TECHNICAL DESCRIPTION: TCEQ 2012 MODELING PLATFORM

Prepared by the

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List of Acronyms

AFS - AIRS Facility Subsystem Format AGL – Above Ground Level AIRS - Aerometric Information Retrieval System AMDA – Air Modeling and Data Analysis Section AMPD – Air Markets Program Database APCA – Anthropogenic Precursor Culpability Assessment ATR – Automatic Traffic Recorder ARR – Austin-Round Rock **BOEM – Bureau of Ocean Energy Management BPA** – Beaumont-Port Arthur **BEIS - Biogenic Emission Inventory System** BELD3 - Biogenic Emissions Landuse Database, version 3 CAMx - Comprehensive Air Model with Extensions CB6 – Carbon Bond Mechanism, Version 6 CB6r2 – Carbon Bond 6 release 2 CB6r2h – CB6 release 2 with halogen chemistry CC – Corpus Christi CCV – Corpus Christi-Victoria CMAQ – Community Model for Air Quality CSAPR – Cross-State Air Pollution Rule DDM - Direct Decoupled Method DFW - Dallas-Fort Worth DV_B – Baseline Design Value DV_F – Future Design Value EDMS - Emissions Dispersion and Modeling System EGU – Electric Generating Utility **EI** – Emissions Inventory ELP – El Paso EPA – United States Environmental Protection Agency EPS3 – Emissions Processing System, Version 3 ERG - Eastern Research Group ERTAC – Eastern Regional Technical Advisory Committee FAA – Federal Aviation Administration FINN - Fire Inventory from NCAR GEOS-Chem - Goddard Earth Observing Systems Chemistry Model GloBEIS – Global Biosphere Emissions and Interactions System GOES – Geostationary Operational Environmental Satellite GOM - Gulf of Mexico GRIMREAPr - Geo-Referenced Interactive Model Results Evaluation and Analysis Program GWEI – Gulf Wide Emissions Inventory HDDM – Higher-Order Direct Decoupled Method HGB - Houston-Galveston-Brazoria HOT - Heart of Texas HPMS – Highway Performance Monitoring System I/M – Inspection/Maintenance **IPM – Integrated Planning Model** km – Kilometer K_v – Vertical Mixing Coefficient LAI – Leaf Area Index

LAIv - Fractional Vegetated Leaf Area Index LCP – Lambert Conformal conic Projection LRG – Lower Rio Grande Valley LTO - Landing/Take-Off LULC – Land-use Land-cover m – Meters MADIS - Meteorological Assimilations Data Ingest System MATS - Modeled Attainment Test Software MCIP – Meteorology-Chemistry Interface Processor MDA8 – Maximum Daily 8-hour Average MEGAN - Model of Emissions of Gases and Aerosols from Nature MM₅ – Fifth Generation Meteorological Model MODIS - Moderate Resolution Imaging Spectroradiometer MOVES - Motor Vehicle Emission Simulator NAAQS - National Ambient Air Quality Standard NAM – North American Model NASA – National Aeronautics and Space Administration NCAR - National Center for Atmospheric Research NCEP – National Centers for Environmental Prediction NEI – National Emissions Inventory **NET - Northeast Texas** netCDF - Network Common Data Form NMIM - National Mobile Inventory Model NO_x – Nitrogen Oxides NO_Y - Total Oxidized Nitrogen Compounds NLCD – National Land Cover Dataset (NLCD) NWS – National Weather Service **OMI – Ozone Monitoring Instrument ON** – Organic Nitrate OSAT – Ozone Source Apportionment Technology PA – Process Analysis PAR - Photosynthetically Active Solar Radiation PBL - Planetary Boundary Layer PFT – Plant Functional Type PiG – Plume in Grid ppb – Parts per Billion QA – Quality Assurance QC - Quality Control RMSE - Root Mean-Square Error **RPO** – Regional Planning Organizations RRC - Railroad Commission of Texas **RRF** – Relative Response Factor RRTM – Rapid Radiative Transfer Model SAT - San Antonio SIP – State Implementation Plan SMOKE – Sparse Matrix Operator Kernel Emissions STARS - State of Texas Air Reporting System TATU – TCEQ Attainment Test for Unmonitored areas TCEQ – Texas Commission on Environmental Quality TD – Technical Description TDM – Travel Demand Model

TexAER – Texas Air Emissions Repository

TexAQS II – Second Texas Air Quality Study

TexN – Texas NONROAD Model

TOPP – Tropospheric Ozone Pollution Project

tpd – Tons Per Day

TTI – Texas Transportation Institute

TxDOT – Texas Department of Transportation

TxLED – Texas Low Emissions Diesel

U.S. – United States

VIC – Victoria

VMT – Vehicle Miles Traveled

VNA – Voronoi Neighbor Averaging

VOC – Volatile Organic Compounds

WAC - Waco

WRF – Weather Research and Forecasting Model

WSMx – WRF Single-Moment x-Class Microphysics Scheme

YSU – Yonsei University

CHAPTER 1: SUMMARY

This Technical Description (TD) presents procedures the Texas Commission on Environmental Quality (TCEQ) has used to develop a 2012 platform for modeling ozone formation in eastern Texas and also describes work that is underway or planned to improve, expand, and utilize this modeling platform. It is envisioned that this platform will be used in several applications including attainment demonstrations for current and future ozone National Ambient Air Ouality Standard (NAAOS), exceptional event demonstrations, and to provide an alternative to the 2011 modeling platform recently developed by the United States Environmental Protection Agency (EPA). Modeling is being conducted primarily with the Comprehensive Air Quality Model with Extensions (CAMx), which is an acceptable photochemical model (U. S. EPA, 2014), although some modeling using EPA's preferred Community Model for Air Quality (CMAO) is also being conducted. Initially, the TCEO is modeling the five-month period associated with highest ozone concentrations across Texas, May through September, and is considering modeling March and April 2012 as well. Plans also include modeling September 2013, when the National Aeronautics and Space Administration (NASA) conducted an extensive field study in the Houston area. Future case anthropogenic emission inventories will be developed as needed for planning based on the meteorological and biogenic emission inputs for 2012 and optionally 2013.

This document is modeled largely on past modeling protocols and contains the major features of such documents. Because much of the development of the 2012 platform has been completed, the TCEQ is referring to this document by the more descriptive term Technical Description. Subsequent protocols may be based on this document for specific modeling applications such as ozone attainment demonstrations.

Like a modeling protocol, this TD should be considered to be a living document since it represents the state of the 2012 platform at only one point in time and may be revised as the platform continues to evolve to incorporate advances in science, improvements in modeling tools, and new or enhanced inputs.

CHAPTER 2: MODELING/ANALYSIS STUDY DESIGN

This Technical Description (TD) describes the procedures that were used in the development of a modeling platform based on 2012 emissions and meteorology. These procedures generally conform to the recommendations set forth in the United States Environmental Protection Agency's (EPA) *Guidance on the Use of Models and Other Analyses for Demonstrating Attainment of Air Quality Goals for Ozone, PM2.5, and Regional Haze* (EPA, 2007), but also reflect the new draft guidance issued in December 2014: Draft Modeling Guidance for Demonstrating Attainment of Air Quality Goals for Ozone, PM2.5, and Regional Haze (EPA, 2014). As per the 2007 EPA guidance for modeling protocols, this TD includes the following sections:

- background for the study;
- schedule and organizational structure for the study;

- rationale for model selection and description of models to be used;
- methods for developing input data;
- methods for evaluating and interpreting model results; and
- documentation to be submitted to the regional EPA office for review.

2.1 BACKGROUND

Texas currently has two areas that are classified nonattainment of the 2008 eight-hour ozone standard of 75 parts per billion (ppb), specifically the ten county Dallas-Fort Worth (DFW) moderate ozone nonattainment area consisting of Collin, Dallas, Denton, Ellis, Johnson, Kaufman, Parker, Rockwall, Tarrant, and Wise counties with a required attainment date of July 20, 2018¹ and the eight-county Houston-Galveston-Brazoria (HGB) marginal ozone nonattainment area consisting of Brazoria, Chambers, Fort Bend, Galveston, Harris, Liberty, Montgomery, and Waller counties with a required attainment date of July 20, 2015. Other areas in Texas occasionally experience ozone concentrations exceeding or approaching the 2008 NAAQS including the San Antonio, Northeast Texas, and Beaumont/Port Arthur areas, while many areas may not be able to attain the recently-announced 2015 ozone National Ambient Air Quality Standard (NAAQS) of 70 ppb. Figure 1: *Texas Ozone Nonattainment Areas and (1998 Ozone Standard)* Air Quality Planning Areas depicts the two nonattainment areas along with air quality planning areas elsewhere in Texas.

¹ Although the attainment date is July 20, 2018, the attainment year is 2017, which is the last full ozone season prior to the attainment date.



Figure 1: Texas Ozone Nonattainment Areas and (1998 Ozone Standard) Air Quality Planning Areas

Previous modeling for the DFW and HGB areas for the 1997 eight-hour ozone standard (84 ppb) and for DFW under the 2008 standard was based on the 2005-2006 modeling platform which coincided with the Second Texas Air Ouality Study (TexAOS II). While the study provided an extremely rich observational data base for model development and evaluation, both emissions and ozone concentrations have dropped significantly across most of Texas since 2006 and a newer basis for future modeling activities is necessary. The EPA recently developed a 2011 modeling platform that it used for its "Good Neighbor" modeling designed to assist states in complying with the ozone transport requirements of the Clean Air Act for the 2008 ozone NAAOS. While this platform is available to states, the TCEQ has not adopted this for Texas because 2011 was the single-worst drought year recorded in Texas since 1895. Figure 2: May through October Average Temperature and Precipitation Ranks, 1895-2011, copied from the EPA's modeling Technical Support Document (U.S. EPA, 2015) illustrates graphically that Texas (along with Oklahoma, New Mexico, and Louisiana) suffered the hottest summer in the 117-year span 1895 through 2011, while the entire Southeast, southern portions of the Midwest, and Arizona were exceptionally hot. While any single year will show local meteorological anomalies, for Texas 2011 is unacceptable for use in

regulatory applications since any conclusions resulting from modeling this extremely atypical year would not likely apply for more normal years.



Figure 2: May through October Average Temperature and Precipitation Ranks, 1895-2011 (<u>http://www.ncdc.noaa.gov/temp-and-precip/us-maps</u>)

2.2 MANAGEMENT STRUCTURE

The Air Modeling and Data Analysis (AMDA) section has the responsibility for planning and conducting the ozone State Implementation Plan (SIP) modeling. AMDA is part of the Air Quality Division of the TCEQ Office of Air. The Office of Air organization chart is shown in Figure 3: *TCEQ Management Organization Chart*.



Figure 3: TCEQ Management Organization Chart

2.3 TECHNICAL AND POLICY ORGANIZATIONS

Because the modeling described in this TD is being developed to serve as a platform for all of eastern Texas, many areas that have air quality concerns may be affected by the outcome of the modeling. The TCEQ plans to share modeling data and results with any organization that requests such, and will keep local intergovernmental bodies apprised of developments as the modeling develops. The Southeast Texas Photochemical Modeling Technical Committee based in Houston is currently the only organization in the state that functions primarily as a technical committee for SIPrelated activities. The Houston area also is represented by the Houston Area Council of Governments' Regional Air Quality Planning Advisory Committee, which is focused on the policy aspects of the SIP process.

Several organizations in the eastern half of Texas have committees and/or hold meetings that combine technical and policy-related functions. These include the North Central Texas Council of Governments (DFW area) and South East Texas Regional Planning Commission (Beaumont-Port Arthur area), as well as several nearnonattainment (Rider 7) areas: East Texas Council of Governments (Tyler-Longview-Marshall area), Alamo Area Council of Governments (San Antonio area), Capitol Area Council of Governments (Austin Area), Golden Crescent Regional Planning Commission (Victoria area), Central Texas Council of Governments (Killeen-Temple area), Heart of Texas Council of Governments (Waco area), and the Coastal Bend Council of Governments (Corpus-Christi area).

2.4 SCHEDULE OF MODELING ACTIVITIES

The schedule of activities for developing the 2012 modeling platform is shown below in **Error! Reference source not found.**. The dates shown are the best current estimates and are likely to change based on problems encountered, emerging research findings, and other requirements. Detailed discussions of most of these activities can be found later in this document.

Table 1: Schedule of Modeling Activities

Modeling Activity	Time Frame
Conduct base case modeling	April 2014 –
• Complete development of conceptual model for eastern Texas	Spring, 2016
Develop base case emissions	
Conduct meteorological modeling	
Conduct emissions modeling and processing	
Conduct model performance evaluations	
Conduct future base modeling with current controls and project future design values	Spring 2016 –
• Develop future base emissions with applicable growth and current controls	
• Project future design values at all regulatory monitors in eastern Texas	

CHAPTER 3: CONCEPTUAL MODEL OF OZONE FORMATION

Under development.

CHAPTER 4: EPISODE SELECTION

4.1 GUIDANCE

The <u>2007 modeling guidance</u> (EPA, 2007) was developed for the 2008 ozone standard and its guidance on episode selection is rather dated. Because of this, we are choosing to use the <u>2014 Draft Guidance</u> (EPA, 2014) to support selection of dates included in the 2012 modeling platform. The Draft Guidance recommends using a recent base year and notes that:

Ozone based research has shown that model performance evaluations and the response to emissions controls need to consider modeling results from relatively long time periods, in particular, full synoptic cycles or even full ozone seasons (Hogrefe et al., 2000; Vizuete et al., 2011). In order to examine the response to ozone control strategies, it may not be necessary to model a full ozone season (or seasons), but, at a minimum, modeling "longer" episodes that encompass full synoptic cycles is advisable. Time periods which include a ramp-up to a high ozone period and a ramp-down to cleaner conditions allow for a more complete evaluation of model performance under a variety of meteorological conditions.

The modeling period for the 2012 platform (May through September) adheres to these recommendations, and also with the following as is discussed below:

Primary ozone (8-Hour Ozone) - 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.

4.2 BACKGROUND

As discussed in Section2.1 2011 is not an acceptable year for Texas because of the extreme drought, extraordinarily high temperatures, and significant wildfires. 2012 was chosen because it is close to the EPA's 2011 modeling platform chronologically and much of the EPA's base inventory could be easily projected one year into the future.

Figure 4: 75 ppb Eight-Hour Ozone Exceedances by Half-Month for Texas Areas from 1990 through 2014 shows how ozone exceedance days of the 75 parts per billion (ppb) standard have historically peaked in June and then from August through early September. All areas shown, except El Paso, exhibit distinctly bimodal patterns with most exceedance days occurring in the May through June and August through September periods. July typically brings strong onshore flow from the Gulf of Mexico, and the result of this pattern is a pronounced dip in the number of exceedance days across eastern Texas. The period of May through September captures a large majority of the high ozone days across eastern Texas. Notably, the Houston-Galveston-Brazoria (HGB) area has historically seen high ozone days as early as March and as late as November.



Days With Eight-Hour Ozone Over 75 ppb in Texas 1990 Through 2014

Figure 4: 75 ppb Eight-Hour Ozone Exceedances by Half-Month for Texas Areas from 1990 through 2014

Figure 5: 75 ppb Eight-Hour Ozone Exceedances by Half-Month for Texas Areas in 2012 shows the same information as the previous figure except for 2012 only. The distinctive "dip" in ozone exceedances in July is evident, with Dallas-Fort Worth (DFW) peaking somewhat earlier than HGB in both graphs. One unusual characteristic of 2012 is the relatively high percentage of exceedances in March and early April, but otherwise the seasonal ozone patterns are well-aligned with those observed between 1990 and 2014. As time permits, the TCEQ will consider expanding the modeling period to include March and April, as well as October, which observed one exceedance day in HGB and in Beaumont-Port Arthur (BPA).





