in the KTF Area frequently occur during periods of

strong southerly winds that bring comparatively less polluted maritime air from the Gulf of Mexico northward into Central Texas.

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 high ozone days shows that transport from the south plays a more important role for days with MDA8 in the 65-70 ppb range at the Killeen CAMS 1047 monitor (Parker et al., 2015).

## 2.4   Regional Transport

EPA Modeling 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 source apportionment modeling for the June 2012 episode was used to estimate transported contributions to ozone at the Killeen CAMS 1047 monitor and the location of the Temple Georgia CAMS 1045 monitor from emissions source regions outside the KTF Area; this included emissions source regions within and outside of Texas (Johnson et al., 2015).

The ozone contribution from KTF Area emissions to MDA8 ozone at Killeen CAMS 1047 and Temple Georgia CAMS 1045 varied from day to day during the June 2012 ozone modeling episode (Johnson et al., 2015).  The KTF area contribution to Killeen CAMS 1047 and Temple Georgia CAMS 1045 ozone ranged from 0.1 - 13 ppb and 0.1 - 12 ppb, respectively; the magnitude of the KTF area contribution depended on each day's weather conditions.  Wind direction is a key factor that determines whether the locally-generated KTF Area ozone plume arrives at the two CAMS.  On average, ozone transported into the KTF Area contributed far more (49-51 ppb) than local KTF Area emissions (3.2 ppb for both monitors) to the daily maximum 8-hour average (MDA8) ozone at the Killeen CAMS 1047 and Temple Georgia CAMS 1045 monitors (Figure 2-4).

The photochemical modeling results indicate that, while ozone at the locations of the Killeen CAMS 1047 and Temple Georgia CAMS 1045 monitors is largely due to transport, local emissions controls can have some benefit in reducing MDA8 ozone at the two monitors. The fact that the local KTF Area contribution to ozone reached 12-13 ppb at Killeen CAMS 1047 and Temple Georgia CAMS 1045 monitors means that local sources can produce intermittent large impacts that are of particular concern because they have the potential to drive up the ozone design value by affecting the monitor on dates that enter into the design value calculation.

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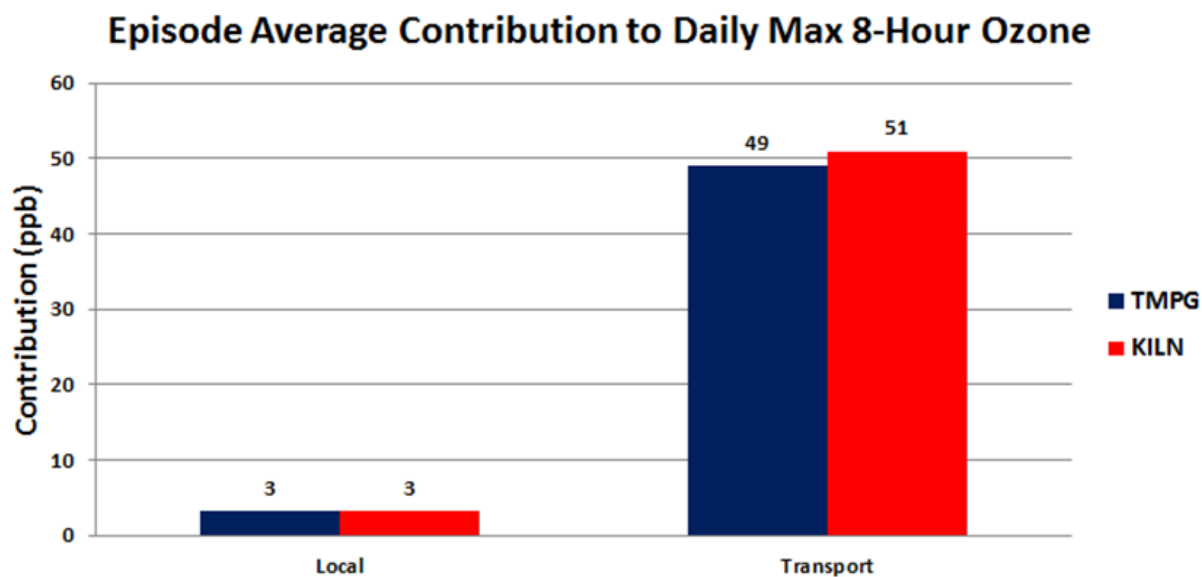


**Figure 2-4. Episode average contribution to daily maximum 8-hour ozone for the location of the Temple Georgia (TMPG; CAMS 1045) monitor and the Killeen (KILN; CAMS 1047) monitor from KTF Area emissions sources ("local") and all emissions sources outside of the KTF Area ("transport").**

## 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 National Emission Inventory (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.


## 3.2  2012 Modeling Episodes

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 all 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 modeling 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[17] 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.

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[17] 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. At the direction of the TCEQ, Ramboll Environ performed CAMx modeling of June 2012 and model performance evaluation focused on the KTF Area, 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. CTCOG is currently using the June 2012 modeling episode in its ozone air quality planning and could 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 the KTF Area and EPA Guidance on episode selection.

Figure 3-1 shows the MDA8 ozone at the Killeen Skylark CAMS 1047 monitor (see Figure 1-1 for monitor location) during the 2012 ozone season, which is defined by the EPA to extend from March-November in Texas[18]. Ozone was generally higher at the Killeen CAMS 1047 monitor during April-June and August-October and lower during March, November and July of 2012. 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. For example, a period of lower ozone follows the June 25-27 high ozone period. Therefore, Criterion 3 is met for the 2012 ozone season. Table 3-1 lists all days during 2012 when the MDA8 ozone at the Killeen CAMS 1047 monitor exceeded 70 ppb. There are two two-day episodes during which the MDA8 exceeded 70 ppb (May 16-17, August 10-11) and a single three-day episode when MDA8 > 70 ppb at CAMS 1047: June 25-27. The 2012 ozone season had 9 days with MDA8 > 70 ppb at the Killeen CAMS 1047 monitor (Table 3-1).
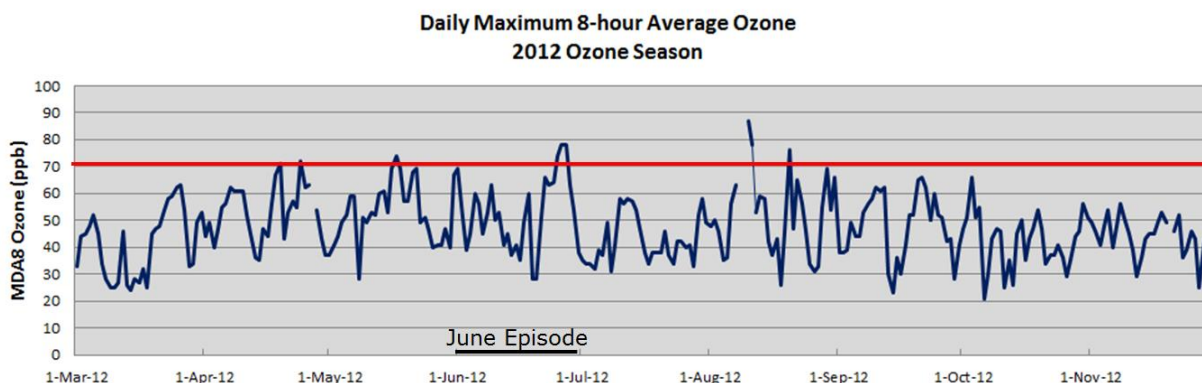


**Figure 3-1. Daily maximum 8-hour average ozone at the Killeen Skylark CAMS 1047 monitor during the 2012 ozone season. Duration of the June 2012 episode is indicated by the black bar and the red bar shows the level of the 70 ppb 2015 NAAQS for ozone. Breaks in the time series indicate periods of missing data. All data have been validated by the TCEQ.**

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[18] https://www.gpo.gov/fdsys/pkg/FR-2015-10-26/pdf/2015-26594.pdf

**Table 3-1. List of 2012 days with MDA8 ozone greater than 70 ppb at the Killeen Skylark CAMS 1047 monitor. Temple monitors were not active in 2012.**

| Location | CAMS | Date | Time of MDA8 Ozone | MDA8 Ozone (ppb) |
|---|---|---|---|---|
| Killeen Skylark Field C1047 | 1047 | April 19 2012 | 11:00 | 71 |
| Killeen Skylark Field C1047 | 1047 | April 24 2012 | 11:00 | 72 |
| Killeen Skylark Field C1047 | 1047 | May 17 2012 | 11:00 | 74 |
| Killeen Skylark Field C1047 | 1047 | June 25 2012 | 10:00 | 74 |
| Killeen Skylark Field C1047 | 1047 | June 26 2012 | 9:00 | 78 |
| Killeen Skylark Field C1047 | 1047 | June 27 2012 | 11:00 | 78 |
| Killeen Skylark Field C1047 | 1047 | August 10 2012 | 12:00 | 87 |
| Killeen Skylark Field C1047 | 1047 | August 11 2012 | 11:00 | 78 |
| Killeen Skylark Field C1047 | 1047 | August 20 2012 | 11:00 | 76 |

Figure 3-2 shows time series of the MDA8 ozone at the Killeen CAMS 1047 monitor for the June 2012 episode, which corresponds to the black bar in Figure 3-1.  There is one multi-day episode of MDA8 ozone > 70 ppb (June 25-27); the high ozone period is preceded by a multi-week lower ozone period and followed by a two-day transition to lower ozone during June 29-30. Therefore, the June 2012 episode satisfies Criterion 3.
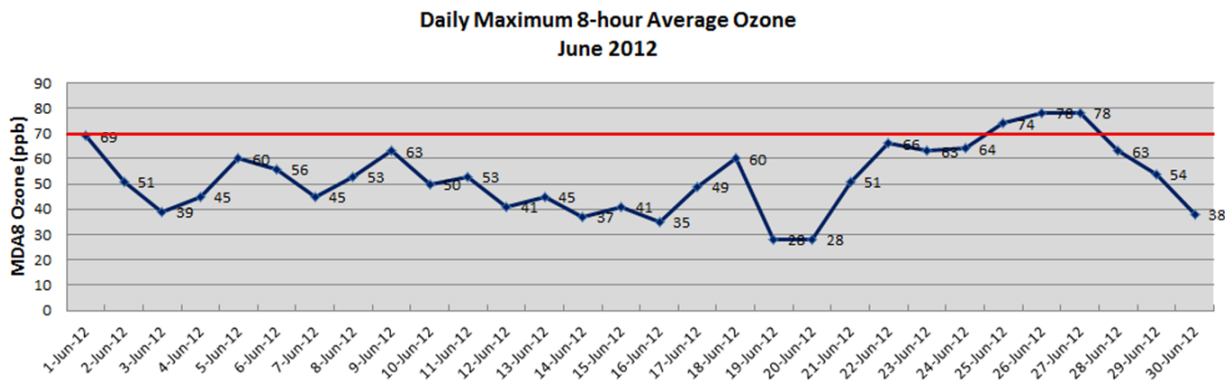


**Figure 3-2. Daily maximum 8-hour average ozone at the Killeen Skylark CAMS 1047 monitor during June 2012 TCEQ modeling episode. Red bar shows the level of the 70 ppb 2015 NAAQS for ozone.**

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 days with the 10 highest modeled MDA8 values in the simulated period at each monitoring site as long as the MDA8 for each day is ≥ 60 ppb.

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A ranked list of the ten days with the highest MDA8 ozone at the Killeen CAMS 1047 monitor 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 the Killeen Skylark CAMS 1047 monitor. Days with MDA8 > 70 ppb are shaded orange. White text indicates June days.**

| Rank | Date | MDA8 Ozone (ppb) |
|---|---|---|
| 1 | 10-Aug-12 | 87 |
| 2 | 26-Jun-12 | 78 |
| 3 | 27-Jun-12 | 78 |
| 4 | 11-Aug-12 | 78 |
| 5 | 20-Aug-12 | 76 |
| 6 | 17-May-12 | 74 |
| 7 | 25-Jun-12 | 74 |
| 8 | 24-Apr-12 | 72 |
| 9 | 19-Apr-12 | 71 |
| 10 | 16-May-12 | 69 |

**Table 3-3. Ranked list of 10 days with highest MDA8 during June 2012 for the Killeen Skylark CAMS 1047 monitor. Days with MDA8 > 70 ppb are shaded orange.**

| Rank | Date | MDA8 Ozone (ppb) |
|---|---|---|
| 1 | 26-Jun-12 | 78 |
| 2 | 27-Jun-12 | 78 |
| 3 | 25-Jun-12 | 74 |
| 4 | 1-Jun-12 | 69 |
| 5 | 22-Jun-12 | 66 |
| 6 | 24-Jun-12 | 64 |
| 7 | 9-Jun-12 | 63 |
| 8 | 23-Jun-12 | 63 |
| '9 | 28-Jun-12 | 63 |
| 10 | 5-Jun-12 | 60 |

Table 3-2 indicates that the 2012 ozone season has 10 days with MDA8 ≥ 60 ppb for the Killeen CAMS 1047 monitor. Therefore, there are enough days meeting the 60 ppb threshold that an RRF can be calculated in accordance with EPA guidance.  The MDA8 on the 10 highest days ranges from 69-87 ppb, which brackets the 73.7 ppb three year average of design values centered on 2012 (Figure 1-4).  Based on the values of the 10 highest MDA8 days at the Killeen CAMS 1047 monitor, 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 three of the seven highest MDA8 values during the 2012 ozone season at the Killeen CAMS 1047 monitor.  All of the days with MDA8 > 70 ppb during June 2012 occurred during the June 25-27 high ozone episode. The ozone MDA8 during the remainder of June was lower than 70 ppb.  The Killeen CAMS 1047 monitor had 10 days with MDA8 ≥ 60 ppb during June 2012, however, seven of these days have MDA8 < 70 ppb.  EPA notes in their 2014 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 has a sufficient number of high ozone days to form an RRF for the Killeen CAMS 1047 monitor that is consistent with EPA Guidance, it would be possible to use June 2012 as an episode for a modeled attainment demonstration; however, it is preferable to use the entire 2012 ozone season if an attainment demonstration is needed for the KTF Area because there are more days with MDA8 ozone values that exceed 70 ppb and are closer to the 2011-2013 average Killeen CAMS 1047 monitor design value.

## 3.3   Review of High Ozone Days in 2012

In this section, we review the June 2012 episode and the entire 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 these two periods. We begin by describing the data und methods used to characterize the high ozone days. We evaluate the winds on and preceding KTF high ozone days to determine whether important source-receptor relationships would be modeled during the selected episode.

### 3.3.1   Back Trajectory Data

The purpose of a back trajectory analysis is to estimate the path that an air mass travelled prior to its arrival at a particular location. Backward trajectory plots provide approximate information regarding possible source regions for pollutants transported to a monitor. However, they may have considerable uncertainty which grows with increasing trajectory length. Backward trajectories should not be interpreted as giving the precise track of air parcels.

We use back trajectories to understand the origin of air masses arriving at the Killeen CAMS 1047 monitor on 2012 ozone season days with MDA8 ozone > 70 ppb.  We examine back trajectories developed with near-surface winds as well as aloft winds.  Parker et al. (2013) reviewed 2012 days with MDA8 > 75 ppb as part of an analysis of the Waco and Killeen airsheds.  75 ppb was used as the threshold for a high ozone day because the NAAQS for ozone was 75 ppb at the time the study was performed.  The back trajectory plots from Parker et al. (2013) are reproduced here.  These back trajectories were developed using TCEQ CAMS surface winds as input to the Corpus Christie back trajectory tool[19] described in McGaughey et al.

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[19] http://dept.ceer.utexas.edu/ceer/ccaqp/trajectory_tool.htm

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(2012). These plots show back trajectories ending at both the Killeen CAMS 1047 and Waco Mazanec CAMS 1037 monitors.

Back trajectories for 2012 days with 70 ppb < MDA8 ozone ≤ 75 ppb were prepared using the TCEQ's AQPlot back trajectory tool[20] driven by TCEQ CAMS surface winds. The AQPlot model determines the trajectory followed by a particle released into the air mass and carried by the CAMS near-surface winds. The AQPlot back trajectories were performed for the Killeen CAMS 1047 monitor only. The AQPlot tool calculates backward trajectories based on observed winds at surface meteorological sites. The major limitation of this method arises when the monitoring network is sparse or a backward trajectory extends to an area without a monitor. In general, AQPlot back trajectories can be considered reliable when the backward trajectory points are relatively close to the set of meteorological monitors used to calculate the backward trajectories. The AQPlot back trajectory is based on surface winds from the Killeen monitor and its uncertainty increases with distance from the monitor.

Aloft back trajectories were prepared using the on-line tools provided by NOAA (Stein et al., 2015)[21]. These tools are based on application of NOAA's Hybrid Single Particle Lagrangian Integrated Trajectory (HYSPLIT) model (Draxler et al., 2015) with archived weather forecast model data from the National Center for Environmental Prediction's North American Mesoscale Forecast System (NAM) forecast model. Uncertainties are introduced by the spatial and temporal resolution of the three-dimensional gridded NAM meteorological data and also by the inherent uncertainties in the analyzed meteorological data. Meteorological data are derived by assimilating high frequency observations such as wind profiler, radar, and aircraft data with modeled predictions. The horizontal spatial resolution of the NAM analysis is 12 km. Large-scale weather patterns are likely well-simulated by the meteorological model but sub-mesoscale weather features may not be captured at the model's resolution. HYSPLIT backward trajectories are therefore likely to be more accurate on days with strong winds driven by large-scale weather features. Days with light, shifting winds are more likely to have backward trajectories with larger uncertainties than days with strong, steady winds. HYSPLIT plots for all days when the Killeen CAMS 1047 monitor recorded MDA8 > 70 ppb are presented together in Figure 3-16.

### 3.3.2    Summary of Back Trajectories on Days with MDA8 > 70 ppb: 2009-2014.

Figure 3-3 shows back trajectories ending above the Killeen CAMS 1047 monitor for all days during 2009-2014 with MDA8 > 70 ppb at the Killeen CAMS 1047 monitor. Backward trajectories were prepared for each high ozone day ending at 500 m above the Killeen CAMS 1047 monitor using the on-line tools provided by the NOAA at http://www.arl.noaa.gov/ready/hysplit4.html (Stein et al., 2015).

The back trajectories show that on days with MDA8 > 70 ppb at the Killeen CAMS 1047 monitor, winds were most frequently from the south, bringing air northward across the Austin and/or

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[20] https://www.tceq.texas.gov/assets/public/implementation/air/am/committees/pmt_set/20060523/20060523-mcdonad-aqplot_mm5_wind.pdf
[21] http://www.arl.noaa.gov/ready/hysplit4.html

San Antonio metropolitan areas before its arrival at Killeen. Several trajectories extend backward over heavily urbanized areas along the Texas Gulf Coast (Houston-Galveston-Brazoria, Corpus Christie, Victoria). The back trajectories indicate that northerly winds also occurred on high ozone days so that air that had traversed the Dallas-Fort Worth and Waco metropolitan areas reached Killeen. Several back trajectories extend over the Tyler-Longview-Marshall area of Northeast Texas. There are two days when air arrived at the Killeen CAMS 1047 monitor from the west on days with MDA8 > 70 ppb, but these back trajectories have a strong curvature and suggest recirculating wind patterns during the days preceding the MDA8 > 70 ppb day. As we consider the June 2012 modeling episode and the potential 2012 ozone season episode, we evaluate whether the wind direction variation shown in Figure 3-3 is reflected in the winds on the days with MDA8 > 70 ppb days in June 2012 and in the full 2012 ozone season. In the next section, we review back trajectories on the days with MDA8 > 70 ppb during 2012.
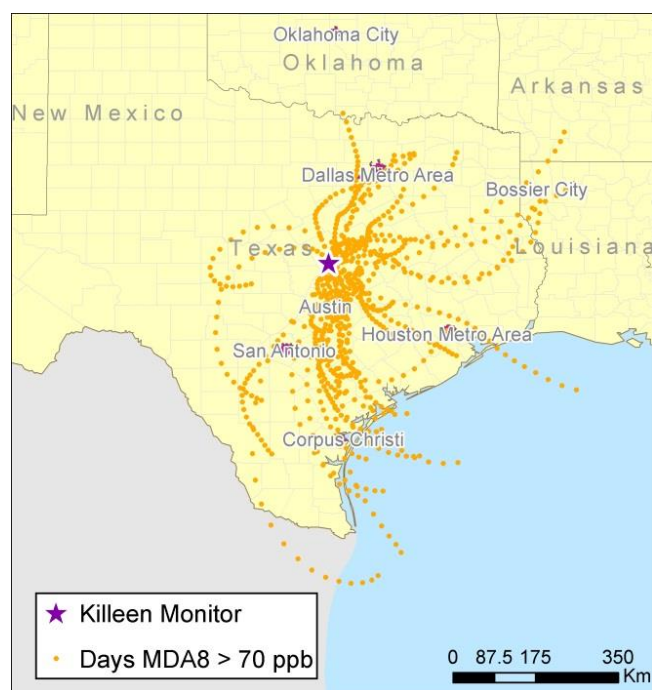


**Figure 3-3. 24-hour HYSPLIT backward trajectory plots ending 500 m above the Killeen CAMS 1047 monitor at 5 pm local time for ozone season days in 2009-2014 for days with MDA8 ozone > 70 ppb.**

### 3.3.3   June 25-27 Episode

June 25-27, 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 (exceeding 90°F). 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., 2014a). June 25-27 was the only period during June

2012 with MDA8 > 70 ppb at Killeen CAMS 1047 and the only 3-day episode of MDA8 > 70 ppb at CAMS 1047 during the entire 2012 ozone season. Figure 3-4 shows a back trajectory
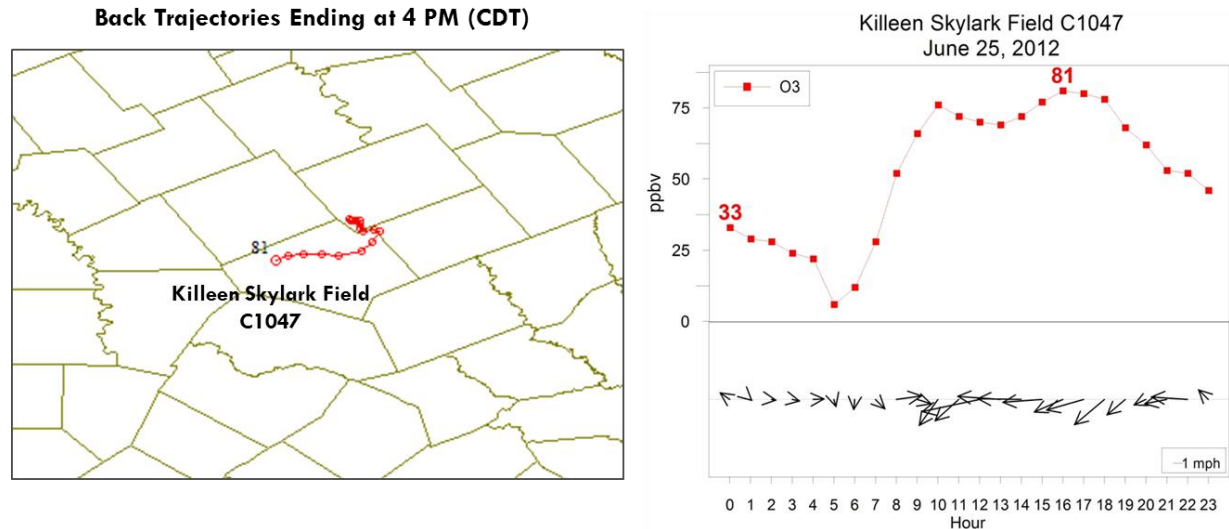


**Figure 3-4. June 25, 2012 high ozone day at Killeen Skylark CAMS 1047. Left panel: AQPlot back trajectories for the Killeen CAMS 1047 monitor for June 25 at the time of peak 1-hour ozone. Right panel: time series of 1-hour ozone (upper panel) and wind vectors (lower panel) at the Killeen CAMS 1047 monitor on June 25.**
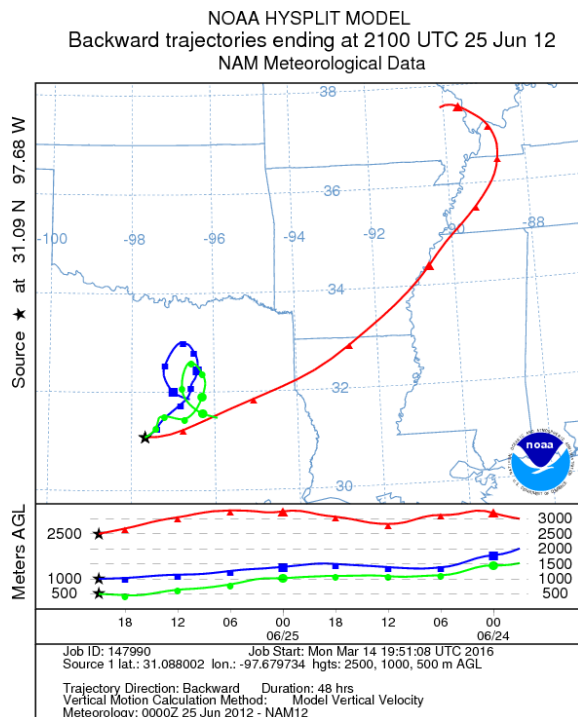


**Figure 3-5. 48 hour HYSPLIT back trajectories ending above the Killeen CAMS 1047 monitor on June 25, 2012.**

developed with the TCEQ's AQPlot tool (left panel) and the hourly ozone concentrations and wind vectors (right panel) measured at the Killeen CAMS 1047 monitor on June 25, 2012. The AQPlot back trajectory for June 25 shows that winds were slow and stagnant leading up to the time of the peak value of 1-hour average ozone at 4 pm. A 48-hour back trajectory developed using HYSPLIT shows that the low-level winds during the two days leading up to June 25 were stagnant and recirculating (Figure 3-5). This flow pattern keeps pollutants in the region rather than dispersing them. Winds aloft were stronger and steadier and from the northeast. This wind direction can bring polluted continental air into Texas (e.g. McGaughey et al., 2012; Parker et al., 2013) and is consistent with the high levels of ozone observed throughout East Texas on June 25.