Figure 6: 75 *ppb Eight-Hour Ozone Exceedance Days by Year for Texas Areas from 1990 through 2014* shows the number of exceedance days for 25 years ending in 2014. Especially notable is the decline in exceedance days from 2005 to 2008. Exceedance days remained low until the exceptional drought year of 2011, which brought an increase statewide, but since that time exceedances per year have decreased. 2012 is seen to be quite representative of the period since 2008, excepting 2011, with relatively high numbers of exceedance days seen in both DFW and HGB.



Figure 6: 75 ppb Eight-Hour Ozone Exceedance Days by Year for Texas Areas from 1990 through 2014 Areas depicted are same as previous figure with addition of Lower Rio Grande Valley (LRG), Victoria (VIC), and Waco (WAC)

4.3 EPISODIC EVALUATION OF 2012 OZONE

Figure 7: *Highest MDA8 Ozone Concentration by Area in 2012* shows time series of area-wide highest maximum daily 8-hour (MDA8) ozone concentrations2 by day for several areas of eastern Texas (excluding far south Texas). Regions are designated as before except that CC and VIC are combined into one (CCV), Hood and Navarro counties are included in DFW along with the 10 counties in the DFW nonattainment area, and the Killeen-Temple-Fort Hood area is combined with the Waco area into a single Heart of Texas (HOT) region. The graph shows several ozone exceedances of the 75 ppb National Ambient Air Quality Standard (NAAQS) between late March and the end of June, and during this period area maximum ozone concentrations in the different areas show a strong correlation, peaking on nearly the same day everywhere. Beginning in July, however, the regional correlation appears weaker.

² The MDA8 value for a monitor is the maximum average value recorded for any eight-hour period on a given day. For example, the peak eight-hour period often occurs during the period of hours 10 through 17, but can occur during any eight consecutive hours during a 24-hour day. The "highest MDA8" ozone concentration for an area is the highest value at any monitor in that area.



Figure 7: Highest MDA8 Ozone Concentration by Area in 2012

To more closely examine the periods of high ozone, the next four figures display the months March through October in two-month segments. Figure 8: *Highest MDA8 Ozone Concentration by Area in March and April 2012* shows a period of high ozone in late March that contained exceedances for HGB (3 days, maximum 113 ppb on March 24), BPA (4 days, maximum 93 ppb on March 24), and DFW (2 days, maximum 84 ppb on March 24). The HGB area also had ozone concentrations greater than 75 ppb on April 6, 7, and 10.

Figure 9: *Highest MDA8 Ozone Concentration by Area in May and June 2012* shows that between May 14 and 22, several areas exceeded 75 ppb: ARR (May 17, 78 ppb), BPA (May 22, 76 ppb), DFW (May 16, 17, 21, and 22, maximum 92 ppb on May 16), HGB (May 14, 15 through 18, 21 and 22, maximum 90 ppb on May 21) and SAT (76 ppb on May 17). In June, both HGB (104 ppb) and DFW (76 ppb) exceeded 75 ppb on June 1. There were also minor exceedances in DFW on June 5 and 8 and in HGB on June 7 and 9.

The major ozone event of 2012, which occurred between June 24 and 28, was preceded by an MDA8 concentration of 83 recorded in DFW on June 22. DFW then exceeded 75 ppb for six straight days with a peak of 110 ppb on June 26, a day on which every area depicted in Figure 9 broke the 75 ppb mark. CCV recorded 84 ppb that day, BPA hit 112 ppb, HGB had 136 ppb (the highest reading of the year anywhere in Texas), ARR reached 87 ppb, HOT saw 78 ppb, NET had 84 ppb, and SAT recorded 89 ppb. June 27 also saw exceedances in every area except CCV.

Both Figure 8 and Figure 9 highlight the high degree of correlation among the different areas' ozone peaks, indicating that ozone during this four-month period was dominated by synoptic-scale meteorological effects that brought ozone-conducive conditions across eastern Texas.



Figure 8: Highest MDA8 Ozone Concentration by Area in March and April 2012



Figure 9: Highest MDA8 Ozone Concentration by Area in May and June 2012

Figure 10: *Highest MDA8 Ozone Concentration by Area in July and August 2012* shows that July was fairly quiet except for some relatively minor exceedances in DFW on July 9, 10, 13, 21 (86 ppb), and 30. Throughout the month of July there appears to be a lower degree of spatial correlation among the areas, with CCV remaining almost flat with values near 20 ppb. In August DFW exceeded 75 ppb on eight of nine days between August 6 and 14, peaking at 109 ppb on August 9. Along with DFW, the

northern portion of eastern Texas experienced high ozone with NET exceeding August 9 through 11 and 14 (maximum 83 ppb on August 11, and HOT seeing exceedances on August 10 and 11 (86 ppb on the latter). The ARR area saw its high MDA8 concentration of the year (94 ppb) on August 11, but SAT did not exceed 75 ppb. The coastal areas of CCV, BPA, and HGB were also largely spared during this period, with only two minor exceedances recorded in HGB on August 6 and 7.

High ozone returned after a short hiatus for a three-day period between August 20 and 22, with two exceedances in DFW (maximum 80 ppb on August 20), two in HGB (maximum 89 ppb), and one in HOT (76 ppb on August 20). SAT exceeded 75 ppb on all three days with a peak concentration of 87 ppb on August 21. Finally, DFW capped the month of August with a reading of 81 ppb on the last day of the month.

Figure 11: *Highest MDA8 Ozone Concentration by Area in September and October 2012* shows relatively fewer and milder ozone exceedances, and shows closer spatial correlation than was evident during the previous two-month period. DFW began the month of September with an 89 ppb one-day episode on September 5, then on September 10 DFW, HGB and SAT exceeded, the latter tying its 2012 peak concentration at 90 ppb. SAT recorded its last exceedance of 2012 (81 ppb) on September 19, then on the following day DFW and HGB began, respectively, three- and five-day periods of relatively mild exceedances (peak for HGB was 87 ppb on September 20). The year's last ozone exceedances occurred on October 3 with BPA recording 78 ppb and HGB seeing 85 ppb.



Figure 10: Highest MDA8 Ozone Concentration by Area in July and August 2012



Figure 11: Highest MDA8 Ozone Concentration by Area in September and October 2012

4.4 SUMMARY OF THE 2012 OZONE SEASON FOR EASTERN TEXAS

The 2012 ozone season started off strong in late March with HGB, DFW and BPA all seeing ozone over the 2008 NAAQS of 75 ppb and HGB seeing its second-highest reading of the year of 113 ppb. The HGB area saw some more minor exceedances in April. Mid-May brought a series of exceedances across most of eastern Texas but none higher than 92 ppb recorded in DFW. After a few days of moderate-to-high ozone in DFW and HGB during the first third of June, the major episode of 2012 arrived a couple of weeks later, culminating in every area shown exceeding on June 26, with the year's highest MDA8 concentration of 136 ppb at the Manvel-Croix Park monitor in HGB. July was very quiet, with only five exceedances, all in DFW.

August 6 through 14 saw widespread ozone over the northern half of eastern Texas, followed by a three day episode beginning on August 20 which affected DFW, HGB, and SAT. The first half of September saw some minor exceedances in DFW and HGB, with SAT tying its annual peak of 90 ppb on September 10. September 19 through 24 brought relatively minor ozone exceedances to first SAT then DFW and HGB, and the 2012 ozone ended on October 3 with minor exceedances in HGB and in BPA.

4.5 CONCLUSION

The 2012 ozone season is representative of recent years in eastern Texas with the possible exception of a rather extreme episode in late March in HGB, DFW and BPA. Since high ozone concentrations were observed in three distant locations, meteorological conditions not usually seen that early in the year were most likely the cause. Because this event is not typical of late winter or early spring, the 2012 modeling platform will not initially include this time period and will begin with May when ozone events typically begin to increase in both frequency and intensity. Both

May through June and August through September include many episodic events typical of their respective time frames. July offers an opportunity to evaluate the model under a different meteorological regime than that characteristic of either May through June or August through September. Because October saw only one day which had mild exceedances in two areas, the modeling platform will not include that month.

In all, the five months May through September 2012 includes 41 days on which an ozone exceedance was recorded in eastern Texas. DFW saw a total of 34 exceedance days with 23 in HGB. SAT saw 8, NET 6, HOT 5, ARR 4, BPA 3, and CCV 1. High ozone in every area was represented to some extent, and well represented in the two current nonattainment areas of DFW and HGB. This period is likely to provide a number of days in most areas of the state with modeled ozone near or over 75 ppb that can be used to calculate relative response factors as per the 2007 and 2014 draft modeling guidance.

CHAPTER 5: MODEL SELECTION

The modeling system is composed of a gridded photochemical air quality model, a meteorological model, and an emissions processing model. Both the meteorological and emissions models provide input to the air quality model. Therefore, the air quality, meteorological, and emission models selected need to interface effectively.

5.1 SELECTION OF AIR QUALITY MODEL

To ensure that a modeling study can be successfully used as technical support for an attainment demonstration State Implementation Plan revision, the air quality model must be scientifically sound and appropriate for the intended application, and be freely accessible to all stakeholders. In a regulatory environment, it is crucial that oversight groups (e.g., EPA), the regulated community, and the interested public have access to and also can be convinced of the suitability of the model. The following three prerequisites were identified for selecting the air quality model to be used in a recent Dallas-Fort Worth attainment demonstration SIP revision:

- must have a reasonably current, peer-reviewed, and scientific formulation;
- must be available at no or low cost to stakeholders; and
- must be consistent with air quality models being used for other Texas nonattainment or near-nonattainment areas.

The only model to meet all three of these criteria is the Comprehensive Air Model with Extensions (CAMx). The model is based on well-established treatments of advection, diffusion, deposition, and chemistry. Another important feature is that nitrogen oxides (NO_x) emissions from large point sources can be treated with the plume-in-grid (PiG) sub-model, which helps avoid the artificial diffusion that occurs when point source emissions are introduced into a grid volume. The model software and the CAMx user's guide are publicly available (http://www.camx.com). In addition, the TCEQ has many years of experience with CAMx. CAMx was used for the recent DFW attainment demonstration SIP revisions, for the Houston-Galveston-Brazoria and Beaumont-Port Arthur areas, as well as for modeling being conducted in other areas of Texas including Austin, San Antonio, and Tyler-Longview-Marshall.

At this time, the TCEQ is using CAMx 6.20, the most recent version available. If subsequent versions are released during development of the 2012 modeling platform, the TCEQ will review each version for potential improvement to the modeling platform. Updated versions of CAMx will likely be used if they offer such improvements and no operational bugs are identified. Compared to version 6.0, CAMx 6.20 includes the following updates:

- optional top boundary conditions input file;
- supports Carbon Bond 6 CB6) release 2 (CB6r2) and CB6r2 with halogen chemistry (CB6r2h);
- extension of the direct decoupled method (DDM) to particulates;
- new surface chemistry and re-emission model; and
- update to the PiG sub-model, which improves speed and total oxidized nitrogen compounds (NOy) mass budget accuracy.

Of particular note is the addition of the CB6r2 and CB6r2h chemistry options. Early work with the June 2012 episode has indicated a strong tendency to over-predict both hourly and Maximum Daily 8-hour Average (MDA8) ozone concentrations, particularly along the upper Texas coast. The CB6r2 chemistry moderates the over-prediction seen with CB6 (release 1) somewhat by partitioning organic nitrates (ON) between gas-phase ON and those ON that can partition into organic aerosols, which then are processed to nitric acid. This in turn increases nitric acid but lessens ozone concentrations. The CB6r2h version adds optional chemistry through which bromine and iodine (halogens) react with ozone over ocean water, further lowering overall ozone concentrations. More information on these updates can be found in Chapter 1 of the <u>CAMx user's guide</u> (Environ, 2015). Henceforth in this document, references to CB6 apply to CB6, CB6r2, and CB6r2h unless otherwise noted.

Significant work has been conducted modeling the June 2012 period prior to modeling the full 5-month period. As will be discussed later in Section Chapter 9: *Model Performance Evaluation*, use of CB6r2h together with selecting appropriate meteorological parameterizations has reduced model over-prediction across eastern Texas and performance is now reasonably good for June, especially in DFW. However, because of over-prediction issues still present in southeast Texas, the TCEQ is testing the Community Model for Air Quality (CMAQ) in an effort to identify and explain the reason for the over-prediction.

The TCEQ plans to use some of the probing tools supported by CAMx 6.20 for sensitivity analyses, including:

Process Analysis (PA) - PA adds algorithms to the CAMx model that store the integrated rates of species changes due to individual chemical reactions and other sink and source processes. By integrating these rates over time and outputting them at hourly intervals, PA provides diagnostic outputs that can be used to explain model simulation in terms of chemical budgets, conversions of chemical species, and effects of transport and other sink and source terms. PA can also improve model validation

and ultimately can assist in the selection of precursor reduction strategies (Tonnesen, 2001).

Ozone Source Apportionment Technology (OSAT) - OSAT provides a method for estimating the contributions of multiple source areas, categories, and pollutant types to ozone formation in a single model run. OSAT also includes a methodology for diagnosing the temporal relationships between ozone and emissions from groups of sources.

Anthropogenic Precursor Culpability Assessment (APCA) - APCA differs from 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 beneficial to identification of potential control strategies. Where OSAT would attribute ozone production to biogenic emissions, APCA reallocates that ozone production to the controllable portion of precursors that participated in ozone formation with the non-controllable precursor. APCA only attributes ozone production to biogenic emissions when ozone formation is due to the interaction of biogenic volatile organic compounds (VOC) with biogenic NO_x. When ozone formation is attributable to biogenic VOC and anthropogenic NO_x under VOC-limited conditions, OSAT would attribute ozone production to biogenic VOC while APCA would redirect that attribution to the anthropogenic NO_x precursors present.

Direct Decoupled Method (DDM) and Higher-Order Direct Decoupled Method (HDDM) – DDM and HDDM provide an efficient and accurate methodology for calculating first-order (via DDM) and second-order (via HDDM) sensitivities between output concentrations and model input parameters.

5.2 SELECTION OF METEOROLOGICAL MODEL

The Weather Research and Forecasting Model (WRF) has gained near-universal acceptance for use in air quality modeling applications. The TCEQ has used WRF version 3.6.1 to develop meteorological inputs for June 2012 and is using 3.7.1 to revise these inputs at this writing. As time and resources allow, newer versions of WRF may be used as they become available to revise these inputs. Updated files with new versions of WRF will first receive a quality assurance review to see if meteorological performance is improved. WRF is supported by a broad user community including the EPA, the Air Force Weather Agency, the National Centers for Environmental Prediction (NCEP), national laboratories and academia, and is currently being used extensively to develop the meteorological inputs for regulatory air quality modeling analyses throughout the United States.

5.3 SELECTION OF EMISSIONS MODELING SYSTEM

Typically, raw emissions inventory databases provide on-road, off-road, non-road, area, biogenic, oil-gas, and point source emission estimates of criteria pollutants, including NO_x and VOC, on an annual, seasonal, daily, and/or hourly basis. The processing of raw emissions data sets into air quality model inputs is accomplished through the use of emission processor tools. These emissions processors temporally distribute, spatially allocate, and chemically speciate the emissions to the resolution and chemical mechanism used by the air quality model. When necessary, emission processors are

also used to apply adjustment factors to specific combinations of county and source types for simulation of control strategy scenarios.

The most common emissions modeling system used to process anthropogenic emissions into the gridded, hourly-resolved, and chemically-speciated inputs needed for an air quality model is Sparse Matrix Operator Kernel Emissions (SMOKE). However, over the last two decades the TCEQ has developed an intricate set of procedures and supporting software that is integrated with the Emissions Processing System, version 3 (EPS3). EPS3 has been used for many air quality modeling projects within Texas, is easily modified to accommodate the complexity of emissions sources and the highly detailed emissions information required, and the TCEQ has years of experience in using EPS3. For on-road emissions inventory development, SMOKE lacks the capability of fully capturing the variable hourly speed associated with vehicle miles traveled (VMT) estimates for each roadway segment from local travel demand models (TDMs). Since vehicle emission rates vary as a function of speed, this is important for obtaining the best possible spatial and temporal resolution of gridded on-road emissions in metropolitan areas.

The biogenic model currently being used is version 2.1 of the Model of Emissions of Gases and Aerosols from Nature (MEGAN). Compared with the Global Biosphere Emissions and Interactions System (GloBEIS) used in previous modeling platforms, MEGAN has shown better isoprene performance in Texas using aircraft measurements and may have emissions estimation advantages for the varying solar radiation and average temperatures that occur at different times of the year. The TCEQ has also conducted modeling using EPA's Biogenic Emission Inventory System (BEIS) and is evaluating its possible use instead of or along with MEGAN.

CHAPTER 6: MODELING DOMAINS

6.1 CAMX MODELING DOMAINS

Figure 12: *CAMx Modeling Domains* depicts the modeling domains currently being used by the TCEQ in CAMx. The horizontal configuration of the CAMx modeling domains is:

- National Regional Planning Organizations (RPO) Domain (outlined in black; also known as the Continental United States or CONUS domain) consists of 36 kilometer (km) × 36 km grid cells covering all of the continental U.S., along with southern Canada, northern Mexico, and portions of the Gulf of Mexico, Atlantic Ocean, and Pacific Ocean;
- **Texas 12 km Domain** (outlined in blue), consists of 12 km × 12 km grid cells covering all of Texas, Arkansas, Louisiana, Oklahoma, along with portions of Alabama, Colorado, Kansas, Kentucky, Mississippi, Missouri, New Mexico, and Tennessee; and
- **Texas 4 km Domain** (outlined in green), consists of 4 km × 4 km grid cells covering most of eastern Texas and small portions of southwestern Arkansas, western Louisiana, southern Oklahoma, and northeastern Mexico.

The Texas 4 km domain is nested within the Texas 12 km domain, which in turn is nested within the National RPO 36 km domain. The National RPO domain is the same

outer domain used in EPA's 2011 modeling platform, which greatly facilitates the sharing of model data among states, RPOs, the EPA, and research organizations that use this modeling domain.



Figure 12: CAMx Modeling Domains

All grids are projected in a Lambert Conformal conic Projection (LCP) with the following parameters:

- Origin: 97° West, 40° North
- First True Latitude (α): 33° North
- Second True Latitude (β): 45° North
- Central Longitude (γ): 97° West
- Spheroid: Perfect Sphere, Radius = 6730 km

The grid dimensions for the CAMx domains are listed in Table 2: *CAMx Modeling Domain Parameters* The locations for the upper right-hand and lower left-hand represent distances (west and south are negative, east and north positive) from the origin, which is by definition location (0, 0) within the LCP projection.

Grid Name	Grid Cell Size	Dimension s (grid cells)	Lower left- hand corner	Upper right-hand corner
National RPO	36 x 36	148 x 112	(-2736, -	(2592,1944)
Texas 12 km	12 x 12	149 x 110	(-984,-1632)	(804,-312)
Texas 4 km Domain	4 x 4 km	191 x 218	(-328,-1516)	(436,-644)

Table 2: CAMx Modeling Domain Parameters

The vertical configuration of the CAMx modeling domains consists of a varying 28layer structure as shown in Table 3: *CAMx Vertical Layer Structure*.

CAM	1x Layer	WRF Laver	Top ³ (m AGL)	Center ³ (m AGL)	Thickness ³ (m)
	28	38	15,179.1	13,637.9	3,082.5
	27	36	12,096.6	10,631.6	2,930.0
	26	32	9,166.6	8,063.8	2,205.7
	25	29	6,960.9	6,398.4	1,125.0
	24	27	5,835.9	5,367.0	937.9
	23	25	4,898.0	4,502.2	791.6
	22	23	4,106.4	3,739.9	733.0
	21	21	3,373.5	3,199.9	347.2
	20	20	3,026.3	2,858.3	335.9
	19	19	2,690.4	2,528.3	324.3
	18	18	2,366.1	2,234.7	262.8
	17	17	2,103.3	1,975.2	256.2
	16	16	1,847.2	1,722.2	249.9
	15	15	1,597.3	1,475.3	243.9
	14	14	1,353.4	1,281.6	143.6
	13	13	1,209.8	1,139.0	141.6
	12	12	1,068.2	998.3	139.7
	11	11	928.5	859.5	137.8
	10	10	790.6	745.2	90.9
	9	9	699.7	654.7	90.1
	8	8	609.7	565.0	89.3
	7	7	520.3	476.1	88.5
	6	6	431.8	387.9	87.8
	5	5	344.0	300.5	87.1
	4	4	256.9	213.8	86.3
	3	3	170.6	127.8	85.6
	2	2	85.0	59.4	51.0
	1	1	33.9	17.0	33.9

Table 3: CAMx Vertical Layer Structure

WRF = Weather Research and Forecasting Model; m = meters; AGL = above ground level

The layer thicknesses are approximate and vary slightly over space and time as a function of local atmospheric pressure and terrain elevation.

6.2 CMAQ MODELING DOMAINS

Preliminary Community Model for Air Quality (CMAQ) modeling is being conducted using the same horizontal grid as CAMx and the same number of vertical layers, but in the case of CAMx the top layer (layer 28) extends from approximately 12967 meters (m) above ground level (AGL) to approximately 15179 m AGL. The top CMAQ layer starts at the same altitude as the top CAMx layer but extends to the top of the WRF domain at approximately 20807 m AGL. This configuration is necessary in order to use converted CAMx boundary condition files in CMAQ, although these may be modified in the future.

³ Layer top, center, and thickness are approximate, based on average over the 4 km domain.

6.3 WRF MODELING DOMAINS

WRF and CAMx share the same LCP grid projection described in above sections, which greatly reduces horizontal interpolation errors. Like the CAMx grids, there are three nested WRF domains composed of 36×36, 12×12, and 4×4 km grid cells, respectively. Each domain overlays the corresponding CAMx domain with between five and ten grid cells appended to the sides of the CAMx domains forming a buffer between each WRF domain and its enclosed CAMx domain. Figure 13: *WRF Modeling Domains* shows:

- North American Domain (outlined in red) consists of 36 km × 36 km grid cells and contains wholly the CAMx National RPO Domain, with at least five buffer cells on each side;
- **South U.S. Domain** (outlined in dark blue) consists of 12 km × 12 km grid cells and contains wholly the CAMx Texas 12 km Domain with a minimum of eight buffer cells on each side; and
- **Texas Domain** (outlined in green) consists of 4 km × 4 km grid cells and contains wholly the CAMx Texas 4 km Domain with a minimum of 17 buffer cells on each side.



Figure 13: WRF Modeling Domains

Table 4: *WRF Modeling Domain Parameters* lists the horizontal grid configurations for the WRF modeling domains. Grid corners are in km (easting, northing) relative to the grid origin at 97 degrees West and 40 degrees North. Respective CAMx grids are nested within each WRF grid. Therefore the 36 km CAMx grid is a smaller portion of the 36 km WRF grid, and the 12 km and 4 km CAMx grids are offset within the respective WRF grids. In this manner WRF meteorological data can be provided to the CAMx boundary grid cells.

Grid Name	Grid Cell Size	Dimension s (grid points)	Lower left- hand corner	Upper right-hand corner
North American	36 x 36	163 x 129	(-2916, -	(2916,2304)
Texas 12 km Domain	12 x 12	175 x 139	(-1188,-1800)	(900,-144)
Texas 4 km Domain	4 x 4 km	217 x 289	(-396,-1620)	(468,-468)

Table 4: WRF Modeling Domain Parameters

As shown in Table 5: *WRF Vertical Layer Structure*, the vertical configuration of the WRF modeling domains consists of a varying 43-layer structure used with all the horizontal domains. The first 21 vertical layers are identical to the same layers used with CAMx, while CAMx layers 22-28 each comprise multiple WRF layers.

Layer	Sigma	Top⁴ (m AGL)	Center ⁴ (m AGL)	Thickness ⁴ (m)
43	0.000	20,806.8	20,362.1	889.6
42	0.010	19,917.3	19,341.4	1,151.7
41	0.025	18,765.6	18,117.9	1,295.3
40	0.045	17,470.3	16,918.8	1,103.1
39	0.065	16,367.2	15,773.2	1,188.1
38	0.090	15,179.1	14,662.7	1,032.8
37	0.115	14,146.3	13,602.4	1,087.8
36	0.145	13,058.5	12,577.6	961.9
35	0.175	12,096.6	11,596.6	1,000.0
34	0.210	11,096.7	10,587.9	1,017.5
33	0.250	10,079.1	9,622.9	912.6
32	0.290	9,166.6	8,752.3	828.6
31	0.330	8,338.0	7,958.1	759.8
30	0.370	7,578.2	7,269.5	617.3
29	0.405	6,960.9	6,671.3	579.2
28	0.440	6,381.7	6,108.8	545.8
27	0.475	5,835.9	5,577.7	516.3
26	0.510	5,319.5	5,108.7	421.6
25	0.540	4,898.0	4,695.9	404.0
24	0.570	4,493.9	4,299.9	388.0
23	0.600	4,105.9	3,919.3	373.3
22	0.630	3,732.7	3,552.8	359.7
21	0.660	3,373.0	3,199.5	347.1

Table 5: WRF Vertical Layer Structure

⁴Layer top, center, and thickness are approximate, based on average over the 4 km domain. In WRF, the actual layers correspond to sigma levels bases on atmospheric pressure.

Layer	Sigma	Top⁴ (m AGL)	Center ⁴ (m AGL)	Thickness⁴ (m)
20	0.690	3,025.9	2,858.2	335.5
19	0.720	2,690.4	2,528.1	324.6
18	0.750	2,365.8	2,234.4	262.8
17	0.775	2,103.0	1,974.9	256.1
16	0.800	1,846.9	1,721.9	249.8
15	0.825	1,597.0	1,475.1	243.9
14	0.850	1,353.2	1,281.4	143.6
13	0.865	1,209.6	1,138.8	141.6
12	0.880	1,068.0	998.1	139.7
11	0.895	928.3	859.4	137.8
10	0.910	790.5	745.0	90.9
9	0.920	699.6	654.6	90.1
8	0.930	609.5	564.9	89.3
7	0.940	520.2	476.0	88.5
6	0.950	431.7	387.8	87.8
5	0.960	343.9	300.4	87.0
4	0.970	256.9	213.7	86.3
3	0.980	170.5	127.7	85.6
2	0.990	84.9	59.4	51.0
1	0.996	33.9	16.9	33.9
0	1.000	0.0	0.0	0.0

Figure 14: *WRF and CAMx Vertical Layer Configuration* compares the WRF and CAMx vertical layer structure. As shown in the right-hand column, the lowest 21 layers are identical. The left-hand column shows all 28 CAMx layers and the middle column the 43 WRF layers. The horizontal lines between the two leftmost columns indicate which WRF layers are collapsed into CAMx layers beginning with layer 22.



Figure 14: WRF and CAMx Vertical Layer Configuration

The recently released CAMx 6.20 allows for time- and space-varying top boundary conditions, and this version is currently being used. Preliminary testing with 38 CAMx layers for June 2012 showed a slight performance improvement but with significantly increased requirements for storage and run time, so there are no plans at this time to conduct routine model runs using the full 38 layers. However, we are currently testing an alternate configuration with 29 vertical CAMx layers with the extra top layer stretching to the top of WRF layer 41, which keeps the top of the CAMx domain above the tropopause – the 28-layer configuration top was low enough to sometimes allow the top of the CAMx domain to be below the tropopause, in which case using stratospheric top boundary conditions from the Goddard Earth Observing Systems Chemistry Model (GEOS-Chem) would be inappropriate.

CHAPTER 7: MODELING INPUT AND OUTPUT

Since the outputs from the WRF model and the emissions modeling system are inputs to the CAMx model, the modeling inputs and outputs for the WRF model and the emissions modeling system are presented before the inputs and outputs for the CAMx model.

7.1 METEOROLOGICAL MODEL INPUT AND OUTPUT

7.1.1 WRF Model Configuration

The TCEQ has tested many physical parameterizations with the WRF modeling platform. The configuration options presented in **Error! Reference source not found.** is currently being used for the June 2012 period with WRF version 3.6.1. As additional months are modeled, the WRF parameters may evolve further, and may even differ from one month to the next. For example, meteorology in July is dominated by southerly breeze from the Gulf and may be better represented by a WRF parametrization different from that which best represents meteorology in June or August.

Grid	Nudging Type	PBL	Cumulu s	Radiatio n	Land- Surface	Micro- physics
36, 12 km	3-D Analysis	YSU	Kain- Fritsch	RRTM / Dudhia	Pleim- Xiu	WSM5
4 km	3-D Analysis Surface Analysis Observational radar profiler	YSU	None	RRTM / Dudhia	Pleim- Xiu	WSM6

Table 6: 2012 Base Case WRF Setup

km = kilometer; PBL = Planetary Boundary Layer; YSU = Yonsei University; RRTM = Rapid Radiative Transfer Model;

WSMx = WRF Single-Moment x-Class Microphysics Scheme

As development of the 2012 modeling platform progresses, the TCEQ plans to test additional features and inputs including:

- updated land-use/land-cover (LULC) data;
- updated soil parameters and data sets;
- alternative radiation and microphysics parameterizations; and
- use of Geostationary Operational Environmental Satellite (GOES) data for cloud assimilation.

7.1.2 Meteorological Model Input

The National Centers for Environmental Prediction North American Model (NCEP NAM, 2009) gridded analysis fields will be used for initial, boundary, and analysis nudging conditions based upon previous experience evaluating model performance in Texas and the southern United States. If archived NAM data sets are incomplete, the North American Regional Reanalysis will be substituted instead. Customized observational radar profiler nudging files will be built from archived data from the Cooperative Agency Profiler network that are available from the Meteorological Assimilations Data Ingest System (MADIS).

7.1.3 Meteorological Model Output

The meteorological model outputs a variety of data fields required by the photochemical model including temperatures, wind components, cloud cover,

humidity, and vertical mixing parameters. The meteorological model output is postprocessed using the program WRFCAMx to convert the meteorological fields to the CAMx grid and input format (Environ, 2013). The WRFCAMx post-processor is run using six different options for calculating vertical mixing (upward/downward transport of pollutants through the model's vertical grid structure). Each of these schemes has been evaluated CAMx using WRF2CAMx output, and so far the best performance for June 2012 has been observed using the Community Model for Air Quality (CMAQ) option (the default scheme in CMAQ), although other options may be used in future work. We are also applying a K_{ν} "patch," which applies a minimum value to the vertical mixing coefficients (K_{ν}) that control how fast air moves vertically within the first 100 meters (m) above ground level (AGL).