On June 26, winds remained light, as indicated by the short length of the surface wind back trajectories in the left panel of Figure 3-6. In the morning, ozone rose rapidly at the Killeen CAMS 1047 monitor and reached a daily maximum 1-hour ozone value of 91 ppb at 10 am (right panel of Figure 3-6). Surface back trajectories indicate stagnant, recirculating winds while aloft back trajectories (Figure 3-16) show slow, shifting winds with an overall northeasterly direction. The Killeen CAMS 1047 back trajectory plot shows a shift in wind direction prior to highest ozone measurement at 10 am. This indicates that local emissions may have accumulated in the air mass and contributed to the high ozone, but regional background levels were also very high (60-65 ppb; Parker et al., 2013).
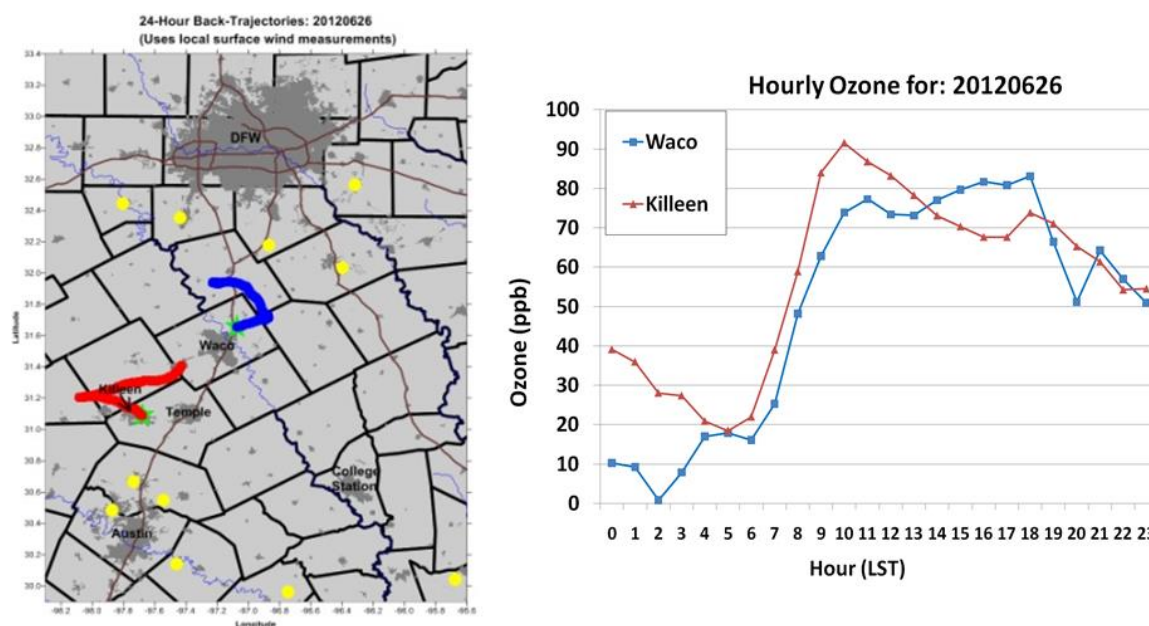


**Figure 3-6. June 26, 2012 high ozone day at Killeen Skylark CAMS 1047. Left panel: 24-hour back trajectories for the Killeen CAMS 1047 monitor (red) and Waco Mazanec CAMS 1037 (blue) for June 26 at the time of peak 1-hour ozone. Yellow circles indicate location of CAMS ozone monitors. Gray shading indicates outline of urban area. Right panel: time series of 1-hour ozone at the Killeen CAMS 1047 monitor and Waco Mazanec CAMS 1037 monitor on June 26. Figures from Parker et al. (2013).**

By June 27, winds had shifted to the southeast and become stronger and steadier near the surface (Figure 3-7) as well as aloft (Figure 3-16). The 500 m and 1,000 m HYSPLIT back trajectories also show southeasterly winds, with trajectories extending back over the Victoria/Corpus Christie areas (Figure 3-16). The 2,500 back trajectory shows winds were from the northwest earlier in the day with a shift to southeasterly winds that aligned with the southeasterly winds at lower levels. Regional background ozone remained high at approximately 70 ppb (Parker et al., 2013).
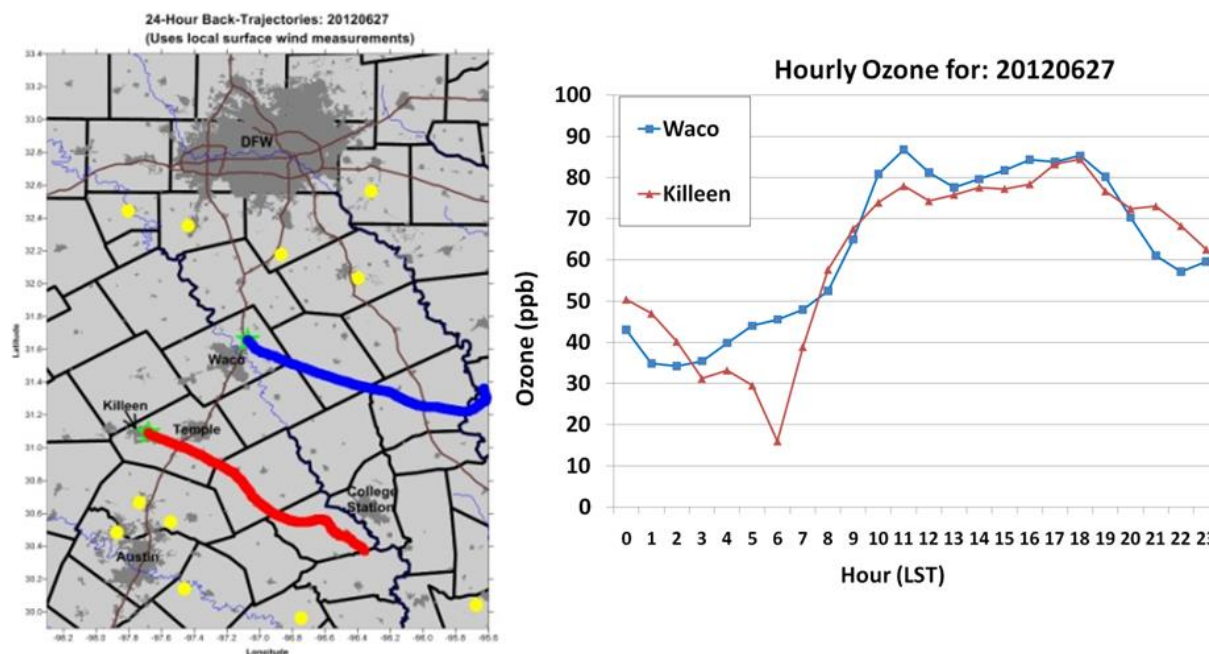


**Figure 3-7. As in Figure 3-6, for June 27, 2012.**

In summary, the three June days when MDA8 > 70 ppb at the Killeen CAMS 1047 monitor were characterized by northwesterly flow aloft and stagnant, recirculating surface winds (June 25-26) or light southeasterly near-surface winds (June 27). This was a period of high temperatures when high background ozone levels affected East Texas and wildfires within and outside Texas likely contributed to the elevated regional background.

### 3.3.4   2012 Days with MDA8 > 70 ppb not in the Month of June

3.3.4.1   April 19, April 24

On April 19, winds were strong and southerly throughout the day (Figure 3-8). The AQPlot surface wind back trajectory shows that air crossed the greater Austin metropolitan area before passing over the Killeen CAMS 1047 monitor. The situation was similar on April 24 (Figure 3-9). Surface winds were light and variable during the early morning hours, but wind speeds increased and winds became southerly just before sunrise. Winds were strong and southerly for the remainder of the day. Aloft winds at the 500 m and 1,000 m levels were southerly on both days (Figure 3-16). On both days, the 2,500 m back trajectory has a westerly component, and indicates the presence of vertical wind shear. Regional background ozone was
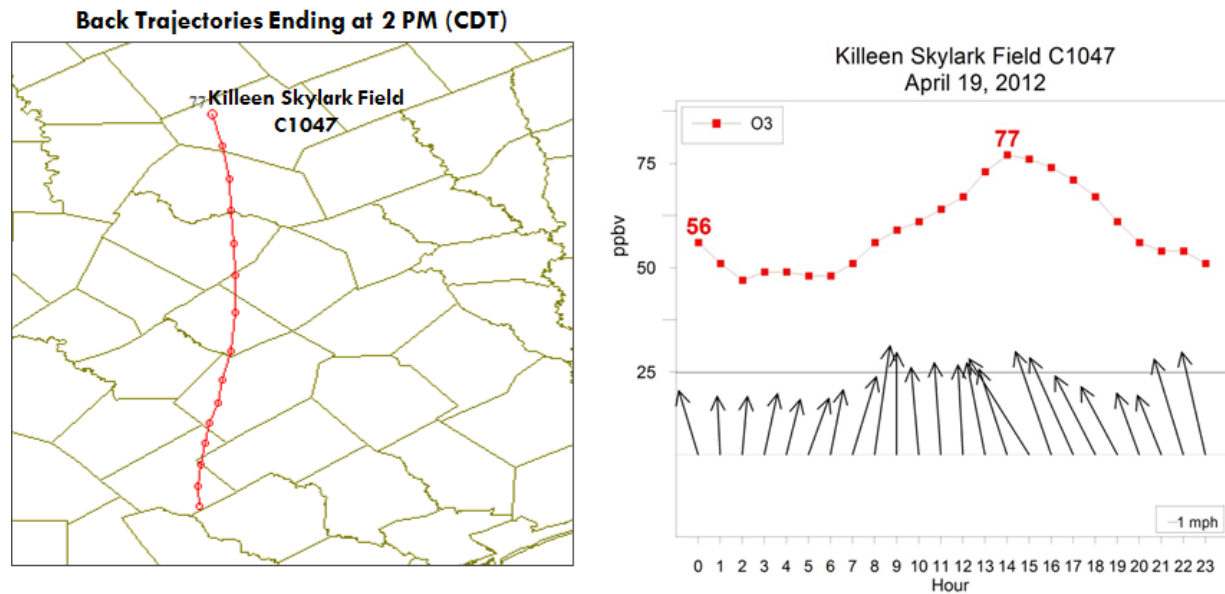
**Figure 3-8. April 19, 2012 high ozone day at Killeen Skylark CAMS 1047. Left panel: AQplot back trajectories for the Killeen CAMS 1047 monitor for April 19 at the time of peak 1-hour ozone. Right panel: time series of 1-hour ozone (upper panel) and wind vectors (lower panel) at the Killeen CAMS 1047 monitor on April 19.**
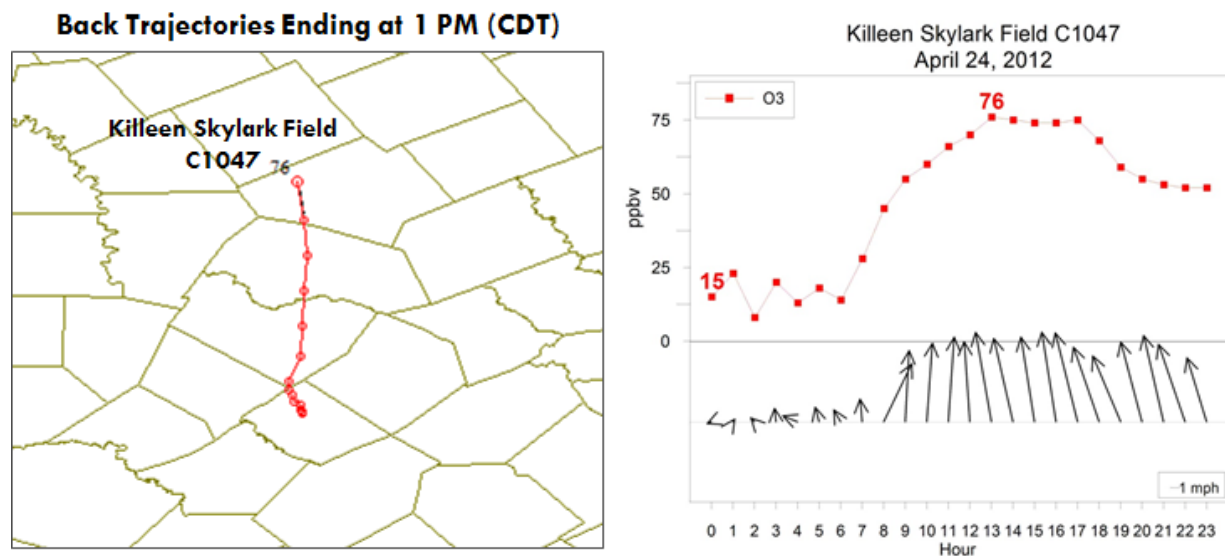


**Figure 3-9. As in Figure 3-8, for April 24, 2012.**

approximately 60 ppb on both days as indicated by the Fayette County CAMS 601 monitor[22], which was upwind of the Killeen urban area and east of the Austin urban plume on both days.

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[22] http://www.tceq.state.tx.us/cgi-bin/compliance/monops/8hr_monthly.pl

These two April days likely indicate the influence of the Austin urban plume on ozone at the Killeen CAMS 1047 monitor superposed on a high regional ozone background. The Killeen urban plume may also have contributed.

### 3.3.4.2   May 16-17

May 14-22 was a period when many monitors across East Texas recorded MDA8 values > 70 ppb, with MDA8 values exceeding 80 ppb in both the Houston and Dallas-Fort Worth areas[23]. At the Killeen CAMS 1047 monitor, only May 16-17 exceeded MDA8 ozone concentrations of 70 ppb.  Both days were characterized by light and shifting winds.  On May 16 (Figure 3-10), surface winds had a clockwise circulation, limiting dispersion of pollutants. Aloft winds were easterly through northerly (Figure 3-16), indicating the influence of continental air, which is associated with higher levels of background ozone in Central Texas (e.g. McGaughey et al., 2010, 2012; Parker et al., 2013).
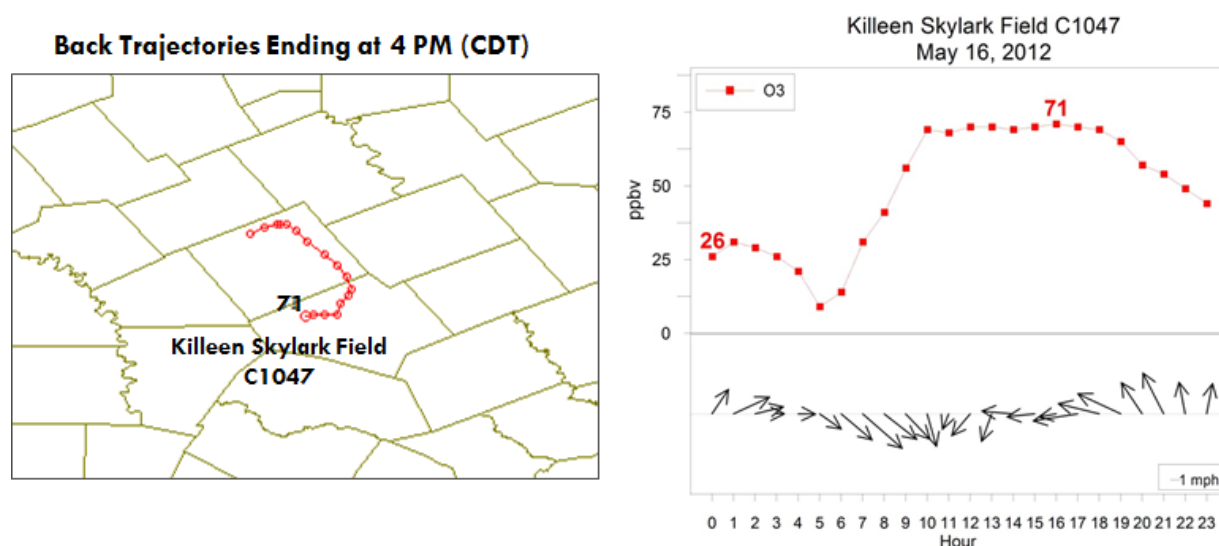


**Figure 3-10. As in Figure 3-8, for May 16, 2012.**

By 9 pm, the winds had become southerly.  Winds were light overnight, but retained a southerly component during most hours.  After day break on May 17, wind speeds rose, but the winds remained southerly. The AQPlot (Figure 3-11) and HYSPLIT (Figure 3-16) back trajectories show the air mass arriving at Killeen had recently travelled over the Austin metropolitan area. These two days are characterized by light, shifting winds and high regional background ozone levels (~60 ppb).  Given the stagnant winds on May 16 and the southerly winds on May 17, it is likely that both local (Killeen/Temple) and regional sources (Austin urban plume on May 17) as well as high levels of incoming background ozone contributed to high MDA8 concentrations at the Killeen CAMS 1047 monitor.

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[23] http://www.tceq.state.tx.us/cgi-bin/compliance/monops/8hr_monthly.pl
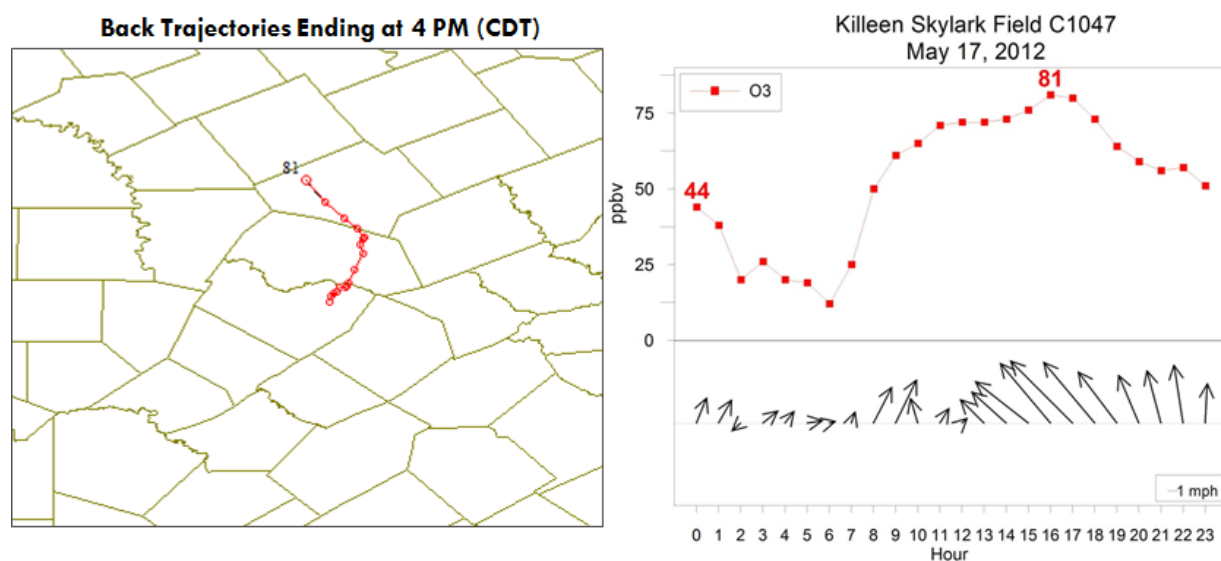
**Figure 3-11. As in Figure 3-8, for May 17, 2012.**

### 3.3.4.3   August 10-11

August 10-11 were part of a multi-day period of high ozone in East Texas that lasted from August 6-14 and was more severe in the DFW area, and briefer and less intense in Houston.  On August 10, the Killeen CAMS 1047 had peak 1-hour ozone of 87 ppb at 1 pm (Figure 3-12). Five DFW monitors and the Lake Georgetown Austin monitor also measured high ozone (MDA8 ≥ 75 ppb) on this day, but areas further south (Fayette County CAMS 601 monitor, Houston area) did not (Figure 3-13; Parker et al., 2013). Back trajectories show northeasterly winds just prior to the peak 1-hour ozone concentrations at Killeen CAMS 1047 (Figure 3-12; Figure 3-16).   The aloft trajectories show relatively strong winds from the northeast whereas the near-surface trajectories show a slower, clockwise, circling wind pattern that transports air from the west and further south to the Killeen CAMS 1047 monitor. The Killeen CAMS 1047 back-trajectory shows differences between the near surface and aloft HYSPLIT trajectories, indicating the presence of vertical wind shear.

No monitor in the Austin area had high ozone except the Lake Georgetown CAMS 690 monitor, which has a 1-hour ozone time series that is similar in shape and magnitude to that of Killeen CAMS 1047, but with a two hour phase delay (Figure 3-13; Parker et al., 2013).  The Killeen CAMS 1047 1-hour ozone peak occurred 4 hours before the Waco CAMS 1037 peak, so it is unlikely that the Killeen CAMS 1047 1 pm peak is associated with transport from DFW on August 10. The origin of the 1-hour peak at Killeen CAMS 1047 and the peak that occurred two hours later at Lake Georgetown CAMS 690 is not clear.  HYSPLIT back trajectories for Killeen CAMS 1047 pass in the vicinity of the DFW and Waco urban areas.  Regional background ozone exceeded 60 ppb on August 10 (Figure 3-13).
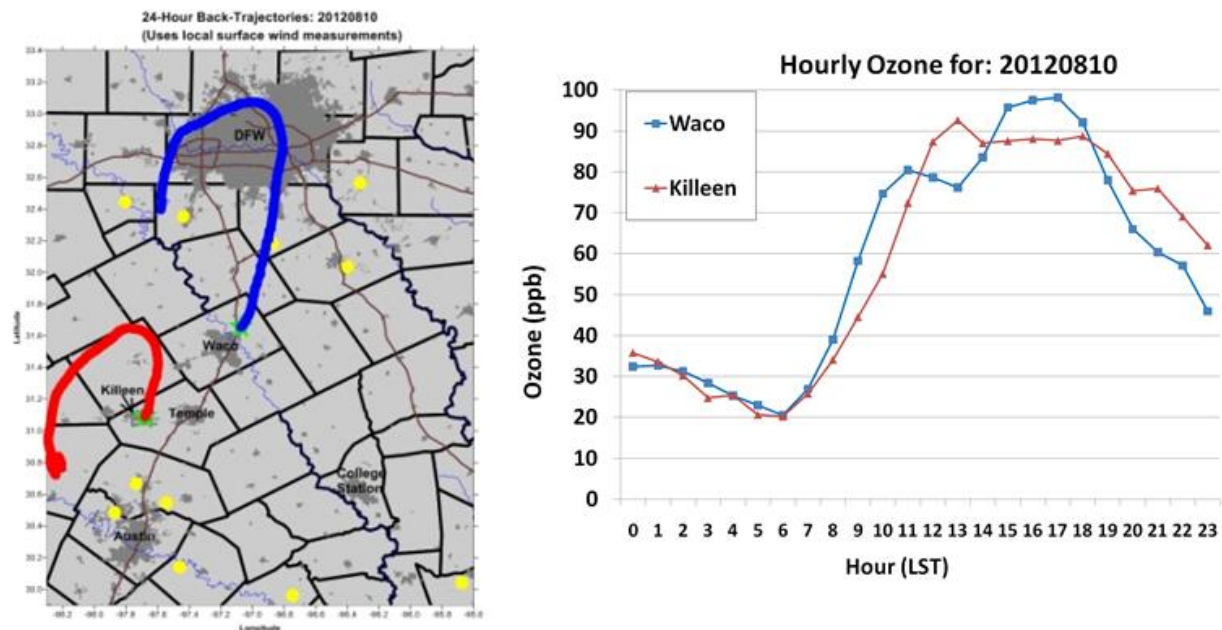
**Figure 3-12. As in Figure 3-6, for August 10, 2012.**
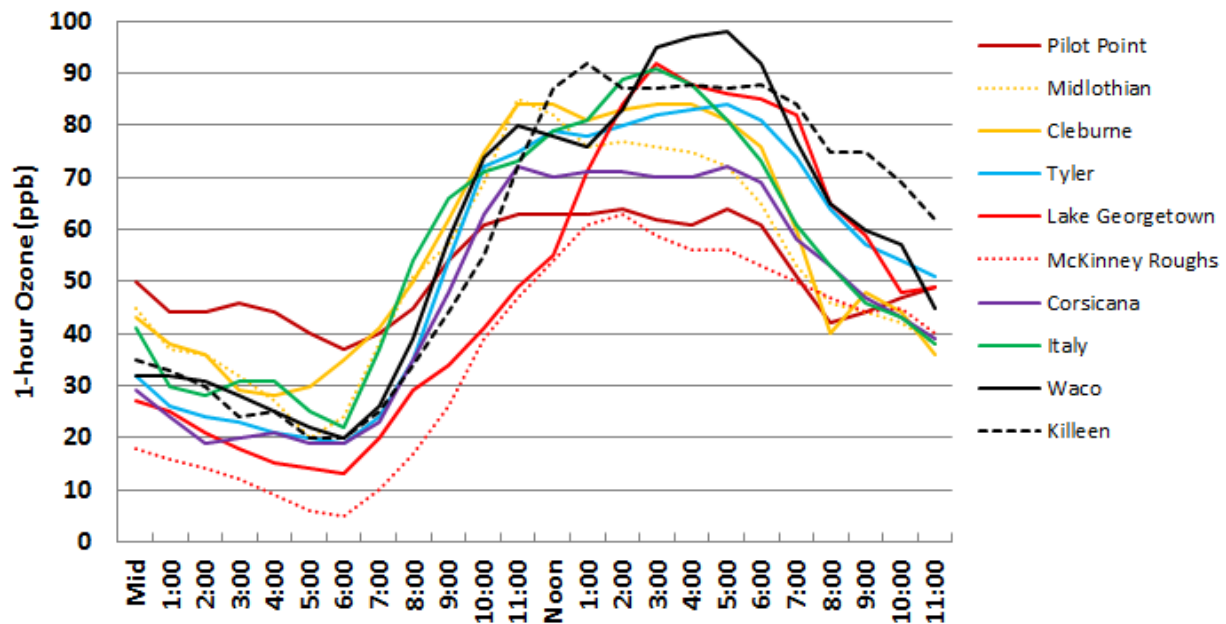


**Figure 3-13. 1-hour ozone time series for Waco Mazanec CAMS 1037 and Killeen Skylark CAMS 1047 monitors and selected East Texas ozone monitors. Dallas-Fort Worth area monitors are shown in orange except Corsicana (purple) and Italy (green). Austin area monitors are shown in red. Figure from Parker et al. (2013).**

On August 11, regional ozone levels remained high; the DFW, Austin and Northeast Texas areas had monitors with MDA8>75 ppb.  Waco CAMS 1037 and Killeen CAMS 1047 have similarly shaped time series except that Killeen CAMS 1047 is consistently about 10 ppb higher than Waco CAMS 1037 throughout the afternoon (Figure 3-14). The MDA8 at Killeen CAMS 1047 was 76 ppb.