Where possible, the output meteorological fields from the WRF model and the postprocessed CAMx input are compared to monitored data to evaluate the model's performance. The TCEQ uses a performance evaluation package designed to interface with WRF that evaluates the four model parameters of wind speed, wind direction, temperature, and humidity. This statistical package generates standardized tables and graphics for each of the four meteorological parameters. Other performance evaluation tools are used to evaluate the meteorological model's ability to represent episode conditions including cloud-fraction plots and trajectory tools. Attachment 1: *Sample WRFCAMX Performance Analysis Graphics for Selected Sites in Eastern Texas, June 2012* provides a sample of graphics showing performance of WRFCAMx post-processed WRF output at selected sites for June 2012. The overall meteorological model performance is quite good except for a few instances where modeled winds are skewed by convective activity misplaced by the model, and in the Houston-Galveston-Brazoria region the specific humidity may exhibit a small positive bias.

7.2 EMISSIONS PROCESSING SYSTEM INPUT AND OUTPUT

For stationary sources (i.e., point and area sources), TCEQ annual emission inventories constitute the major inputs to the emissions modeling system. For on-road mobile, non-road mobile and biogenic sources, estimates are derived from specific emission models. For example, link-based, on-road mobile source emissions are derived from vehicle miles traveled (VMT) estimates coupled with emission rates from the EPA's Motor Vehicle Emission Simulator (MOVES) model. Non-road mobile source emission estimates are estimated with both the Texas NONROAD (TexN) model and the EPA's National Mobile Inventory Model (NMIM). Models such as Biogenic Emission Inventory System (BEIS) and Model of Emissions of Gases and Aerosols from Nature (MEGAN) are used to estimate biogenic emissions.

With the exception of biogenic emission models that directly output as CAMx modelready emissions, the emissions for the other source categories are processed using the Emissions Processing System, version 3 (EPS3) to generate CAMx model-ready emissions that are day-specific, gridded, chemically speciated, and temporally allocated by hour.

In past modeling for attainment demonstration purposes a separate baseline inventory was created, which replaced some base case emission variability, most notably daily-varying Electric Generating Utility (EGU) emissions and wildfires, with average emissions since these conditions are unlikely to recur in the future. However, the latest draft guidance (EPA, 2014) no longer recommends this approach, although it does
indicate that some accommodation for extreme events such as large wildfires may be needed when predicting future design values. Accordingly, this Technical Description (TD) does not consider development of a separate baseline inventory.

7.2.1 Point Source Emissions

Point source emissions are from stationary sources with emissions large enough to be reported individually, ranging from dry cleaning facilities to power plants and refineries. Point source modeling emission inventories are based on a number of regional data sets available: the EPA's Air Markets Program Database (AMPD), the Bureau of Ocean Energy Management's (BOEM) Gulf-Wide Emissions Inventory (GWEI), the EPA's National Emissions Inventory (NEI), the Mexico NEI, and the Canada NEI, along with state-level data sets such as the State of Texas Air Reporting System (STARS) and local sources.

For the 2012 base case, point source emission estimates for U.S. regions outside of Texas are derived from the 2011 NEI data sets adjusted as appropriate to 2012 with substituted hourly AMPD emissions. Non-U.S. point source emission estimates come from sources including the 2011 GWEI, the 2008 Mexico NEI, and the 2006 Canada NEI (soon to be replaced with a 2010 version). Emissions from these sources are projected to 2012 if projection data are available. Within Texas, the TCEQ 2012 STARS data is used for most sources except AMPD units, which are assigned hourly emissions from the AMPD. The TCEQ will incorporate updates to these data sets as they become available.

Relevant fields are extracted from each of these data sets to develop Aerometric Information Retrieval System (AIRS) Facility Subsystem (AFS) files, which are point source inputs to the EPS3 PREPNT module. For each point source, these AFS files include all of the appropriate source identifiers; source type and classifications; spatial, temporal, and chemical information; and stack parameters used by the model. To reduce the number of points to be modeled explicitly, sources with a nominal plume rise of 30 m or less are consigned to the lowest model layer and combined with the other low-level sources into grid-cell total emissions. Some sources are always treated as elevated regardless of plume rise, including all AMPD sources, ships, and fires. The plume-in-grid (PiG) feature of CAMx is used for large point sources, based on a threshold nitrogen oxides (NO_{x)} emission value; sources in Texas that emit at least 5 tons per day (tpd) of NO_x are flagged as PiGs, increasing to 25 tpd for the farthest regional states, Mexico, and Canada. The PiG feature provides for more realistic treatment of chemistry occurring within concentrated plumes that are small relative to the grid cell containing the plume. As the plume disperses over time its contents are released incrementally into the grid until the plume contents are finally dumped into the grid. Sources located near one another may be combined to reduce the number of PiG sources that the model must track.

For future year point source emissions outside of Texas, the TCEQ plans to use data from the EPA's most recent modeling platform. Emissions from the platform's future year, closest to the TCEQ's future case year, will be used. For EGUs, Cross-State Air Pollution Rule (CSAPR) allowances will be used in conjunction with the latest available (currently 2014) AMPD data. If a substitute program is proposed to replace CSAPR, it will be incorporated as time allows. Other EGU tools, such as Eastern Regional Technical Advisory Committee's (ERTAC) EGU projection tool, may also be given consideration as an alternative to CSAPR allocations. The TCEQ plans to use the EPA's modeling platform data for future case Mexico and Canada point source emissions, unless superior information becomes available. Offshore (Gulf of Mexico) emissions will be from the most recent available GWEI from BOEM.

Within Texas, the TCEQ plans to use the most currently available STARS data, with Eastern Research Group (ERG) composite growth factors applied for projecting non-EGU point source emissions to the future year. To project EGUs within Texas, the TCEQ plans to start with the latest AMPD units, then incorporate the latest information for new EGUs and retirement status for existing EGUs obtained from the TCEQ permit database, Public Utilities Commissions, Energy Information Administration, and the Electric Reliability Council of Texas. Emissions for newly permitted EGUs that are planned to be operational prior to or during the future year will be used, and units retiring prior to the future year will have their emissions removed. Emissions for both new and existing EGUs will be constrained to the CSAPR statewide allowance. Where necessary, other on-the-books controls, rules, programs and consent decrees applicable to the future year will supersede and limit projected emissions for EGUs and non-EGUs.

Although the current plan is to use the aforementioned techniques for projecting EGUs, these plans might vary. Consideration may be given to other projection methods such as the ERTAC EGU projection tool and the Integrated Planning Model (IPM).

Figure 15: *Tile Plots of Elevated and Low-Level Point Source NOX Emissions for June 6, 2012* displays two tile plots pf point source NO_x emissions for June 6, 2012 on the Texas 4 kilometer (km) domain. The left-hand plot shows elevated anthropogenic point source emissions while the right-hand plot shows emissions from point sources assigned to the first model layer. Additional plots along with a more detailed description of the plots themselves may be viewed in Attachment 2: *Quality Assurance/Quality Control (QA/QC) Plan* for the TCEQ 2012 modeling platform. These plots include emissions from ships with stacks high enough to be treated as elevated points (see Section 7.2.3 below).



Figure 15: Tile Plots of Elevated and Low-Level Point Source NO_x Emissions for June 6, 2012

7.2.2 Area Source Emissions

Area sources are stationary sources too small or numerous to be inventoried individually, including home heating and cooking, gas stations, road paving, painting, etc. Since the exact locations of these sources are not usually known, area sources usually are allocated to grid cells using spatial surrogates such as population, urban area, etc. Area source emissions for Texas use 2011 data from the Texas Air Emissions Repository (TexAER) database (TCEQ, 2010b) projected to 2012 using ERG composite growth factors (also housed in TexAER). Emissions data from these inventories are processed with EPS3 to generate CAMx model-ready emissions that are day-specific, gridded, speciated and temporally allocated by hour. Surrogates for basic area sources are based on EPA data. Future years will be projected from the same sources using the most current data available.

An ERG-developed calculator (ERG, 2011) is updated annually using detailed countybased Railroad Commission of Texas (RRC) production and drilling data. Oil and gas emissions are calculated for over 20 categories including many compressor types, flares, completions, and numerous fugitive source types. The 2012 oil and gas emissions inventory (EI) is based on actual 2012 annual data for production, drilling and spatial data. Future year emissions will be based on 2015 or the most current RRC data projected by shale play (Barnett, Eagle Ford, and Haynesville) using ERG shale play-based projection data (ERG study, 2012) also housed in TexAER. Future year drilling rig emissions will be developed by applying projected drilling rig emission rates to the 2015 or most current EI. Surrogates derived from RRC spatial data are unique for oil production, gas production (well-head density by type), flare location and drilling (new well-head density) by respective year.

For regions outside of Texas, the TCEQ is using area source emissions data from the EPA's 2011 NEI. The NEI data sets are projected to 2012 using ERG and available EPA factors as appropriate. Future year emissions for these regions will be projected from the 2014 version of the NEI when it becomes available (or the 2011 NEI if necessary). Additional non-Texas area source inventory data sets currently used include the 2008 Mexico NEI, 2011 GWEI, and the 2006 Canadian NEI, but these will be updated if newer data become available. Since no projections for these emissions are available at this time the TCEQ will use them as is in future case modeling unless projections become available.

Figure 16: *Tile Plots of Area Source VOC Emissions for a June, 2012 Weekday*; (L) All Sources Except Oil and Gas Production, and (R) Oil and Gas Production Only displays two tile plots of area source volatile organic compounds (VOC) emissions for a June 2012 weekday; on the left is shown area source emissions excluding oil and gas production, while the right-hand plot shows only oil and gas production for the 4 km Texas domain.



Figure 16: Tile Plots of Area Source VOC Emissions for a June, 2012 Weekday; (L) All Sources Except Oil and Gas Production, and (R) Oil and Gas Production Only

7.2.3 Non-Road and Off-Road Source Emissions

Non-road emissions are associated with non-stationary sources such as boats, construction equipment, lawn mowers, and drilling rigs, and like area sources are

typically allocated to the modeling grid using spatial surrogates. Both 2012 base and future case non-road source emission estimates within Texas are developed with the TexN model, which runs the EPA's NONROAD model "under the hood" for 25 distinct equipment sub-categories within each county. TexN 1.7.1 is the most current version that is available. Updated versions of TexN will be used to develop revised estimates for 2012 and future years if they become available. 2012 base and future case non-road source emission estimates outside of Texas are developed with the EPA's <u>NMIM</u> model, which provides output for each U.S. county. For the non-U.S. portions of the modeling domain, the 2008 Mexico NEI and 2006 Canada NEI data sets are being used, and will be updated if newer information becomes available.

Non-road emission files are processed with EPS3 to generate CAMx model-ready emissions that are day-specific, gridded, speciated, and temporally allocated by hour. Since the NONROAD model cannot account for the effects of variable temperature and humidity on NO_x emissions from diesel engines, the EPS3 CNTLEM module is used to apply these adjustments by hour for Texas counties.

Figure 17: *Tile Plots of Non-Road NOX Emissions for a June 2012 Weekday*; (L) All Sources except Drilling Rigs, and (R) Drilling Rigs Only shows non-road NO_x emissions from non-road sources for a June 2012 weekday; the left panel shows all non-road emissions except drilling rigs while the right shows drilling rigs only.



Figure 17: Tile Plots of Non-Road NO_x Emissions for a June 2012 Weekday; (L) All Sources except Drilling Rigs, and (R) Drilling Rigs Only

Off-road emissions are a subset of the larger non-road category that are treated separately and consist of emissions from aircraft, airport equipment, locomotive, and

commercial marine sources. While these emissions may be allocated spatially using surrogates, at least some emissions can be modeled using bottom-up location data such as specific airport landings and take-offs during the base period. The Federal Aviation Administration (FAA) Emissions Dispersion and Modeling System (EDMS) is used for estimating emissions from the aircraft and airport equipment source categories within Texas. EDMS reports emissions separately for aircraft, ground support equipment, and auxiliary power units. 2012 base case emissions are based on historical landing/take-off (LTO) activity, while future case LTO activity will be based on Terminal Area Forecast projections done by the FAA. Some of this work has already been developed under an ERG study entitled Aircraft Emissions Inventory for Texas Statewide 2014 AERR Inventory and 2008 to 2040 Trend Analysis Years, July 2015. The 2012 locomotive emission inventories within Texas are based on an ERG study entitled 2014 Texas Statewide Locomotive Emissions Inventory and 2008 through 2040 Trend *Inventories*, August 2015. These studies will be used to develop future emissions unless more up-to-date data become available. CAMx model-ready emissions that are day-specific, speciated, and temporally allocated by hour are prepared using EPS3. Since aircraft and associated inventories are developed for each Texas airport rather than at the county-level, the emissions are allocated to the grid cell(s) where each airport is located. Locomotive emission inventories are spatially allocated to appropriate switcher yards and railway lines.

Commercial marine emissions for HGB, Beaumont-Port Arthur (BPA), the Gulf of Mexico (GOM) and oceans are modeled as elevated points, or "elevated links" mapped to points by EPS3, since many of these vessels have stacks tall enough to exceed the 30 m cut-off threshold. The emissions are essentially based on annualized trips and reflect actual traffic patterns for large vessels from sea buoys to ports for HGB and BPA (as displayed in Figure 15). The GOM emissions in the Texas 4 km domain incorporate the results of a contract project that based emissions on the onboard location transponders installed on most modern ships by tracking speed and course based on minute to minute location data (report pending). In addition to being more current than those shown in Figure 15: Tile Plots of Elevated and Low-Level Point Source NOX Emissions for June 6, 2012, the revised emissions are more highly resolved spatially as shown in Figure 18: *Revised 2014 Elevated Marine Emissions in Texas 4 km Grid* (L) Ships at Anchor, (R) Ships Underway. These emissions were back-cast to 2012 and will be forecast to future years as appropriate.



Figure 18: Revised 2014 Elevated Marine Emissions in Texas 4 km Grid (L) Ships at Anchor, (R) Ships Underway

For non-Texas off-road emissions, the 2012 aircraft, airport equipment, locomotive, and commercial marine, inventories are based on the 2011 NEI data sets from EPA; future years will be based on the 2014 (or latest available) NEI data. As described above, the 2005 GWEI non-road and off-road emissions are included in the area source category. Figure 19: *Tile Plots of (L) Non-Road and (R) On-Road NOX Emissions for* a June 2012 Weekday shows June 2012 weekday non-road NO_x emissions (ship emissions outside U.S. territorial waters are not shown) and also on-road emissions (discussed in the next section).



Figure 19: Tile Plots of (L) Non-Road and (R) On-Road NO_x Emissions for a June 2012 Weekday

7.2.4 On-Road Mobile Source Emissions

On-road mobile source emission estimates for the DFW area, HGB area, the remaining portions of Texas, and all non-Texas U.S. counties are based on the latest version of the EPA's <u>MOVES</u> model, which is currently MOVES2014a. All of the on-road emission inventories developed include the benefits of current on-the-books rules such as new vehicle emission standards, reformulated gasoline, low Reid Vapor Pressure gasoline, Texas Low Emissions Diesel (TxLED), and vehicle inspection/maintenance (I/M).

The TCEQ contracted with the Texas Transportation Institute (TTI) to develop non-link on-road emission inventories with the MOVES2014 version of the model using Highway Performance Monitoring System (HPMS) data as the basis for VMT estimates for 19 different roadway categories. These MOVES on-road emission inventory data sets include the day types of Monday through Thursday average weekday, Friday, Saturday, and Sunday for both school and summer (i.e., non-school) seasons. The result is eight different combinations of season and day type for all 254 Texas counties based on automatic traffic recorder (ATR) data regularly collected by the Texas Department of Transportation (TxDOT). The summer season inventories are used for the June, July, and August months, while the school season inventories are used for the May and September months. These MOVES on-road inventories are available on the <u>TCEQ on-road emissions FTP site</u>.