The back trajectories (Figure 3-14, Figure 3-16) indicate that winds were northeasterly and steady and also that Killeen CAMS 1047 was downwind of both the Waco and Temple urban areas; this may account for ozone at Killeen CAMS 1047 being higher than ozone at Waco CAMS 1037. On August 11, both the Waco CAMS 1037 and Killeen CAMS 1047 monitors were affected by high regional ozone levels, with enhancements at each monitor due to different sources:  a power plant impact for Waco CAMS 1037 and a possible Waco and/or Temple urban plume impact for Killeen CAMS 1047.

### 3.3.4.4  August 20

On August 20, DFW, Houston, Austin and San Antonio monitors had high ozone as well as Killeen CAMS 1047.  1-hour ozone concentrations at Killeen CAMS 1047 were consistently higher than at Waco on this day, and in the late afternoon Killeen CAMS 1047 was about 15 ppb higher than Waco (Figure 3-15). Back trajectories (Figure 3-15, Figure 3-16) show northeasterly winds, with Killeen CAMS 1047 generally downwind of DFW. The surface level back trajectories for Killeen CAMS 1047 extend back through the DFW area.  The Killeen CAMS 1047 aloft back trajectories, however, pass over the central DFW metropolitan area, while the surface back trajectories pass just west of the DFW area. The Killeen CAMS 1047 back trajectories for both near-surface and aloft levels pass through the Waco and Temple urban areas.  The increased ozone at Killeen CAMS 1047 relative to Waco may therefore be due to greater influence of the DFW urban plume and/or additional contribution from the Waco and Temple urban plumes.

### 3.3.5  Summary of 2012 Ozone Season

Comparison of the HYSPLIT back trajectories for the 10 highest days during the 2012 ozone season (Figure 3-16) with Figure 3-5 shows that the days with MDA8 > 70 ppb during the 2012 are reasonably representative of the entire population of Killeen CAMS 1047 high ozone (MDA8 > 70 ppb) days from 2009-2014. Winds from the north, northeast, and south as well as stagnant days occurred in 2012.  During the 2012 ozone season, the Killeen CAMS 1047 monitor was influenced by the DFW, Austin, San Antonio, Victoria and Corpus Christie urban plumes as well as transport from Northeast Texas.  However, transport from the Houston-Galveston-Brazoria area on a day when the MDA > 70 ppb at the Killeen CAMS 1047 monitor is not represented in the 2012 ozone season.

June 2012 has three high ozone days with a mix of stagnant winds and northeasterly and southeasterly winds.  There are days with winds from the south and north during this episode, but they do not have observed MDA8 > 70 ppb at the Killeen CAMS 1047 monitor.  Therefore, transport from the Austin/San Antonio and DFW areas on high ozone days would not be

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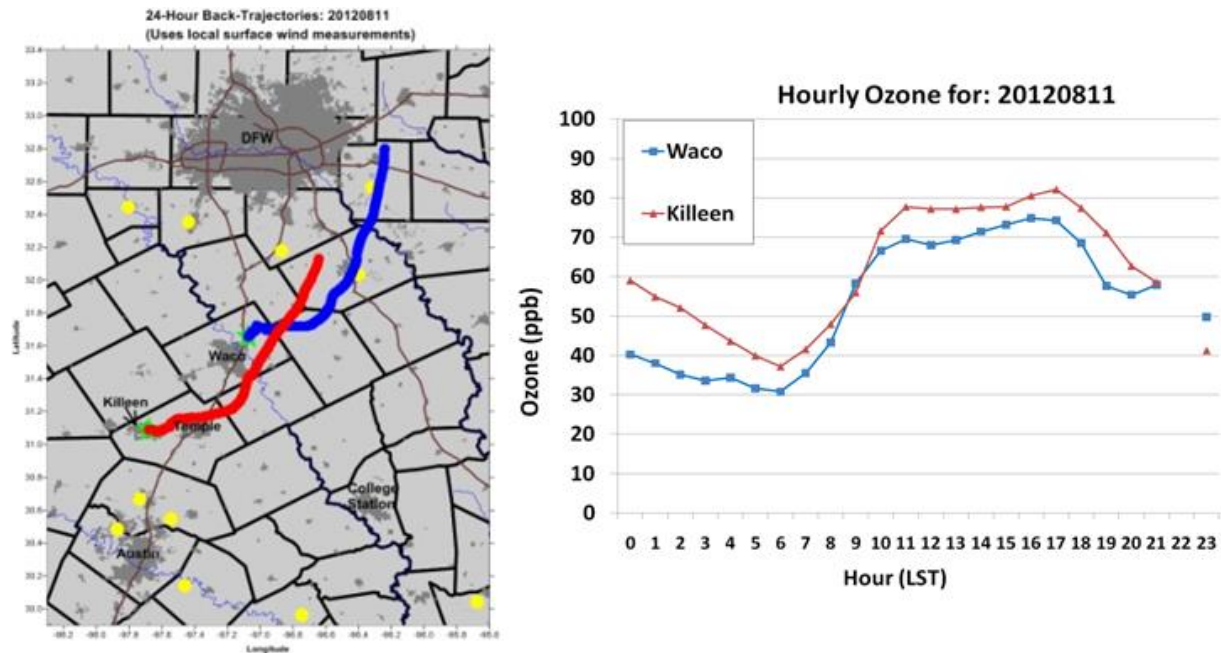


**Figure 3-14. As in Figure 3-6, for August 11. 2012.**
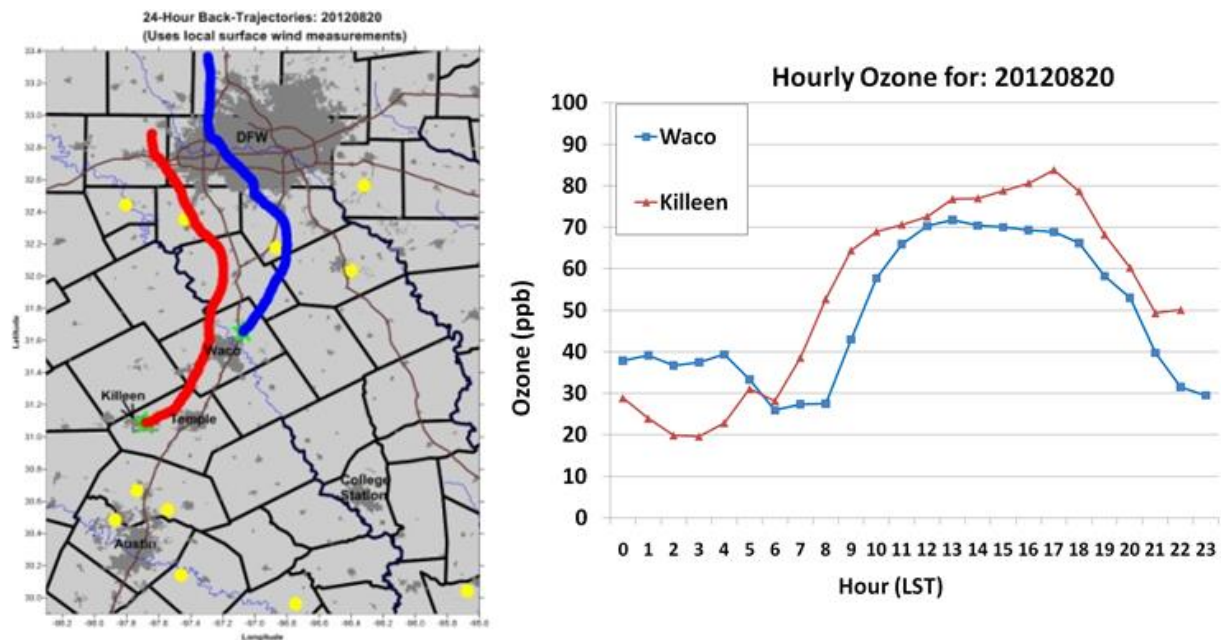


**Figure 3-15.  As in Figure 3-6, for August 20, 2012.**

modeled and these areas have been shown to contribute to high ozone at Killeen CAMS 1047 in both ozone source apportionment modeling (Parker et al., 2013) and ambient data analyses (Kemball-Cook et al., 2015).  We conclude Criterion 4 is better addressed if the entire 2012 ozone season is modeled rather than June 2012 only.

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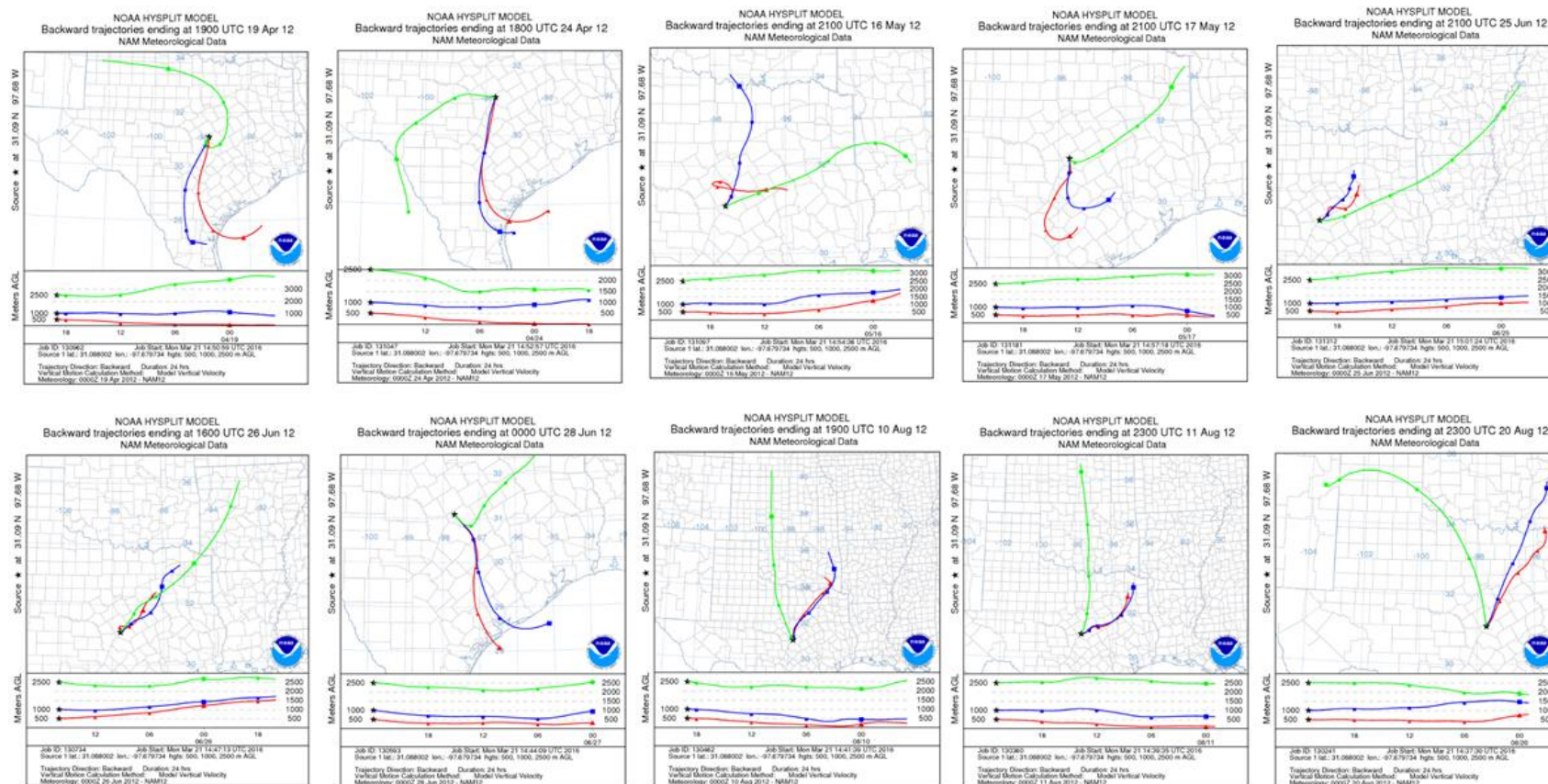


**Figure 3-16. HYSPLIT 24-hour back trajectories using the NAM 12 km Analysis ending at 500 m, 1,000 m and 2,500 m above the Killeen CAMS 1047 monitor. The days shown had the 10 highest values of the MDA8 ozone at the Killeen CAMS 1047 monitor during the 2012 ozone season.**

## 3.4   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, 2, and 3, but not Criterion 4, because some source-receptor relationships did not occur on days with MDA8 > 70 ppb at the Killeen CAMS 1047 monitor during June 2012.  For example, there is no day with southerly or northerly winds and MDA8 > 70 ppb at the Killeen CAMS 1047 monitor during June 2012.  Analysis of the 2009-2014 high ozone days and ozone source apportionment modeling (Figure 3-16, Parker et al., 2013) shows that the Austin and DFW urban plumes can contribute to ozone at the Killeen CAMS 1047 monitor during periods of southerly and northerly winds, respectively. While the June 2012 episode remains useful for air quality planning and analysis for the KTF Area, 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 greater number of days with MDA8 close to the Killeen CAMS 1047 base year 2012 design value for an attainment demonstration, if that were to become necessary for the KTF Area.

## 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 Model of Emissions of Gases and Aerosols from Nature (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[24].

## 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

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[24]

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

other users;  however, following the release of its successor, WRF, MM5 is no being longer 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, and fire 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 MEGAN model (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 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 this ozone modeling study, 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 the KTF Area 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 KTF Area 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 KTF 7-county area, and includes nearby electric generating units (EGUs), as well as the DFW and Austin urban areas that can influence ozone at the Killeen CAMS 1047 monitor. The KTF Area conceptual model (Kemball-Cook et al., 2015) also indicates that transport from the Houston-Galveston-Brazoria nonattainment area can affect the Killeen CAMS 1047 monitor. 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 the KTF Area, 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 a balance between computational efficiency and accuracy in simulating processes that determine ozone levels in Central 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[25]. 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 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.

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

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**Table 5-1. WRF and CAMx model layer structure. TCEQ figure[26].**

## 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 |

(Right side charts: "All 28 Layers" with vertical axis from 0 to 16000; "Lower 21 Layers" with vertical axis from 0 to 3500.)

- AGL - Above Ground Level.

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

## 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. Additional WRF modeling may be necessary in FY16-17 to refine WRF model performance and thereby improve ozone performance at the Killeen CAMS 1047 monitor. Therefore, we outline the model performance evaluation strategy for any WRF modeling that is performed by Ramboll Environ during the KTF Area 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.

**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<br>4 km: 3-D and surface |
|   **Winds** | $3\times10^{-4}$ |
|   **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** | $6\times10^{-4}$ |
|   **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)<br>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.  We will evaluate the initial TCEQ WRF run and any new WRF runs performed for the KTF ozone modeling 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 Central Texas such as the CAMS 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 the KTF Area and regions that are often upwind on high ozone days at the KTF Area monitors.  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 the initial TCEQ 2012 WRF run and 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).
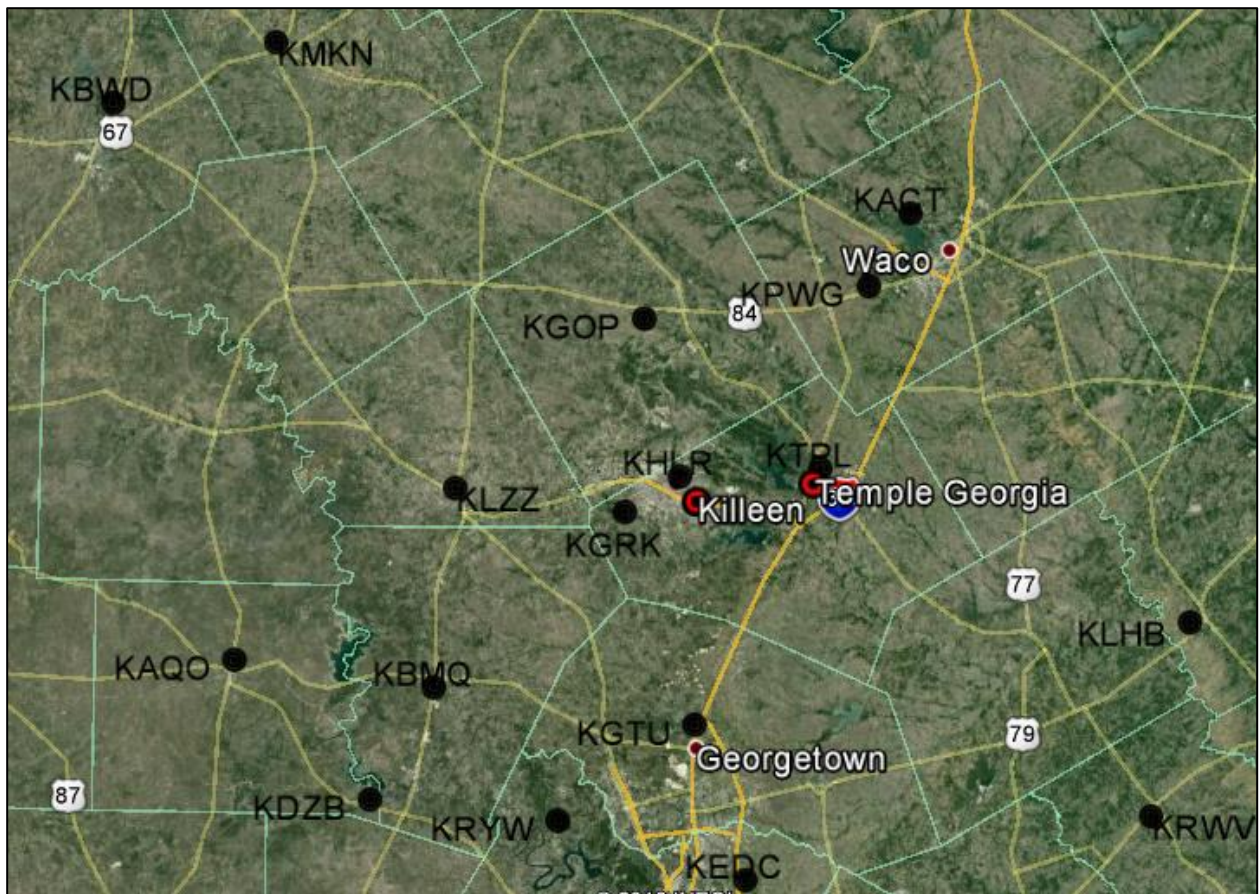
**Figure 6-1. Map of KTF Area and surrounding counties showing ds3505 airport monitoring locations (black circles) and KTF Area CAMS (red circles).**
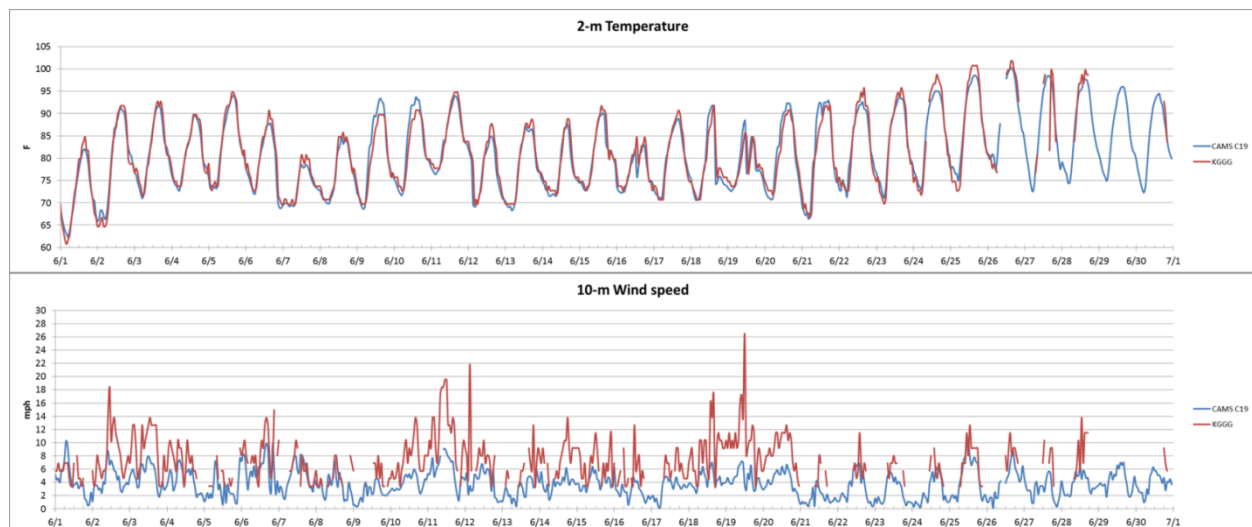


**Figure 6-2. Time series of observed 2-m temperature (top) and 10-m wind speed (bottom) at the Longview CAMS 19 (blue) and East Texas Regional Airport (red) monitoring sites.**

WRF v3.7.1 Temperature at All Sites; June 1-30, 2012
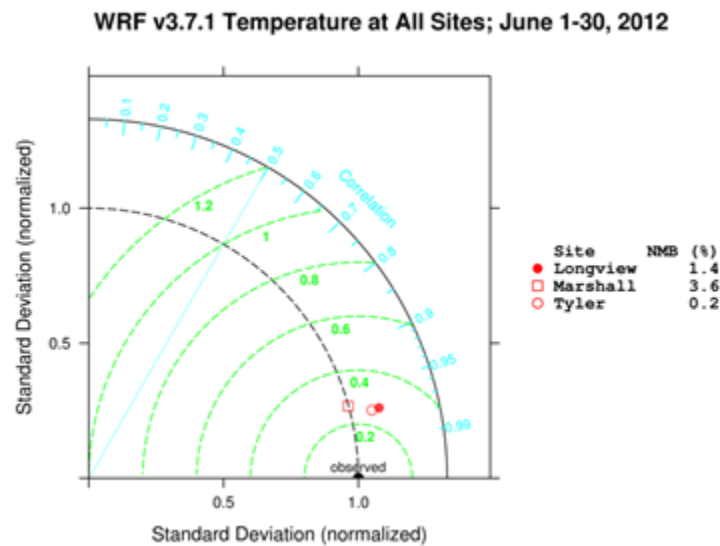
**Figure 6-3. Example of statistical evaluation comparing multiple WRF simulations. June 2012 Taylor diagrams for the W0 (filled circle), W4 (square) and W5 (open circle) WRF simulations for near-surface wind speed at the KGGG (left), KTYR (middle) and KASL (right). Figure from Johnson et al. (2015).**

WRF daily precipitation totals can be evaluated by comparing them with daily PRISM (Parameter-elevation Relationships on Independent Slopes Model[27]) 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. An example of a WRF precipitation evaluation from Johnson et al. (2015) is shown in Figure 6-4.

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[27] ftp://rattus.nacse.org/pub/prism/docs/appclim97-prismapproach-daly.pdf
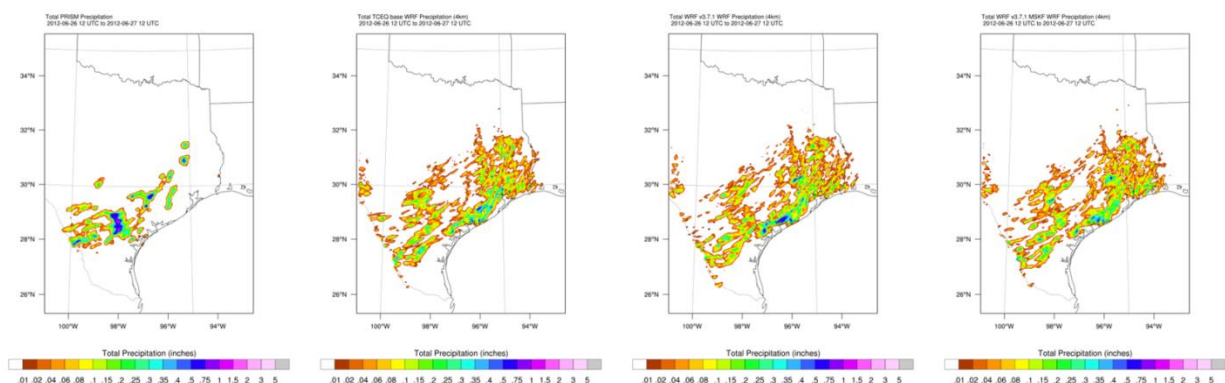
**Figure 6-4. Example of precipitation evaluation. June 26, 2012 precipitation comparison. From left to right: PRISM daily precipitation total and WRF daily precipitation totals for three different WRF simulations labelled W0, W4 and W5.**

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 1-hour average ozone values at the Central Texas monitors (Kemball-Cook et al., 2015). An example of comparison of observed and modeled cloud fields is shown in Figure 6-5.
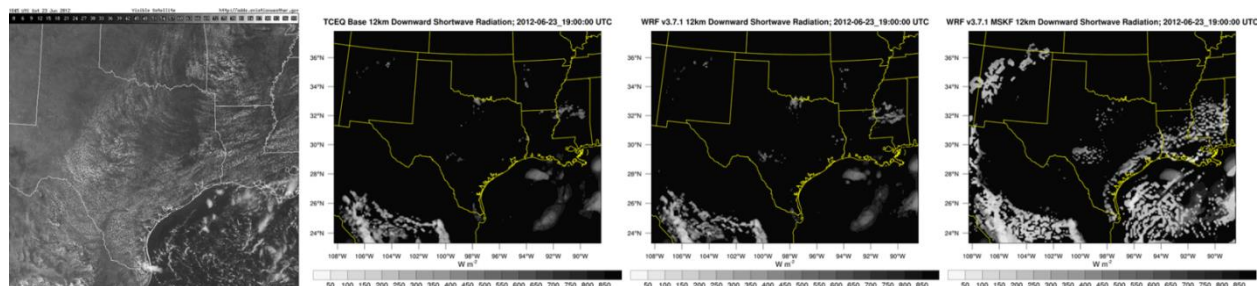


**Figure 6-5. GOES visible satellite image (left panel) and WRF 12 km grid DSW for the W0, W4 and W5 (right panels) simulations for June 23, 2012, 19 UTC.**

Each new WRF run will be compared to observations and previous model runs for the episode (i.e. the initial TCEQ run). The best-performing run will be used in subsequent CAMx air quality modeling. Depending on the outcome of the model performance evaluation, the CTCOG Air Quality Advisory Committee may elect to refine WRF model options or input data and perform additional runs in order to improve model performance over the KTF Area. Results from the local and regional evaluations may suggest any necessary modifications needed in the WRF configuration.