The TCEQ is using a 2012 link-based on-road emission inventory developed by TTI using the MOVES2014 model. A 2012 link-based inventory is also being developed for the ten-county DFW area by the North Central Texas Council of Governments

(NCTCOG). Future year link-based on-road emission inventories will be developed using the latest version of the MOVES model available.

The TCEQ has already run MOVES2014 in default mode for all non-Texas U.S. counties for a July average weekday in both 2012 and a future year (in this case, 2017). The Texas-based on-road emission inventories are aggregated by year, season, day type, and hour to develop pollutant-specific temporal emission factor ratios that are applied to the MOVES2014 default July average weekday emissions using the EPS3 TMPRL module. The net result is non-Texas on-road CAMx inputs that vary by season, day type, and hour in the same manner as the Texas inventories developed with high resolution by TTI. If a future year other than 2017 is needed, similar procedures will be followed.

The 2006 Canadian NEI includes annual on-road emission estimates that are divided by 365 days to develop average weekday totals. In order to obtain 2012 and future year Canadian on-road inputs, MOBILE6-Canada⁵ is run to obtain emission rate adjustment factor ratios that vary by pollutant and vehicle type between 2006 and 2012, and 2006 and 2017. Until superior information is made available, the TCEQ will assume an average annual VMT growth rate of 2% between 2006 and future years. The combination of emission rate ratios and activity growth is applied to the 2006 Canadian on-road inventory to obtain both 2012 and future year estimated emissions. The Texas pollutant-specific temporal factors are applied to the Canadian on-road inventories to obtain all the necessary combinations of season and day type.

A similar approach is being taken with the 1999 on-road emission inventories available from the Mexico NEI. MOBILE6⁵-Mexico is run to develop 2012/1999 and future year/1999 emission rate adjustment factor ratios that vary by pollutant and vehicle type. Similar to Canada, an average annual VMT growth rate of 2% is assumed from 1999 to 2012 and 1999 to a future year until superior information becomes available. Also, the Texas pollutant-specific temporal factors are applied to the Mexican on-road inventories to obtain all the necessary combinations of season and day type.

The on-road emissions from each of the different regions is processed with EPS3 to generate season and day-type specific CAMx model ready emissions that are gridded, temporally allocated by hour, and speciated for the CB6 mechanism using profiles available from the EPA's <u>SPECIATE</u> database. Since the Texas on-road emissions received from TTI are already provided by hour, EPS3 processing preserves the hourly distribution of the emissions. Within Texas, the on-road emissions processing is generally divided into processing streams for each area: roadway link-based when such inventories are available; roadway HPMS-based when link-based inventories are not available; off-network estimates for start emissions and evaporative VOC from parked vehicles; and extended idling emission estimates for combination long-haul diesel trucks. Allocation of emissions for link-based inventories is applied to specific roadway segments. For non-link on-road emission inventories, spatial allocation is done with spatial surrogates for interstates, state highways, arterials, population, etc.

⁵ MOBILE6 was the predecessor to MOVES. MOBILE6-Canada and MOBILE6-Mexico are versions on MOBILE6 customized for use in the two countries, respectively.

A more complete description of how this is done is contained within a <u>ReadMe file</u> available on the <u>TCEQ on-road mobile FTP site</u>.

Table 7: *Development Summary of On-Road Mobile Source Emissions* summarizes pertinent features of the planned development of on-road mobile emissions in the different regions of the modeling domain as described above.

On-Road Inventory Development Parameter	Texas Metropolitan Areas	Texas Rural Areas	Non-Texas U.S. Counties
VMT Source	Travel Demand Models (TDMs)	HPMS Data Sets	MOVES Default
VMT Resolution	Roadway Links From TDM	19 Roadway Categories	MOVES Road Types
Season Types	School and Summer (i.e., non-School)	School and Summer	School and Summer
Day Types	Weekday, Friday, Saturday, and Sunday	Weekday, Friday, Saturday, and Sunday	Weekday, Friday, Saturday, and Sunday
Hourly VMT	Yes	Yes	No
VMT Mix Variation By Day/Time Period	Yes	Yes	No
Roadway Speed Distribution	Varies by Hour and Link	Varies by Hour and Roadway Type	MOVES Default
Spatial Resolution	Excellent	Very Good	Good
Temporal Resolution	Excellent	Very Good	Good
MOVES Source Use Types	13	13	13
MOVES Fuel Types	Gasoline and Diesel	Gasoline and Diesel	Gasoline and Diesel

Table 7: Development Summary of On-Road Mobile Source Emissions

7.2.5 Biogenic Emissions

The TCEQ is using MEGAN v. 2.1 to estimate emissions from biogenic emission sources, although overall CAMx modeling with MEGAN tends to over-predict isoprene concentrations at most sites by up to two times the observation. The TCEQ has also used EPA's BEIS, but BEIS under-predicts isoprene by about 50% in most cases. The TCEQ is currently investigating these discrepancies and how they may be mitigated.

The MEGAN model requires inputs by model grid cell area of:

• Emission factors for nineteen chemical compounds or compound groups;

- Plant Functional Types (PFTs);
- Fractional Vegetated Leaf Area Index (LAIv); and
- Meteorological information including air and soil temperatures, photosynthetically active solar radiation (PAR), barometric pressure, wind speed, water vapor mixing ratio and accumulated precipitation.

7.2.5.1 Emission Factor and PFT Inputs

The TCEQ is using the default emission factors and PFTs that are provided with the model for the entire globe in Network Common Data Form (netCDF) format. To process the emission factors and PFTs to the TCEQ air modeling domain structures, raster layers of each emission factor file were created in ArcMap version 9.3 using the Make NetCDF Raster Layer tool. The Zonal Statistics as Table tool was then used to tabulate averages per grid cell for each compound class and CAMx domain.

7.2.5.2 Fractional Vegetated Leaf Area Index Input

Leaf Area Index (LAI) is the one-sided leaf coverage over the same area of land. Fractional vegetated Leaf Area Index (LAIv) is LAI divided by the fraction of land defined as vegetated, and files for every eight-day period of 2008 are provided on the MEGAN website. The TCEQ created 2012-specific LAIv data using the level-4 Moderate-Resolution Imaging Spectroradiometer (MODIS) global LAI MCD15A2 product. For each eight-day period, the satellite tiles covering North America in a sinusoidal grid were mosaicked together using the MODIS Reprojection Tool. Urban LAI cells, which MODIS excludes, were filled according to a function that follows the North American average for four urban land cover types. An urban LAI maximum was chosen based on Loughner et al. (2012). MODIS' quality control flags were applied to use only the high quality data from the main retrieval algorithm. The resultant LAI was divided by the percentage of vegetated PFT per grid cell to yield the final LAIv.

7.2.5.3 Meteorological Input

The Weather Research and Forecasting (WRF) meteorological model is currently being used to provide the meteorological data needed for MEGAN input, including PAR. The WRF output was processed through the Meteorology-Chemistry Interface Processor (MCIP). Some PAR data derived from GOES observations is available and may be used in the future, possibly augmented with WRF predictions. Figure 20: *Tile Plots of Biogenic Isoprene (L) and NOX (R)* Emissions, June 22, 2012 shows biogenic emissions for a day in June 2012.



Figure 20: Tile Plots of Biogenic Isoprene (L) and NO_x (R) Emissions, June 22, 2012

7.2.6 Wildfires

Wildfire emissions were estimated from the daily Fire Inventory from National Center for Atmospheric Research (NCAR) (FINN) version 1.5 product for 2012 (Wiedinmyer, 2011). The FINN fire estimates were projected to the model's Lambert Conformal conic Projection modeling projection and grouped if fires were within 5 km. Each fire was treated as a point source and processed using the EPS3 PREFIR, CHMSPL, TMPRL, and PSTFIR modules following the methodology of Ramboll Environ (2008). The fire emissions were temporally allocated according to the temperate North American diurnal cycle of fires from Mu et al. (2011). Figure 21: *Tile Plots of Elevated Wildfire NOX Emissions on the 4 km Grid (L) and VOC Emissions on the 36 km Grid (R*), June 22, 2012 shows wildfire emissions for June 22, 2012, an active wildfire day in Oklahoma, Kansas, and Louisiana.



Figure 21: Tile Plots of Elevated Wildfire NO_x Emissions on the 4 km Grid (L) and VOC Emissions on the 36 km Grid (R), June 22, 2012

7.3 CAMX MODEL INPUT AND OUTPUT

7.3.1 Model Input

The outputs from EPS3/MEGAN and WRF serve as the CAMx inputs for emission rates and meteorological parameters, respectively. Additional CAMx inputs include initial and boundary conditions, spatially resolved surface characteristic parameters, spatially resolved opacity, and photolysis rates.

7.3.1.1 Initial and Boundary Conditions

The TCEQ is using initial and boundary conditions for CAMx developed with the Goddard Earth Observing System model with Chemistry (GEOS-Chem). Boundary conditions were developed with GEOS-Chem for each grid cell along all four edges of the 36 km domain (i.e. the four "walls" of the outer domain) and each vertical layer for each episode hour. CAMx 6.2 also allows boundary conditions on the top of the domain (the "ceiling") to be used, although this is not required. The TCEQ is currently evaluating using the top boundary conditions with CAMx 6.2 for the 2012 ozone season and will obtain revised boundary/initial conditions generated using a newer version of GEOS-Chem that includes halogen chemistry. These updates should help alleviate persistent model over-prediction of ozone in air brought onshore from the Gulf and other salt water bodies.

Figure 22: *GEOS-Chem Derived Ozone Boundary Conditions for June 12, 2012, 09:00-12:00 CST* shows an example of boundary conditions for the four "walls" of the 36 km modeling domain. These values are updated every three hours throughout the simulation. Most CB6 species are provided, but because the GEOS-Chem chemistry differs from CB6 some species are are set to constant values.



O3 Concentration of Lateral Boundary Conditions Envrion's GEOS-CHEM (a0) for rpo_36km domain (base 2012)

Figure 22: GEOS-Chem Derived Ozone Boundary Conditions for June 12, 2012, 09:00-12:00 CST

7.3.1.2 Land-Use and Surface Characteristics

Surface characteristic parameters, including roughness, vegetative distribution, and water/land boundaries, are input to CAMx via a land-use file. The land-use file provides the fractional contribution (0 to 1) of 26 land-use categories (see Zhang et al, 2003). Land-use data from <u>National Land Cover Dataset (NLCD)</u> and <u>Biogenic Emissions Landuse Database, version 3 (BELD3)</u> are used for areas outside Texas; the updated land-use data (Popescu et al., 2008), which were derived from more highly resolved LULC data collected by the Texas Forest Service and the University of Texas Center for Space Research, are used for Texas. The land-use categories of source data are cross-referenced to Zhang's 26 land-use categories.

7.3.1.3 Ozone Column and Photolysis Rates

Spatially-resolved total atmospheric ozone column data and photolysis rates are input to CAMx via ozone column and photolysis files. Episode-specific satellite data from the Ozone Monitoring Instrument (OMI) are used to prepare the ozone column data files. The photolysis rates are also specific to the chemistry parameters of the CB6 mechanism.

7.3.2 Model Output

CAMx outputs CB6 species in molar concentration units of parts per million by volume. Some of the CB6 species are actual chemical species and include ozone, nitric oxide, nitrogen dioxide, isoprene, carbon monoxide, ethane, ethene, formaldehyde and acetaldehyde, while others represent molecular bonds which do not map directly to actual chemicals. Typically, CAMx is executed to output hourly average concentrations, which are comparable to hourly monitored aerometric parameters. CAMx also outputs limited diagnostic files, including instantaneous concentration files for the last two simulation hours (typically used for restarts), PiG output files (typically used for restarts, but can be used for diagnostic analyses), and a deposition file (typically used for diagnostic analyses).

CAMx can also be executed to output process analysis (PA) and source apportionment results. PA, including chemical PA and integrated process rate analysis, provides indepth details of ozone formation showing the various physical and chemical processes that determine the modeled ozone concentrations at specified locations and times. PA modeling output is typically used as a part of the performance evaluation. Source apportionment, using tools such as Ozone Source Apportionment Technology (OSAT) and Anthropogenic Precursor Culpability Assessment (APCA), estimates the culpability of sources from various regions contributing to local ozone concentrations. Source apportionment modeling output can also be used as a part of the performance evaluation, but more typically, it is used with the future year modeling to quantify the region/source type contributions to the projected future design values.

CAMx can also output analysis results of first and higher order sensitivities of modeled concentrations to model input parameters via the Direct-Decoupled Method (DDM) and Higher-Order Direct Decoupled Method (HDDM) tools. DDM and HDDM calculate CAMx's sensitivity to changes in inputs directly as the model is executed, and can be used to evaluate base case performance as well as to assist in control strategy evaluation for future year modeling.

CHAPTER 8: QUALITY ASSURANCE/QUALITY CONTROL (QA/QC) PLAN

The TCEQ's QA/QC plan focuses primarily on the data input to the models and procedures, and post-processing of the output data used for decision making. The TCEQ conducts extensive QA/QC activities when developing modeling inputs, running the models, and analyzing and interpreting the output. The TCEQ has developed a number of innovative and highly effective QA/QC tools that are employed at key steps of the modeling process. The QA/QC plan is consistent with EPA guidance to ensure the scientific soundness and defensibility of the modeling.

CHAPTER 9: MODEL PERFORMANCE EVALUATION

The performance evaluation of the base case modeling measures the adequacy of the model to correctly replicate the relationship between levels of ozone and the emissions of ozone precursors such as nitrogen oxides (NO_{x_1} and volatile organic compounds (VOC). The model's ability to correctly replicate this relationship is necessary to give confidence in the model's prediction of the response of ozone to various emission changes.

The TCEQ conducts two types of performance evaluations, operational (e.g., statistical and graphical evaluations) and diagnostic (e.g., sensitivity evaluations). As recommended by the EPA (EPA, 2007 and 2014), these evaluations are considered as a whole in a weight-of-evidence approach, rather than individually, to gauge the adequacy of the model.

The TCEQ has incorporated the recommended eight-hour performance measures into its routine evaluation procedures, but continues to focus primarily on one-hour performance analyses. The high-resolution meteorological and emissions features characteristic of areas in eastern Texas, both urban and rural, require model evaluations be performed at the highest resolution possible to determine whether or not the model is getting the right answer for the right reasons. On the other hand, the volume of model output for a regional-seasonal application like the 2012 platform requires significant numerical and graphical summarization to make the model results comprehensible to humans. These summarizations provide an overall evaluation of model performance, and at the same time help identify areas that need to be analyzed in detail.

9.1 OPERATIONAL EVALUATIONS

9.1.1 Statistical Measures

Statistical measures provide a quantitative evaluation of model performance, and by definition summarize information into more easily understood numerical values. Data in photochemical grid modeling applications are typically aggregated by day across defined sub-areas of the modeling domain, such as individual non-attainment areas or contiguous groups of urban counties which are in danger of becoming non-attainment. The TCEQ routinely calculates summary statistics for Dallas-Fort Worth, Houston-Galveston-Brazoria, Beaumont-Port Arthur, San Antonio, Austin-Round Rock, and

Northeast Texas by day. We plan to further summarize some model performance statistics by month.

The following statistics are recommended in the draft guidance (EPA, 2014) for evaluating performance of the base case modeling and the following descriptions are copied verbatim from the draft guidance, except for correcting the description of root mean-square error (RMSE). Formulae for calculating these metrics are not shown here but can be found in the draft guidance.