## 7.0 CAMX AIR QUALITY MODELING

In this section, we describe air quality model configuration and inputs for the KTF Area 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 ozone modeling of the June 2012 episode. If a new version of CAMx is released during the KTF Area 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 the KTF Area or regions that may influence it.

### 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 at the Killeen CAMS 1047 monitor.

## 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 Central 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 CTCOG, TCEQ 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 KTF Area 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 Ramboll Environ with emphasis on performance in the KTF Area.  Ramboll Environ's evaluation focused on the Killeen CAMS 1047 monitor and is documented in Johnson et al. (2015) and Kemball-Cook et al. (2015).  New CAMx runs aimed at improving model performance the Killeen CAMS 1047 monitor 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 the KTF Area.  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.

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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. 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) | $$\frac{\sum_{i=1}^{N}\left|P_i - O_i\right|}{\sum_{i=1}^{N}O_i}$$ | Reported as % |
| Root Mean Square Error (RMSE) | $$\left[\frac{1}{N}\sum_{i=1}^{N}\left(P_i - O_i\right)^2\right]^{1/2}$$ | Reported as % |
| Mean Error (ME) | $$\frac{1}{N}\sum_{i=1}^{N}\left|P_i - O_i\right|$$ | Reported as concentration (e.g., ppb) |
| Mean Bias (MB) | $$\frac{1}{N}\sum_{i=1}^{N}\left(P_i - O_i\right)$$ | 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.

### 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 KTF Area 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 8-3, Figure 8-4, and Figure 8-5)
  - Animations of predicted ozone and precursor concentrations for periods of interest (not shown)
- Comparison of observed and predicted precursor emissions or species concentrations.
- Comparison of model performance among different runs using statistical metrics displayed in Taylor Diagrams (Figure 6-3).

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.
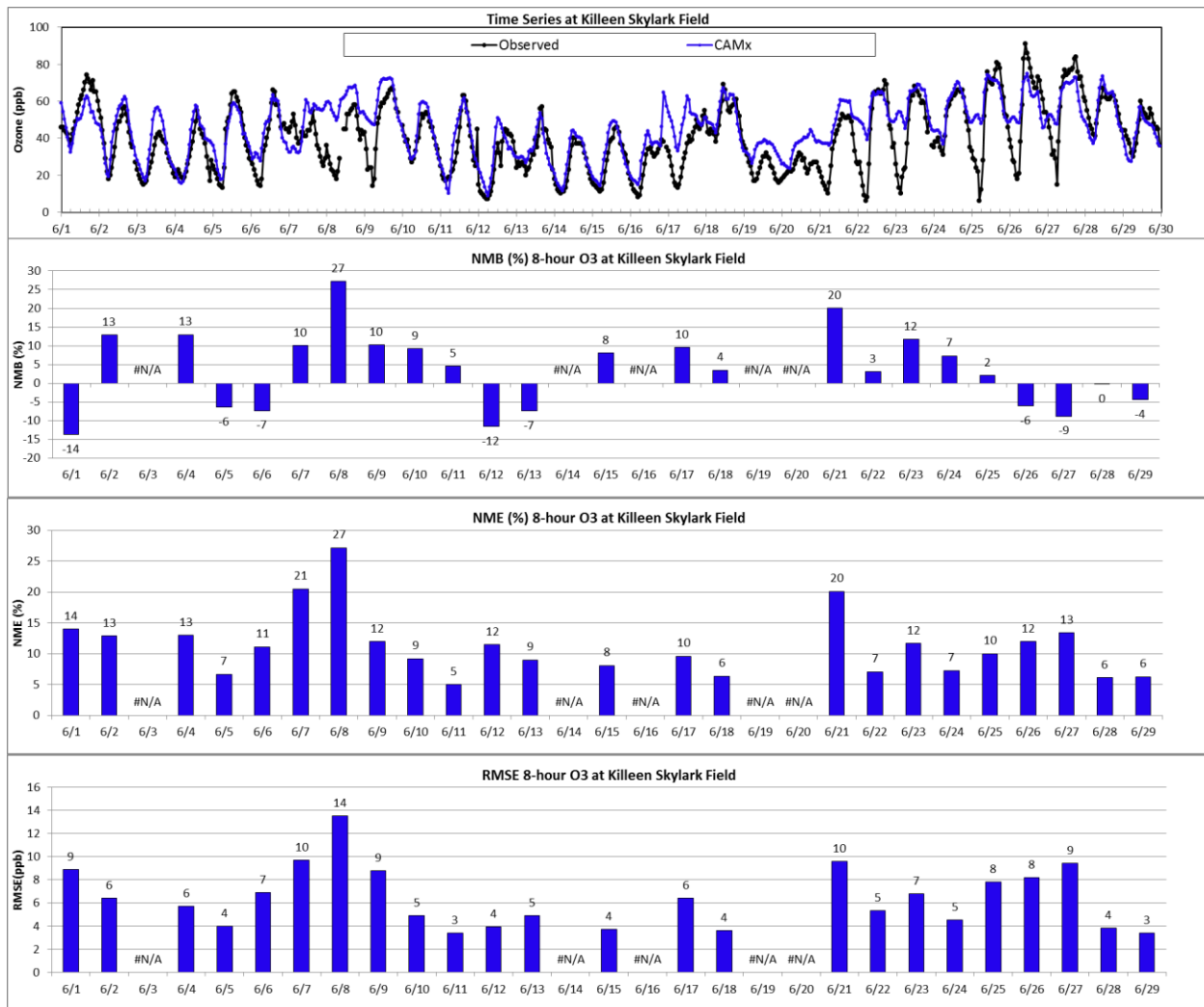
**Figure 8-1. Top panel: observed 1-hour ozone (black) at the Killeen CAMS 1047 monitor versus modeled 1-hour average surface layer ozone during the June 1-29, 2012 period. Lower three panels: normalized mean bias (NMB), normalized mean error (NME) and root mean squared error (RMSE) for the Killeen CAMS 1047 monitor.**

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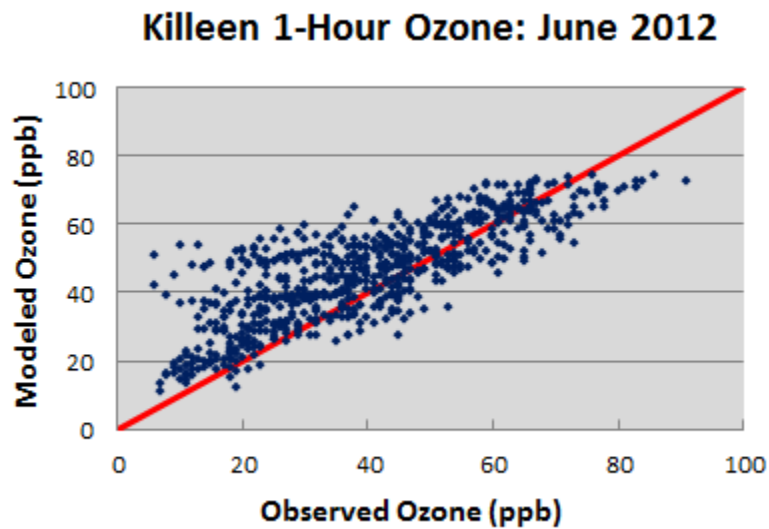


**Figure 8-2. Scatter plot comparison of predicted and observed daily maximum 8-hour ozone concentrations during June 2012 at the Killeen CAMS 1047 monitor.**
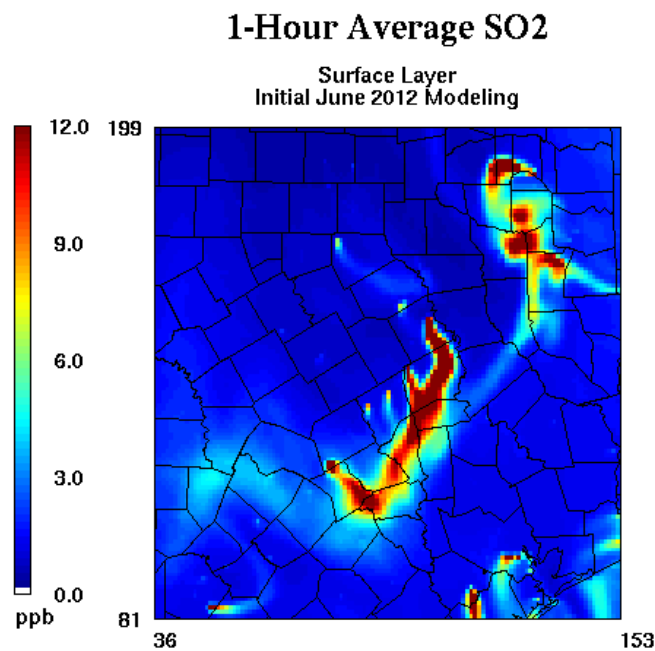


**Figure 8-3. CAMx SO$_2$ concentrations for June 26, 2012 at 10:00 CST, time of 1-hour ozone maximum at the Killeen CAMS 1047 monitor.**

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## 1-Hour Average Ozone

### Surface Layer
### Initial June 2012 Modeling
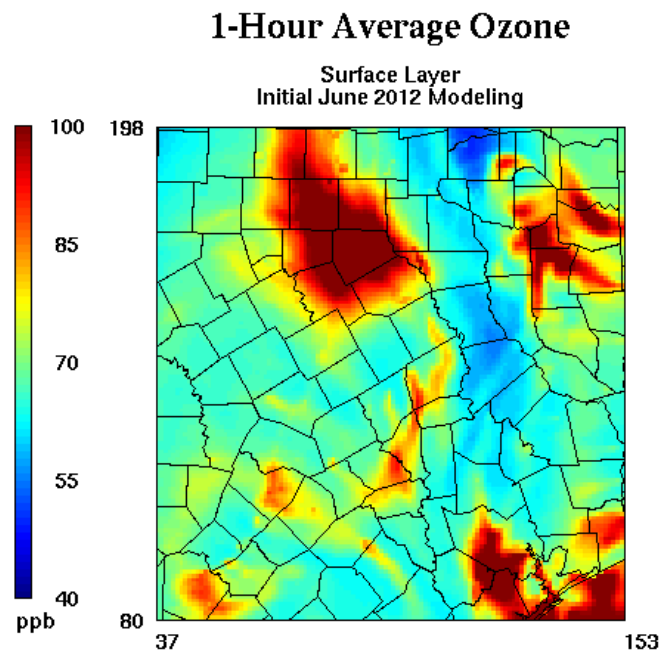


**Figure 8-4. CAMx ozone concentrations for June 26, 2012 at 10:00 CST, time of 1-hour ozone maximum at the Killeen CAMS 1047 monitor.**

## 1-Hour Average NOx

### Surface Layer
### Initial June 2012 Modeling
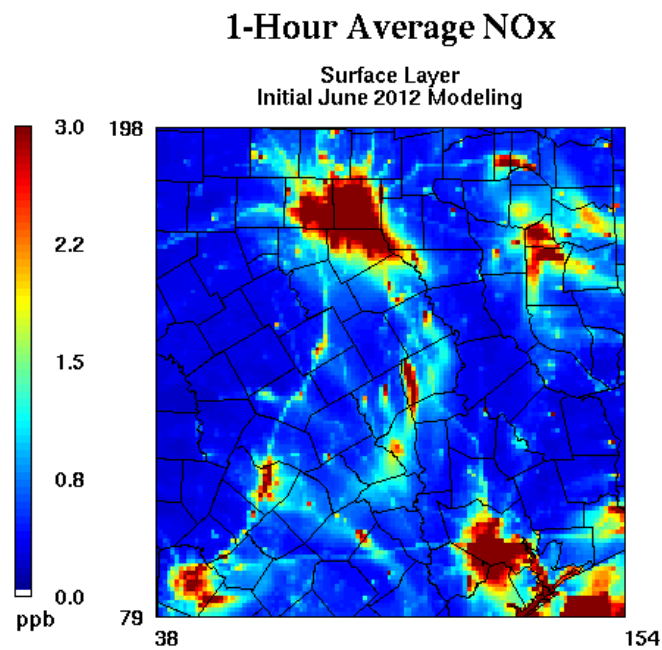


**Figure 8-5. CAMx NOx concentrations for June 26, 2012 at 10:00 CST, time of 1-hour ozone maximum at the Killeen CAMS 1047 monitor.**