Mean Bias (MB): This performance statistic averages the model/observation residual paired in time and space. A value of zero would indicate that the model overpredictions and model under predictions exactly cancel each other out. An advantage of this metric is the bias is reported in the unit of measure (ppb or μ g/m³) making interpretation simpler.

Mean (Gross) Error (ME/MGE): This performance statistic averages the absolute value of the model/observation residual paired in time and space. A value of zero would indicate that the model exactly matches the observed values at all points in space/time. An advantage of this metric is the bias is reported in the unit of measure (ppb or μ g/m³) making interpretation simpler.

Root Mean Square error (RMSE): This performance statistic (ppb or $\mu g/m^3$) is a measure of the average distance between predicted and observed values. It is calculated by squaring the difference between each model-observation pair, averaging the squared differences, then taking the square root of the result, which yields a measure in the same units as the original data (ppb or $\mu g/m^3$). RMSE is similar to MGE, except that squaring the differences puts more weight on the pairs with the largest errors.

Normalized Mean Bias (NMB): This statistic (given in units of percent) normalized MB to the average observed value. NMB values range from -100% to +infinity. Consequently, negative and positive bias values using this metric are not symmetrical around 0. NMB is a useful model performance indicator because it avoids over inflating the observed range of values.

Normalized Mean Error (NME): This performance statistic (given in units of percent) is used to normalize the mean error relative to the average observation. This statistic averages the absolute value of the difference (model - observed) over the sum of observed values. NME values range from 0 to +infinity. NME is a useful model performance indicator because it avoids over inflating the observed range of values.

(Mean) Fractional Bias (MFB/FB): Fractional bias is determined by normalizing the MB by the average of observed and modeled concentrations. Since normalized bias can become very large when a minimum threshold is not used, fractional bias may be used as a substitute. The range of FB is -200% to +200%. The fractional bias for cases with factors of 2 under- and over- prediction are -67 and + 67 percent, respectively (as opposed to -50 and +100 percent, when using normalized bias). Fractional bias is a useful indicator because it has the advantage of equally weighting positive and negative bias estimates (underestimates and overestimates are symmetrical around 0).

The single largest disadvantage is that the predicted concentration is found in both the numerator and denominator.

(Mean) Fractional Error (MFE/FE): Fractional error is determined by normalizing the ME by the average of observed and modeled concentrations. Since normalized error can become very large when a minimum threshold is not used, fractional error may be used as a substitute. The range of values for FE is 0 to 200%. It is similar to the fractional bias except the absolute value of the difference is used so that the error is always positive.

Correlation Coefficient (R²): This performance statistic measures the degree to which two variables are linearly related. A correlation coefficient of 1 indicates a perfect linear relationship; whereas a correlation coefficient of 0 means that there is no linear relationship between the variables.

The TCEQ currently calculates all of the above statistics for every base case model run except RMSE and R², and plans to add RMSE to its suite of performance measures soon. The TCEQ does not plan to add R², however, since it measures only correlation, not predictive skill. For example, a model that predicted exactly twice the observed values would score an R² of 1.0, but would probably be a poor predictor of the future value. All statistics are calculated for both hourly averaged and Maximum Daily 8-hour Average (MDA8) ozone concentrations.

These statistical measures are used primarily for ozone concentrations, although they may be applied to some of the ozone precursors. In addition, the TCEQ may use statistical measures other than those listed above as deemed necessary in the performance evaluation. Neither the 2007 nor 2014 draft guidance specify acceptable ranges for statistics, but the latter refers to a paper by Simon, et al (2012) which summarized photochemical model performance for applications published in the perreviewed literature between 2006 and 2012. This reference will be used as a guideline but the TCEQ may also apply traditional performance criteria that have been used in previous Texas modeling applications.

9.1.2 Graphical Measures

Graphical measures provide a qualitative evaluation of model performance. The TCEQ post-processing routines develop the following graphical representations for each base case model run, including most of those listed above.

Time Series Plots - For each monitor, the monitored and bi-linearly interpolated modeled concentrations can be compared visually for each hour in an episode. This comparison assesses how well the model predicts diurnal and/or daily variation in the ozone concentrations at specific monitor locations as well as how well the model predicts the magnitude of the observed concentrations.

For every base case model run the TCEQ develops hourly time series plots for ozone (O3) and most CB6 species including nitric oxide (NO), nitrogen dioxide (NO2), isoprene (ISOP), olefins (OLE), formaldehyde (FORM), etc. and where available plots hourly observations together with the modeled concentrations. Comparing the modeled versus monitored concentrations of precursors, intermediate products, and reaction

products can indicate whether the model is correctly replicating the physicochemical processes by which ozone was actually generated.

The display routines allow two model runs to be compared, or if a single run is evaluated, the plot shows the minimum and maximum values in the 3×3 array of grid cells containing each monitor. Figure 23: *Time-Series Hourly Ozone (O3) Plot for Denton,* June 2012 **shows an example of this type of plot** produced by the TCEQ post-processing routines.



Figure 23: Time-Series Hourly Ozone (O3) Plot for Denton, June 2012

Site Daily Maximum Plots: Site daily maximum plots compare peak modeled and observed ozone concentrations at a site, either one-hour or MDA8, and are useful tools to identify over-prediction bias of peak concentrations at specific locations. The "error bars" shown for the modeled values indicate the 3×3 grid cell minimum-maximum. Figure 24: *Example MDA8 Ozone Plot for Denton, June 2012* shows an example of this type of plot produced by the TCEQ post-processing routines.



Figure 24: Example MDA8 Ozone Plot for Denton, June 2012

Scatter Plots - Scatter plots of hourly monitored and bi-linearly interpolated modeled ozone and precursor concentrations show the same data displayed on corresponding time-series plots, except modeled concentrations are plotted against observed concentrations for the same hour. These plots are useful in analyzing model bias and how it varies as a function of observed concentration. Quantile/Quantile (Q/Q) plots

indicating the rank distribution of the monitored versus modeled ozone concentrations are optionally displayed. Figure 25: *Example Scatter Plot with Q-Q Plot Showing Observed and Modeled Isoprene Concentrations at the Hinton Street Monitor* in June 2012 is an example of these plots produced by the TCEQ post-processing routines.



e camx610p1_cb6r2.tx.bc12_12jun.reg3.2012_wrf361_p2a_i2_kvCMAQ.tx_4km(Q-Q)

Figure 25: Example Scatter Plot with Q-Q Plot Showing Observed and Modeled Isoprene Concentrations at the Hinton Street Monitor in June 2012

Vertical Profile Plots – Though infrequently available, vertical profile plots of ozone concentrations are invaluable for assessing how well the model replicates the vertical distribution of ozone concentrations through the troposphere. These plots are located at the sites of ozone sonde launches conducted as part of the Tropospheric Ozone Pollution Project (TOPP), a multi-year effort to characterize tropospheric ozone in the United States. Figure 26: *Example Vertical Profile Plot Showing Observed and Modeled Ozone Concentrations for a Sonde Launch in June 2012* shows an example produced by the TCEQ post-processing routines.





Figure 26: Example Vertical Profile Plot Showing Observed and Modeled Ozone Concentrations for a Sonde Launch in June 2012

Peak Ozone Spatial Plots – Peak ozone spatial plots show maximum daily hourly or MDA8 ozone concentrations across a selected area using custom software developed at the TCEQ that overlays modeled concentrations over a Google Maps display. Observed concentrations are also displayed to provide a visual comparison to the model results. The display can be zoomed in to any area to the limits of the underlying map and several display options are available. This software replaces the static tile plots used previously. The concentration data are smoothed automatically and grid cell boundaries are no longer evident. The program allows the difference between two model runs to be displayed allowing the results of changing model inputs or parameterizations to be quantified and located spatially within the model grid. Figure 27: *Example MDA8 Ozone Spatial Plot for Eastern Texas, June 26, 2012* shows an example of the plots that can be quickly produced using the TCEQ post-processing software.



Figure 27: Example MDA8 Ozone Spatial Plot for Eastern Texas, June 26, 2012

Hourly Concentration Plots and Animations – Hourly concentration plots of ozone and several precursors can be produced through software analogous to that described above, except that instead of displaying only the peak value for a day this type of plot displays concentration data simulated for every hour. The display program allows the hourly images to be automatically run sequentially to provide an animated display of the concentration data. This feature is very useful to track the development, transport, and destruction of ozone and ozone precursors. Besides displaying pollutant concentrations, the hourly mapping program includes several optional displays including radar (from the National Weather Service, NWS) and satellite overlays, back trajectories, and wind observations. Figure 28: *Example Hourly Ozone Concentration Spatial Plot for Eastern Texas, 15:00, June 26, 2012, with NWS Radar Overlay* shows an example of this type of plot produced with the TCEQ's post-processing software called Geo-Referenced Interactive Model Results Evaluation and Analysis Program (GRIMREAPr).



Figure 28: Example Hourly Ozone Concentration Spatial Plot for Eastern Texas, 15:00, June 26, 2012, with NWS Radar Overlay

9.2 DIAGNOSTIC EVALUATIONS

9.2.1 Sensitivity Analyses

Sensitivity analyses are designed to check the response of the modeled ozone to changes in model inputs including meteorological parameters and precursor emissions. The results of these analyses indicate the sensitivity of the model to various inputs and can identify which inputs must be scrutinized most closely. In addition, sensitivity analyses can also indicate which modeling inputs may be hindering the performance of the model.

The TCEQ has tested different model inputs, configurations, and parameterizations to try to obtain the best model performance possible for June 2012, consistent with current science. These tests include running CAMx with:

- Chemical mechanisms CB6, CB6r2, and CB6r2h, as well as with the older CB05;
- CAMx versions 6.00, 6.10, and 6.20;
- 85% and 40% reductions to isoprene emissions;
- WRF 3.5 and WRF 3.61;
- Vertical mixing (Kv) with O'Brien and cloud adjustment, YSU, and CMAQ schemes;
- With and without sub-grid cloud parameterization;

- With hourly and 15 minute WRF input;
- Southeast ocean boundary condition ozone reduced by 10 ppb, reduced by 50%;
- With and without asymmetric vertical mixing v. 2 (ACM2) diffusion in CAMx;
- With and without Goddard Earth Observing Systems Chemistry Model (GEOS-Chem)-derived top boundary conditions (CAMx 6.2); and
- Alternative vertical layer structures (WRF and CAMx, and CAMx alone).

As additional months are modeled, additional sensitivity tests will likely be needed to optimize overall model performance. These tests may include very-high-resolution modeling (1 km or 1.33 km) for selected areas, alternative boundary conditions, new biogenic emission estimates, and alternative meteorological characterizations among others.

9.2.2 Diagnostic Analyses

Diagnostic analyses tend to focus more directly on the model's change in predicted ozone to changes in the ozone precursor emissions. At a minimum, the TCEQ plans to conduct the following diagnostic analyses:

Observational Methods - These methods compare changes in modeled ozone associated with changes in emissions input to the model to changes in monitored ozone associated with changes in actual emissions. The primary analysis of this type that the TCEQ plans to conduct is a modeling scenario to compare the weekday versus weekend differences in ozone and emissions to the monitored weekday versus weekend differences for the area. Another analysis of this type that the TCEQ may conduct involves comparing the changes in the modeled versus monitored NO_x-limitation or VOC-limitation both geographically and temporally over eastern Texas.

Probing Tools - Probing tools are embedded procedures in the CAMx model used to discern the contribution to ozone formation from the various inputs. The primary probing tool the TCEQ plans to use is process analysis (PA). The TCEQ plans to conduct source apportionment analyses (e.g., Anthropogenic Precursor Culpability Assessment (APCA), Ozone Source Apportionment Technology (OSAT)) on the base and future case modeling to understand the contribution from source categories in various source regions to the predicted ozone concentrations.

Retrospective Analyses – A retrospective analysis is intended to examine the ability of the model to respond to emission changes by comparing a recent trend or change in observed ozone concentrations to the model-predicted ozone concentration trend or change over the same period. The TCEQ plans to use the model and the attainment test procedure to project year 2006 ozone design values (i.e., back-cast from the 2012 base case to year 2006), using previously-developed 2006 emissions data. The model-projected year 2006 ozone design values will be compared to the actual design values calculated from the ambient measurements.

These diagnostic analyses should establish the reliability of the model to adequately predict the response of ozone to changes in the emissions, which is paramount in testing possible control measures.

CHAPTER 10: ATTAINMENT YEAR MODELING

This Technical Description is intended to apply generically to the development of the 2012 modeling platform and not to any specific attainment demonstration. A 2017 statewide modeling inventory was prepared for the Dallas-Fort Worth attainment demonstration submitted to EPA in June 2016, and will be the basis for any additional 2017 modeling. The TCEQ will update the 2017 inventory and develop additional future years as necessary.

As per EPA guidance, the TCEQ will first calculate each nonattainment regulatory monitor's 2012 baseline design value (DV_B). The 2012 baseline for a monitor is the average of three design values from 2012, 2013, and 2014, each of which is itself a three-year average of fourth-high maximum daily 8-hour average (MDA8) ozone concentrations at that monitor. Each of these three design values includes the 2012 fourth-high in its three-year average. The 2012 baseline DV_B can thus be thought of as a five-year weighted average of fourth-high MDA8 ozone concentrations with weighting factors of 1, 2, 3, 2, and 1 applied to the fourth high values for 2010, 2011, 2012, 2013, and 2014, respectively; 2012 is given the most weight, followed by 2011 and 2013, with 2010 and 2014 receiving the least weight. The future design value (DV_F) is found by multiplying the DV_B by a modeled relative response factor (RRF) calculated as described below.

Each monitor's RRF will be calculated in accordance with the 2014 EPA draft modeling guidance. For a given monitor, the process is as follows: for each day modeled, locate the highest modeled MDA8 concentration "near" the monitor, specifically within a 3 x 3 grid cell array containing the monitor in the central cell. Next identify the ten (if available) days with the highest concentrations "near" the monitor, provided those concentrations are ≥ 60 parts per billion (ppb) (if fewer than five days have nearby MDA8 ozone concentrations ≥ 60 ppb, then no RRF will be calculated for that monitor). For the selected days, average the modeled baseline MDA8 concentrations and separately average the future modeled concentrations (using the modeled future case concentration from the grid cell having the maximum baseline concentration "near" the monitor). The monitor's RRF is then the ratio of the average future case MDA8 concentration to the average base case concentration.

The TCEQ will evaluate performance on each day selected for RRF calculations, and may in some cases replace days with poor performance at a monitor with days showing better model performance, as suggested in EPA's 2014 <u>Draft Modeling</u> <u>Guidance</u>.

Prior to release of the EPA's Modeled Attainment Test Software (MATS), the TCEQ developed its own procedure for calculating RRFs and DV_F values called the TCEQ Attainment Test for Unmonitored areas (TATU). Like MATS, TATU performs a spatial interpolation, so it can also be used to analyze unmonitored areas (i.e., an out-of-network test). While conceptually similar to MATS, TATU was designed specifically to be integrated into the TCEQ's CAMx modeling process, runs on Linux, and does not

require geographic coordinates be converted into Latitude/Longitude. This integration facilitates the calculation of RRFs, DV_F projections, and spatial interpolation. TATU originally was based on the familiar kriging process for spatial interpolation, but recently has been adapted to use the Voronoi Neighbor Averaging (VNA) technique employed in MATS. While kriging works very well in urban-scale applications it is difficult to apply in regional applications where data points tend to be relatively tightly clustered in widely-separated urban areas, so we anticipate using the VNA approach for modeling using the 2012 modeling platform but may also apply kriging in some circumstances.