## 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 8-6 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 Killeen CAMS 1047 monitor.
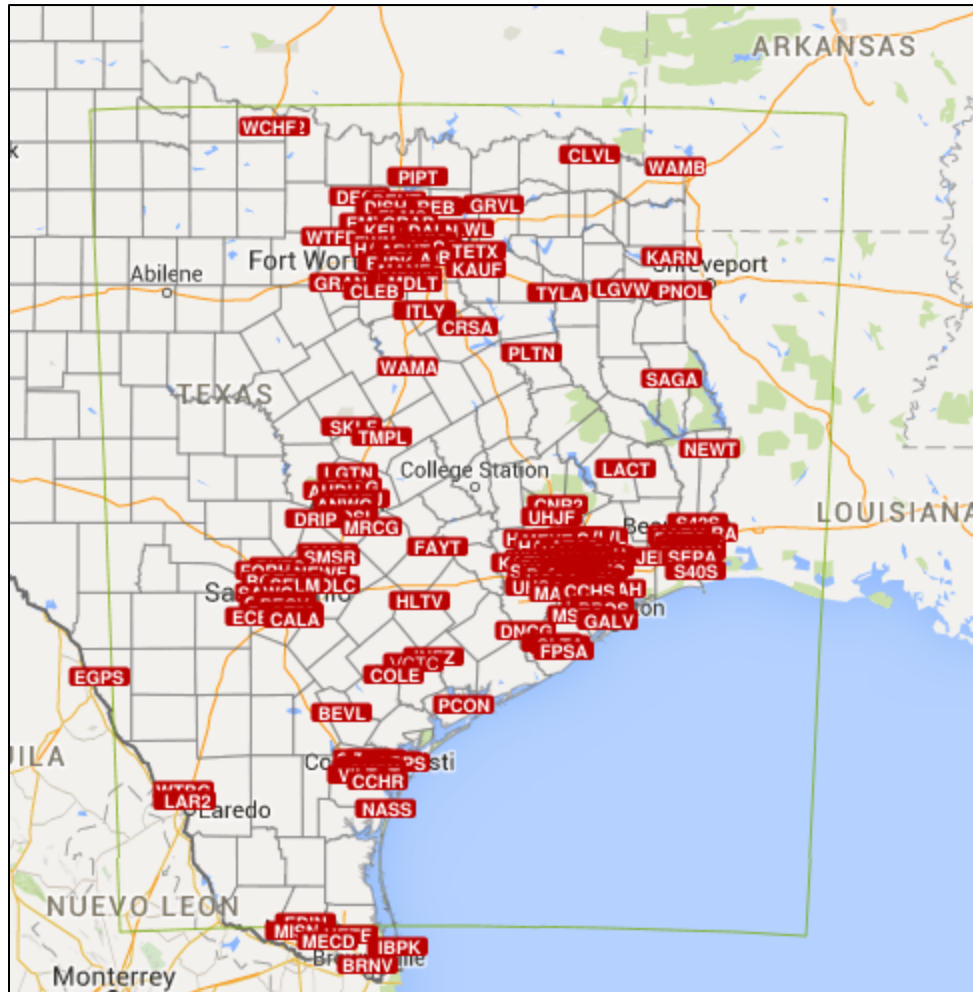


**Figure 8-6. TCEQ CAMS on 4 km grid, which is outlined in light green.  Note that not all monitors shown have data available for June 2012.  Green outline shows the 4 km CAMx modeling domain. TCEQ figure[28].**

We will evaluate the model's simulation of ozone transport into the KTF Area by assessing model performance in areas upwind of the 7-county area 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

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

against ground level observations from Clean Air Status and Trends Network (CASTNET) sites within the 36 km grid (Figure 8-7) and rural/suburban sites in the EPA AQS network (not shown).



**Figure 8-7. CASTNet Sites. EPA figure.**[29]

## 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.

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

### 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 the CTCOG Air Quality Advisory Committee and TCEQ staff in periodic telephone conferences.

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 new sources of emissions within the area,
- 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 8-8.
- sensitivity to reductions/increases in anthropogenic VOC and/or NOx emissions from specific urban areas and source regions (e.g., distant or local).
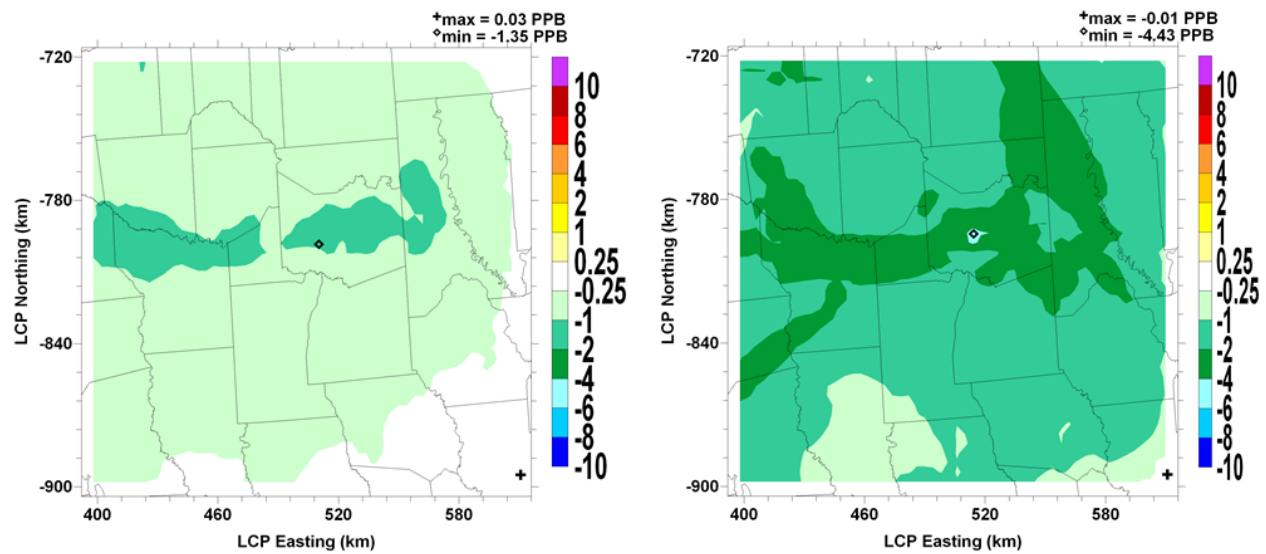
Figure 8-8. Change in 8-hour average surface layer ozone for 30% reduction in on-road mobile source NOx emissions.   Left hand panel:  Average change in 8-hour ozone.  Right hand panel: Maximum change in 8-hour ozone.  Differences calculated only for times when the surface layer ozone concentration was > 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 the KTF Area as well as the transport of ozone and precursors into the region.  The model will be used to carry out supplemental analyses.  The goal of the supplemental analyses is to provide the CTCOG Air Quality Advisory Committee and the TCEQ with information regarding emissions control strategies that will reduce ozone levels in the KTF Area 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 KTF Area 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 the KTF Area.

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 KTF Area Ozone Modeling Study

APCA will be used to determine source regions and emissions source categories that contribute to high modeled ozone at KTF Area ozone monitors during the June 2012 simulation. The KTF Area 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 Central 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).

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 2012 is shown in Figure 9-1.  The green bar shows the contribution to the Killeen CAMS 1047 MDA8 from emissions sources within the 7-county KTF Area.  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 7-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.
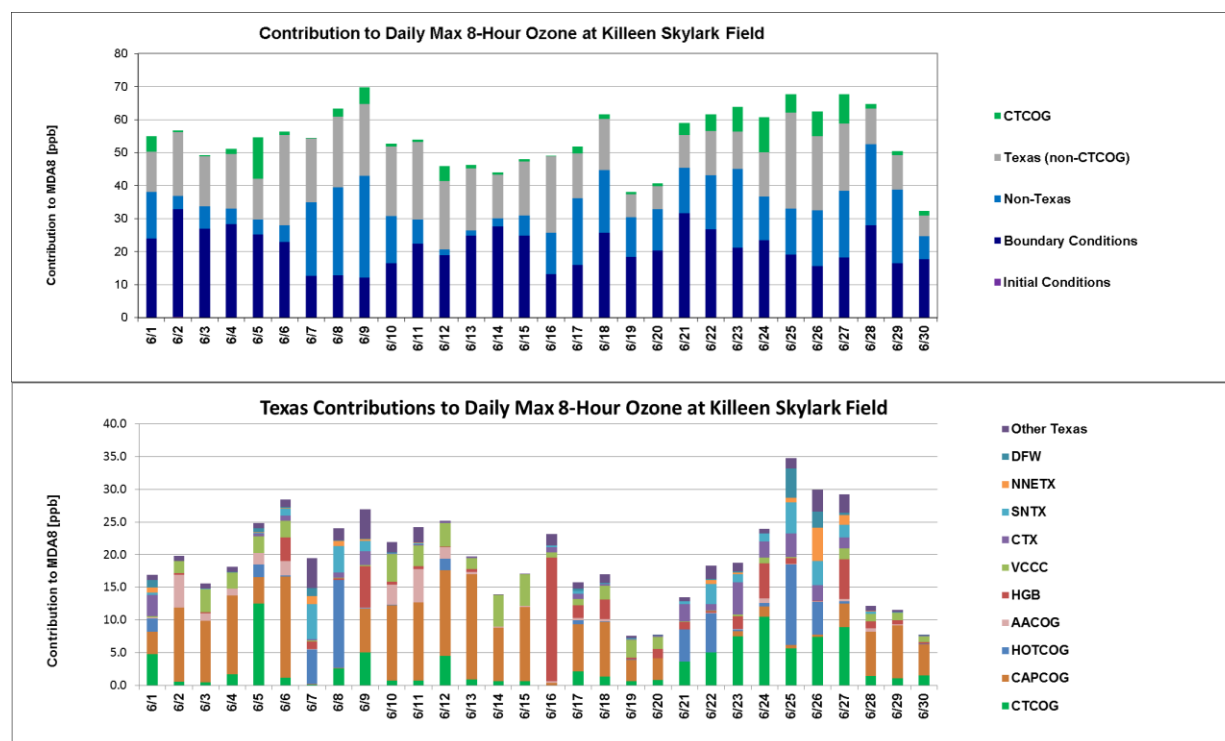


**Figure 9-1. Example of CAMx APCA results for the June 2012 episode.**

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 (Kemball-Cook et al., 2014b). 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.

## 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 KTF Area 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 KTF Area analysis, if the effect of an emissions change on ozone at the Killeen CAMS 1047 and Temple Georgia CAMS 1045 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 TCEQ modeling 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.
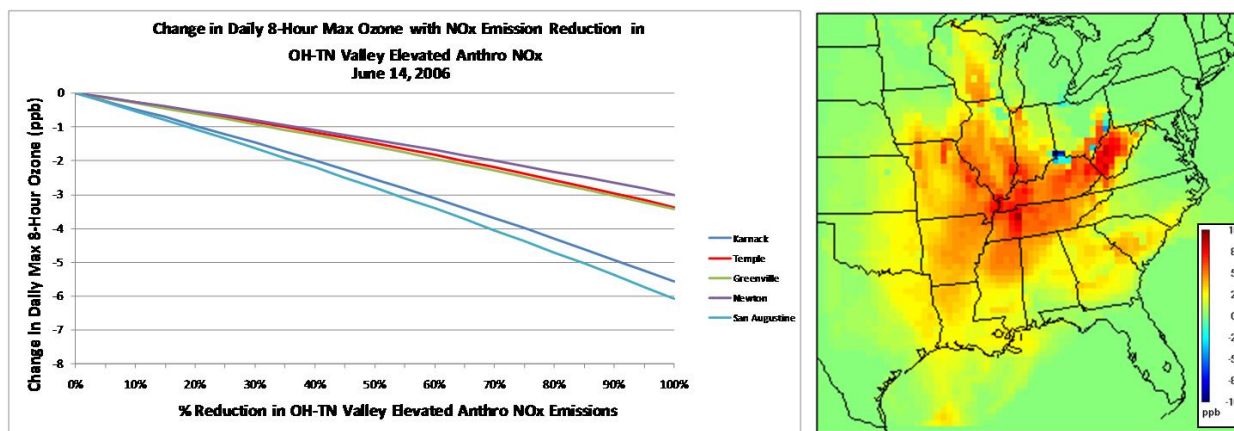
**Figure 9-2. Left panel: Change in daily max 8-hour ozone at rural Texas monitors with NOx emissions reductions from point sources in the Ohio and Tennessee Valleys. Right panel: June 13-15, 2006 average model ozone sensitivity to point source NOx emissions in the Ohio and Tennessee Valleys. Positive (negative) values indicate ozone increases (decreases) if NOx emissions increase (decrease).**

### 9.3.2   Application of the HDDM Tool in the KTF Area Ozone Modeling Study

In the KTF Area 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.

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

1.  The geographic applicability is limited to the 7-county CTCOG 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 the KTF Area 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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