CHAPTER 11: MODELING DOCUMENTATION AND ARCHIVE

11.1 DOCUMENTATION

The following supporting documentation will be developed to support the 2012 modeling platform:

Modeling Technical Description (this document) - Establishes the scope of the analysis and encourages stakeholder participation in both the study development and the study itself.

Modeling Reports – For specific applications of the 2012 modeling platform, reports describing in depth the development of emissions and meteorological inputs for base and future years, model application, model results, and conclusions will be developed as required.

11.2 MODELING ARCHIVE

The TCEQ plans to archive all documentation and modeling input/output files generated as part of the 2012 modeling platform. Interested parties can contact the TCEQ for information regarding data access or project documentation.

CHAPTER 12: BIBLIOGRAPHY

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ATTACHMENT 1: SAMPLE WRFCAMX PERFORMANCE ANALYSIS GRAPHICS FOR SELECTED SITES IN EASTERN TEXAS, JUNE 2012

This attachment compares Weather Research and Forecasting Model (WRF) output temperature, wind speed and direction, and humidity with observations at selected sites in eastern Texas for June 2012. All sites with available humidity data are included, as well as sites selected to provide a broad geographic representation.

DENTON (DFW)



GRAPEVINE (DFW)



ALDINE (HGB)


CLINTON DRIVE (HGB)



PARK PLACE (HGB)





AT1-7

DEER PARK (HGB)



MAURICEVILLE (BPA)



SABINE PASS (BPA)



LONGVIEW (NET)



CAMP BULLIS (SAT)



AUDOBON (ARR)



ARANSAS PASS (CCV)



ATTACHMENT 2: QUALITY ASSURANCE/QUALITY CONTROL (QA/QC) PLAN FOR THE TCEQ 2012 MODELING PLATFORM

In order to ensure that its photochemical modeling is conducted to the highest possible standards, the Texas Commission on Environmental Quality (TCEQ) performs a series of QA procedures on the input files to the various modeling components. All data, whether produced internally or externally by contractors, are examined. This document specifically addresses five aspects of the photochemical modeling process: emissions inputs, meteorological data inputs, photochemical model inputs, model execution, and output interpretation.

CHAPTER 1: EMISSIONS INPUTS QA/QC

Emissions inputs to the photochemical model are aggregated from a large number of sources and undergo many steps on the way to developing the spatially gridded, chemically speciated, hourly emissions arrays in FORTRAN binary file format that are read by the Comprehensive Air Quality Model with Extensions (CAMx) used by the TCEQ for regulatory modeling applications. Effectively managing the process by which these input files are created requires a great deal of scrutiny at each step; fortunately, the Emissions Processing Software, v.3 (EPS3) used for processing all anthropogenic emissions data has excellent reporting capabilities that facilitate performing thorough QA/QC on the data. In addition, most EPS3 modules create an ASCII output file containing records that were not processed because of missing or bad data called the Emissions Model ASCII Records (EMAR) file. Biogenic emissions of Gas and Aerosols from Nature (MEGAN).

Much QA/QC is based on examining plots that show emissions as they are allocated to the grid using visualizations tools developed at the TCEQ and elsewhere. *Figure 29: Tile Plot definition panel for QA/QC of CAMx-ready emission files* below shows the panel used to select the options for creating tile plots of emissions in CAMx input format. Plots can be created for selected episode, episode day, emission version, CAMx domain, emission category, and chemical species. The tile plot shown is for the 4 km Texas domain for Friday June 1, 2012 and shows on-road emissions of NO. Along with showing the spatial distribution of emissions in the 4 km domain (Mexican emissions are not shown), the plot also displays the temporal distribution of emissions and provides totals for nonattainment areas and other areas that have ozone concentrations approaching the NAAQS.

CAMx Modeling Emissions Inventory (CB6)

2012jun: June 1 - 30, 2012



Figure 29: Tile Plot definition panel for QA/QC of CAMx-ready emission files

1.1 ELEVATED SOURCE EMISSIONS

Unlike other emission sources that are allocated to specific grid cells in the first model layer, point sources are identified by their geographic location and emissions are allocated to horizontal and vertical grids by CAMx during processing. Horizontal grid allocation is determined simply by which grid cell (in each nested grid) the point lies in, but vertical cell positioning is performed dynamically for each hour of the simulation based on wind speed and vertical mixing coefficient.

1.1.1 Elevated Point Sources

The largest component of the elevated source input is point sources. Point source emissions come from several sources, including the State of Texas Air Reporting System (STARS), the Air Markets Program Data (AMPD), the EPA's 2011 modeling platform, and the Bureau of Ocean Energy Management's 2011 Gulf-Wide Emissions

Inventory (GWEI). The AMPD emissions are provided on an hourly basis, while other sources are supplied as either ozone season or yearly averaged daily emissions.

The STARS inventory contains emissions data for Texas major stationary sources including location, stack parameters, annual emissions rate, and in some cases typical hourly and daily operations. The TCEQ Emissions Assessment Section manages the STARS inventory, quality checks the results and maintains a database of the results. For any given year, modeling staff take several downloads (extracts) of the STARS database, and each download is compared to others from the same year to confirm that the download is complete. The number of point sources and emission totals for each pollutant is compared for the three most recent years. The number of points reporting emissions to the STARS database should not vary much from year to year, and any changes in the emission totals must be reasonable and assignable. To investigate the latter, the TCEQ compares the large NO_x , VOC, and SO_2 point sources over the last three years to identify sources that may require additional scrutiny. It is not unusual to have changes as point sources shut down, start up, or have upsets. Location and stack parameters are also screened for accuracy. Unreasonable stack dimensions and/or operating conditions are given default values. If a point is located more than three miles from the median of other points at the same site, then the point is relocated at the median.

Point source emissions from outside of Texas are acquired from EPA's 2011 Modeling Platform, which has been thoroughly peer-reviewed by Texas and other states affected by EPA's rules on interstate pollution transport. For all sources that report to the AMPD, the TCEO uses reported hourly NOx and SO2 emissions data from the AMPD to provide hourly emissions to the photochemical model. Procedurally, the hourly emission records replace their daily emission counterpart in the STARS sourced emission records. To assure that all of the AMPD data are successfully converted, annual pollutant emission totals are compared by site, hour, and day. The site comparison is the annual total for the year, the hour comparison is the hourly average over the entire year, and the day comparison is for each day of the year. In addition, the hourly emissions for a single (arbitrary) day are compared for each point source reporting emissions for that day. To keep from double counting emissions, the TCEQ maintains a cross reference file that links AMPD boiler identifiers (ORISPL and BLRID⁶) to STARS point source identifiers (FIPS, plant, stack, point). The cross reference is updated each time there is a new year of AMPD data to account for new sources. After QA of the above data is complete, the next step for all point source data is to read the raw data and write it out in the Aerometric Information Retrieval System (AIRS) Facility Subsystem (AFS) format. The TCEQ has written code in SAS and other computer languages to extract data from the various data sources and convert it to AFS format. Data quality checks performed to assure fidelity of the conversion process include comparing output emissions totals with input totals and with emissions totals from previous years.

Once the point source data have been successfully converted to AFS format, data are processed through the TCEQ's customized version of <u>EPS3</u>. The AFS records are input to the EPS3 entry module PREPNT, where the emissions are first screened to determine

⁶ ORISPL refers to the Office of Regulatory Information Systems Plant Location identifier; BLRID refers to Boiler identification code.

which sources will be treated as low-level and later dumped into the first-level grid using a conservative estimate of plume rise for the point. Currently a 30 meter (m) plume rise cutoff is used, which is slightly lower than the top of the first model layer (~34 m). Low-level points are not tracked individually and are treated like other lowlevel sources by EPS3. AMPD sources are always treated as elevated sources for EPS3 processing⁷.

PREPNT produces message files warning of processing errors or data issues, and produces a stack report; these reports are scanned for problems along with checking the EMAR file⁸. Next, the emissions are chemically speciated (i.e., VOC is disaggregated into Carbon Bond species) using the SPCEMS module. While some sources use default speciation profiles from EPA's Speciate database, most major Texas point sources (excluding electric generation units (EGUs), which emit only small amounts of VOC) report reasonably complete speciation of emissions by process. Custom speciation profiles are generated for these sources, translating the original hydrocarbon components into Carbon Bond species. After SPCEMS completes, input and output totals by category are checked for consistency and all discrepancies are investigated. SPCEMS also performs simple speciation for direct emissions of fine particulate matter $(PM_{2.5})^{9}$.

The next step is allocation of emissions temporally using the TMPRL module. AMPD sources are already reported as hourly totals, hence are not temporally allocated further. For the remaining sources any information available through STARS, such as operating hours per day or days per week are used to make reasonable guesses as to actual operating hours. The vast majority of non-EGU point sources are treated as operating 24/7. Again at this step input and output emission totals are checked for consistency. At this point the TMPRL output contains both low-level and elevated points. Processing of the low-level points will be discussed later.

After temporal and spatial allocation and chemical speciation are completed, the emissions are next read by the point source post-processing program PSTPNT, which drops sources identified by PREPNT as low-level, performs some additional error checks, and creates input files for the last step of processing for elevated points called PIGEMS. PIGEMS is run initially to create a master stack list, which is necessary for Plume-in-Grid (PiG) processing. This is because not all point sources may have emissions on every day modeled, so every single-day point source emissions file must be read into PIGEMS to create a complete master stack list¹⁰. PIGEMS is then executed

⁷ Note that elevated sources may still be assigned to the lowest model layer in CAMx, and it would be theoretically possible to treat all sources as elevated and let the model make the vertical layer assignment for each. The reason for maintaining low-level sources is that all low-level emissions in a grid cell are combined before input to CAMx, greatly reducing the number of individual sources that the model must account for.

⁸ The EMAR file is checked for erroneous records for all subsequent modules so will not be discussed henceforth.

⁹ Particulate matter chemistry is optional in CAMx and the TCEQ does not routinely run with it to save computational resources, but is required by the Community Model for Air Quality (CMAQ) which the TCEQ also runs to help inform the modeling process.

¹⁰ CAMx tracks individual plumes across days, and the master stack list allows plumes emitted on one day to be tracked even if the source had no emissions the following day.

again to provide day-specific emission files in CAMx-ready format. PIGEMS reports input and output emissions totals, which are checked for consistency.

1.1.2 Ship and Fire Emissions

Ships are modeled as elevated sources because their emissions may rise above the first model layer. Most emissions data for ships in and near Texas were developed under contract with the TCEQ, while emissions for more distant ocean waters are derived from the Ship Traffic, Energy and Environmental Model (STEEM). Emissions from larger vessels are spatially located along shipping lanes or in ports, while smaller vessels may be more spread out. The PRESHP preprocessor assigns the emissions to the center points of model grid cells. All offshore ship emissions are treated as elevated sources, but at this time emissions from ships on inland waterways such as the Mississippi River and Intracoastal Canal are assigned to the first model layer (these are included in the low-level off-road source emissions data, discussed below). The emissions are then processed through the SPECEMS and TMPRL processors for speciation and temporal allocation. The offshore shipping emissions are then finally post-processed into a CAMx-ready input file using the PSTSHP processor, which also distributes ship plumes vertically within the first two model layers based on ship classification.

Day-specific fire emissions are derived from the Fire Inventory from the National Center for Atmospheric Research (FINN). These emissions are entered into EPS3 via the PREFIR preprocessor as point sources. PREFIR assigns a time varying plume height to each fire and a recent update now allows fire plumes to be distributed among several vertical layers according to the size and intensity of the fire. The fire emissions are then processed through CHMSPL and TMPRL for speciation and temporal allocation, and then are written out in CAMx-ready format by the PSTFIR processor. Each of these modules used to process ship and fire emissions produces message files and reports which are scanned for potential problems.

1.1.3 Merged Elevated Emissions

All elevated emissions files are merged together for each modeled day using the PTSMRG processor. The output of this program is scanned for errors.

One of the biggest QA challenges is accounting for the large number of emissions files that must be assembled for each day modeled. Because elevated emissions derive from a myriad of sources, and because several of these are day-specific (e.g. AMPD emissions), the TCEQ creates summary lists of the files and tracks emissions of several pollutants as the files are merged into CAMx-ready inputs. These reports are assembled automatically by scanning the voluminous output from PIGEMS and consolidating the key information. Figure 30: *Sample Summary Report from Merging Elevated Emissions for June 8, 2012* shows a single-day excerpt from a report from one recent merge.

After ensuring that all elevated source emissions have been processed with no errors and emission totals have remained consistent throughout the several steps of processing, the model-ready elevated point-source emission files are plotted into a series of day-specific tile plots showing both the spatial and temporal distribution of emissions on each grid for each CB6 species. These plots are spot-checked to ensure the spatial and temporal allocations are reasonable and no anomalies are seen. Figure 31: *Elevated Source Emissions of NOX and VOC for June 14, 2012 in the CONUS (RPO) 36 km Domain,* Figure 32: *Elevated Source NO Emissions for June 14 and 25, 2012 in the Texas 12 km Domain, and* Figure 33: *Elevated Emissions of the CB6 Species PAR and ETH for June 25, 2012 in the Texas 4 km Domain* illustrate these plots for different days, domains, and precursors. Ship emissions are shown as linear features evident over ocean waters (shipping lanes). Fires are notable by their often intense but short-lived emissions; such a feature is noted by red circles in Figure 32 indicating the presence on June 14, 2012 and subsequent disappearance of a large fire in south-central New Mexico.

Component Files	NOx	VOC	ETHA	co
/ei/point/rpo eps3/pstpnt/tx ard/pstpnt.out.cb6p.120607.conus 36km.tx ard bc12e june hgb 8co.15Jun08	24,6017	1.5719	1.0308	25.6809
/ei/point/rpo eps3/pstpnt/tx ard/pstpnt.out.cb6p.120607.conus 36km.tx ard bc12e june dfw 10co.15Jun08	4.5435	1.0909	1.2472	8.8347
/ei/point/rpo eps3/pstpnt/tx ard/pstpnt.out.cb6p.120607.conus 36km.tx ard bc12e june no h d 18co.15Jun08	309.8680	9.5221	2.4487	454.7621
/ei/point/rpo eps3/pstpnt/tx osd/pstpnt.out.cb6p.120606.conus 36km.tx osd bc112d.mamp hqb 8co.14Jun25	58.1499	11.1701	3.1019	34.4806
/ei/point/rpo eps3/pstpnt/tx osd/pstpnt.out.cb6p.120606.conus 36km.tx osd bc112d.mamp dfw 10co.14Jun25	26.7942	9.8918	7.2488	32.0098
/ei/point/rpo eps3/pstpnt/tx osd/pstpnt.out.cb6p.120606.conus 36km.tx osd bc112d.mamp no h d 18co.14Jun25	309.1141	56.4467	35.1259	216.1837
/ei/point/rpo eps3/pstpnt/tx osd/pstpnt.out.cb6p.120606.conus 36km.tx osd bc112d.mamp fl hgb 8co.14Jun25	5.1255	22.4413	2.9434	22.7514
/ei/point/rpo eps3/pstpnt/tx osd/pstpnt.out.cb6p.120606.conus 36km.tx osd bc112d.mamp fl dfw 10co.14Jun25	0.2109	0.2691	0.0432	0.9112
/ei/point/rpo eps3/pstpnt/tx osd/pstpnt.out.cb6p.120606.conus 36km.tx osd bcl12d.mamp fl no h d 18co.14Jun25	7.1811	26.2483	3.7166	32.9265
/ei/point/rpo eps3/pstpnt/reg ard/pstpnt.out.cb6p.120607.conus 36km.reg ard bc12d june.15Jun08	4317.9755	72.1078	10.6490	1262.1636
/ei/point/rpo eps3/pstpnt/reg osd/pstpnt.out.cb6p.120608.conus 36km.ar osd b2011b.14Apr15	76.7227	20.6965	2.2664	86.6949
/ei/point/rpo eps3/pstpnt/reg osd/pstpnt.out.cb6p.120608.conus 36km.la osd b2011b.14Apr15	299.8634	40.7922	8.9238	199.7803
/ei/point/rpo_eps3/pstpnt/reg_osd/pstpnt.out.cb6p.120608.conus_36km.ok_osd_b2011b.14Apr15	171.4066	36.6386	1.3349	117.8905
/ei/point/rpo eps3/pstpnt/reg osd/pstpnt.out.cb6p.120608.conus 36km.no westarlacktx osd b2011b.14Apr15	2487.0868	414.5691	46.4788	3888.5008
/ei/point/rpo_eps3/pstpnt/reg_osd/pstpnt.out.cb6p.120608.conus_36km.west_azcaorwa_osd_b2011b.14Apr15	147.6332	17.2521	1.9596	260.0315
/ei/point/rpo eps3/pstpnt/os/pstpnt.out.cb6p.110601.conus 36km.gwei2011a.15Feb18	200.1846	43.7987	4.6465	156.2801
/ei/point/rpo eps3/pstpnt/mex/pstpnt.out.cb6p.120612.conus 36km.mex fy2012b MexID.15Jun18	978.4474	289.7415	7.6725	672.3840
/ei/point/rpo_eps3/pstpnt/reg_ont/pstpnt.out.cb05.060606.conus_36km.canada_2006.110ct12	1300.0675	2465.9203	1.5784	2527.1473
/ei/offroad/pstshp/el pstshp.out.cb6p.hg 1km.HGB 2007.fy2012b.15Aug03	23.9396	1.0781	0.0376	3.6296
/ei/offroad/pstshp/el_pstshp.out.cb6p.tx_4km.HGB_2007.fy2012b.15Jul31	3.8021	0.1635	0.0057	0.5778
/ei/offroad/pstshp/el_pstshp.out.cb6p.tx_4km.BPA_2011.by2012a.15Aug03	12.0702	0.5840	0.0204	2.5053
/ei/offroad/pstshp/el_pstshp.out.cb6p.tx_4km.epa_nearport_TX_CRUSM.fy2012a.15Aug05	16.4965	0.5348	0.0187	1.3426
/ei/offroad/pstshp/el_pstshp.out.cb6p.tx_12km.epa nearport TX_CRUSM.fy2012a.15Aug05	0.2385	0.0077	0.0003	0.0195
/ei/offroad/pstshp/el pstshp.out.cb6p.tx 4km.epa nearport noTX.fy2012a.15Aug05	2.9040	0.1192	0.0042	0.8679
/ei/offroad/pstshp/el_pstshp.out.cb6p.tx_12km.epa_nearport_noTX.fy2012a.15Aug05	52.0404	1.6536	0.0577	4.3721
/ei/offroad/pstshp/el_pstshp.out.cb6p.us_36km.epa_nearport_noTX.fy2012a.15Aug05	183.2944	6.0337	0.2105	16.3988
/ei/offroad/pstshp/el pstshp.out.cb6p.rpo 36km.epa nearport noTX.fy2012a.15Aug05	125.0437	4.3505	0.1518	11.5909
/ei/offroad/pstshp/el_pstshp.out.cb6p.tx_4km.STEEMships.fy2012a.15Aug05	99.2627	3.2174	0.1122	8.1469
/ei/offroad/pstshp/el_pstshp.out.cb6p.tx_12km.STEEMships.fy2012a.15Aug05	164.6428	5.3366	0.1862	13.5133
/ei/offroad/pstshp/el_pstshp.out.cb6p.us_36km.STEEMships.fy2012a.15Aug05	1134.0064	36.7554	1.2822	93.0743
/ei/offroad/pstshp/el_pstshp.out.cb6p.rpo_36km.STEEMships.fy2012a.15Aug05	1276.6310	41.3771	1.4434	104.7775
./ptsrc.finn_fires.RandTMPRL_PlumeDist2.20120607.tx.bc12_12all.rpo_36km.cb6	986.1862	2616.8043	61.7841	19100.0000
Totals (tons/day)	14800.0000	6258.1851	207.7311	29300.0000
USERIN file :TMP.userin.cb6.20120608.rpo 36km.17jun2015.camx				
Input master stack list file :master stk.pigems.cb6p.rpo 36km.bc12.r3d2.15Nov20				

Figure 30: Sample Summary Report from Merging Elevated Emissions for June 8, 2012



Figure 31: Elevated Source Emissions of NO_{x} and VOC for June 14, 2012 in the CONUS (RPO) 36 km Domain

Texas Elevated Point El, bc12_12jun.reg2i, 20120625: NO

(12x12km cells)

Texas Elevated Point El, bc12_12jun.reg2i, 20120614: NO

(12x12km cells



Figure 32: Elevated Source NO Emissions for June 14 and 25, 2012 in the Texas 12 km Domain



Figure 33: Elevated Emissions of the CB6 Species PAR and ETH for June 25, 2012 in the Texas 4 km Domain

1.2 LOW-LEVEL EMISSIONS

Low-level emissions consist of low-level points, area sources, non-road mobile sources, and on-road sources. Biogenic emissions are also low-level but are discussed separately. On-road emissions are divided into link-based and non-link-based emissions. Area, non-road, and non-link-based emissions are reported at the county or equivalent level and must be spatially allocated to grid cells using surrogates, while link-based emissions are assigned to grid cells based on the geographic coordinates of the roadway links. Low-level point source emissions are allocated based on their reported locations by PREPNT, as discussed above.

1.2.1 On-road Mobile Sources

For most cities, on-road mobile sources are the most important low-level emission source for air quality applications on an urban scale. The TCEQ devotes considerable resources to developing processing and quality-assuring this critically important input to the CAMx model.

1.2.1.1 Link-based on-road mobile source emissions

For the two largest urban areas in Texas, Houston-Galveston-Brazoria (HGB) and Dallas-Fort Worth (DFW), emissions are based on the travel-demand models used for a variety of urban planning purposes. Travel-demand models provide traffic volume by roadway segment (or "link") by time period, such as morning rush-hour. The traffic volume is the basis for calculating average speed by link, using factors such as roadway type and capacity, which in turn is fed into the MOVES model to provide emissions by link by period or hour. An important factor is vehicle mix, particularly fraction of heavy-duty diesel vehicles, which varies by time period. Emissions are developed separately for school year/non-school year and for specific days (Friday, Saturday, Sunday, and Weekday (Monday through Thursday)), and are provided for each hour of the day. The 2012 link-based emissions for DFW were developed by the North Central Texas Council of Governments (NCTCOG), and those for HGB by the Texas Transportation Institute (TTI), but under contract with and supervision of the TCEQ. Both organizations follow strict QA/QC protocols for developing these estimates.

The link-based emission files are first input to the LBASE module of EPS3, which allocates emissions to the modeling grid cells. The files are then speciated into CB6 species by SPCEMS profiles from EPA's SPECIATE database for on-road gasoline and diesel vehicles. The EPS3 message files and reports are scanned for errors, warnings, and inconsistencies.

1.2.1.2 Non-link-based on-road mobile source emissions

Link-based emissions are not developed for neighborhood streets by NCTCOG or TTI. Rather, neighborhood-level emissions are provided as county totals which must be spatially allocated using a spatial surrogate (population by census block) by the GRDEM module of EPS3. In the DFW and HGB areas, these are later added to the gridded link-based emissions using the MRGUAM module of EPS3. For all Texas counties outside the DFW and HGB areas, county-level emissions are provided by TTI for three day-types (Saturday, Sunday, Weekday) for school and non-school days for different roadway classifications, such as interstate highways, other freeways, and major highways. Emissions for major roads are spatially allocated according to roadway type while the remaining emissions are allocated to population. The emissions are allocated temporally using TMPRL and chemically speciated using the SPCEMS module. Message files and reports are scanned at each processing step for errors, warnings, and inconsistencies. For non-Texas on-road mobile emissions, the MOVES model is run in default mode for all U.S. counties to develop modeling inventories.

The final step in processing on-road mobile source emissions is to merge the linkbased and non-link based emissions using MRGUAM¹¹. The merged emissions are plotted in the same fashion as elevated points and the plots are checked visually for consistency and to identify any possible anomalies. Figure 34: *Summer Weekday On-Road NOX (L) and VOC (R) Emissions for* CONUS 36 km Domain (U.S. sources only), Figure 35: *Summer Weekday (L) and Sunday (R) On-Road Emissions of NO on the* **Texas 12 km Domain** (U.S. sources only), and Figure 36: *Summer Sunday On-Road Emissions of PAR (L) and ETH (R) on the* Texas 4 km Domain (U.S. sources only) illustrate these emission plots for different days, grids, and ozone precursors. A notable feature in Figure 34 is the seeming lack of a bimodal distribution for NO_x emissions for the CONUS domain, although the VOC temporal profile does show a morning peak associated with the morning rush hour. This seeming anomaly is the result of two

¹¹ Link-based and non-link-based on-road emissions are merged for the purpose of generating graphics and emissions tables used for illustration and QA/QC, but these merged files are not themselves used in making the final CAMx input files. Instead, all anthropogenic components are merged in a single MRGUAM run for each model day as described in Section 1.2.5

factors: first, the NO_x profile for the 12 km domain (**Figure 35**) shows a modest morning peak, while VOC emissions on the smaller grid (not shown) have a more pronounced peak. Second, the CONUS 36 km domain encompasses all four U.S. time zones, which smooths out the rush hour peaks when emissions for a single modeled hour are aggregated. Because the VOC peak is more pronounced, this smoothing effect does not completely erase its signature. This example illustrates the value of the emission tile plots as a QA tool in emissions modeling.



Figure 34: Summer Weekday On-Road NO_x (L) **and VOC** (R) **Emissions for CONUS 36 km Domain** (U.S. sources only)



On-road Mobile EI, MOVES, bl12,14Dec17, Sunday, summer; NO

On-road Mobile EI, MOVES, bl12,14Dec17, Weekday, summer; NO

Figure 35: Summer Weekday (L) and Sunday (R) On-Road Emissions of NO on the Texas 12 km Domain (U.S. sources only)



Figure 36: Summer Sunday On-Road Emissions of PAR (L) **and ETH** (R) **on the Texas 4 km Domain** (U.S. sources only)

1.2.2 Other low-level anthropogenic emissions

The remaining low-level emissions (excluding biogenic) fall into four broad categories: 1) Low level points consist of stationary sources that are emitted near ground-level and remain in the first vertical model layer. These include industrial plant fugitive emissions, small stationary engines, emergency generators, etc. Point source emissions are written to an EPS3 file by PREPNT, which identifies points to be treated as low-level. Most Texas low-level points from industrial facilities have source-specific VOC emission profiles from STARS. 2) *Non-road mobile sources* include boats, farm equipment, construction equipment, lawn and garden equipment, etc. Emissions for these sources are produced by the Texas Non-road (TexN) model for Texas sources and from the National Mobile Inventory Model (NMIM)¹² elsewhere except for two specific types of sources, locomotives and aircraft landing and takeoffs (often called, collectively with ships, *off-road mobile sources*). The former is produced by the Texas Railroad Emission Model, and the latter by TCEO contractors and local planning organizations. Emissions for Texas airports are airport-specific, and are provided by county for the rest of the country. 3) Area sources include a variety of sources (primarily VOC) including paints and solvents, service stations, and household natural gas usage, etc., and are retrieved from the Texas Air Emissions Repository (TexAER). 4) *Oil and gas sources* are treated separately because the emissions and spatial allocation are derived directly from data from the Texas Railroad Commission.

EPS3 again allocates emissions temporally with TMPRL and speciates them with SPCEMS. The final step in making CAMx-ready low-level files is GRDEM. It properly allocates emissions spatially to the model grids for run-streams that start as points, links or commonly, county totals. For example, GRDEM reads the point source emissions flagged by PREPNT as low-level and places emissions from sources identified as low-level points into the grid cells containing the respective point locations. Emissions starting with county totals, like most non-road and area sources, are assigned to grid cells by GRDEM using surrogate files. As an example, a surrogate like navigable water within a county is used for distributing boating emissions proportionally to only grid cells within a county containing lakes and rivers. Message files and reports are scanned at each processing step for errors, warnings, and inconsistencies. Prior to being merged into the CAMx-ready low emissions input files, several sub-categories are pre-merged and examined visually using emission tile plots similar to those shown earlier. Example plots of several categories are shown in Figure 37: U.S. Oil and Gas Production VOC Emissions on the CONUS 36 km Domain (L) and Texas Drilling NOX Emissions on the 12 km Domain (R), Figure 38: U.S. Non-Road Mobile *Source NOX Emissions (Excluding Oil and Gas Drilling) on the Texas 12 km Domain (L)* and Airport CO Emissions on the Texas 4 km Domain (R)., and Figure 39: U.S. Off-Road Mobile Source NOX Emissions (Railroads and Airports) on the Texas 12 km Domain (L) and Area Source Propane Emissions on the Texas 12 km Domain (R)below.

¹² NMIM was used to produce the non-Texas emissions currently in the 2012 platform, but future work will utilize the newly-available capabilities now available in the MOVES model.



Figure 37: U.S. Oil and Gas Production VOC Emissions on the CONUS 36 km Domain (L) and Texas Drilling NO_X Emissions on the 12 km Domain (R) Texas Non-road Mobile (No Olifare Drill Fight EL, bit 2, bit 3, Weekday, CO



Figure 38: U.S. Non-Road Mobile Source NO_x Emissions (Excluding Oil and Gas Drilling) on the Texas 12 km Domain (L) and Airport CO Emissions on the Texas 4 km Domain (R).



Figure 39: U.S. Off-Road Mobile Source NO_x Emissions (Railroads and Airports) on the Texas 12 km Domain (L) and Area Source Propane Emissions on the Texas 12 km Domain (R)

1.2.3 Biogenic Emissions

Biogenic emissions are developed using the Model of Emissions of Gases and Aerosols from Nature (MEGAN) emissions model. The TCEQ selected the MEGAN model because it is actively used and updated by a broad community and unlike the previously-used Global Biogenic Emissions Inventory System (GloBEIS), MEGAN runs on Linux. We have also run EPA's Biogenic Emissions Inventory System (BEIS) model and have compared emissions between the two systems. In general, MEGAN tends to over-predict isoprene emissions while BEIS under-predicts isoprene.

Inputs used include the default plant functional type (PFT) data and emission factors supplied with the model, leaf area index (LAI) values derived from the Moderate-Resolution Imaging Spectroradiometer (MODIS) global LAI MCD15A2 product, and photosynthetically-active radiation (PAR) extracted from the WRF runs. All output and message files and reports are scanned at each processing step for errors, warnings, and inconsistencies.

Tile plots are generated for each day, domain, and constituent of the emissions, and these are examined visually to check for inconsistencies, obvious errors or omissions, and other visible anomalies in the modeling. Figure 40: *Tile Plots of Biogenic Isoprene Emissions for June 1, 2012*: (L) **CB6 Emissions Generated Using MEGAN**, (R) **CB05 Emissions Generated Using BEIS**; Note different scales on diurnal profile plots compares emissions of isoprene generated by MEGAN with those generated by BEIS. While BEIS only outputs CB05 emissions, isoprene is treated identically by the two

mechanisms, so the spatial densities are comparable (note that the diurnal profile plots have different scales, however). The map totals show that for this day MEGAN generates nearly twice the emissions of isoprene as BEIS, and there are subtle differences in the shapes of the temporal profiles with BEIS emissions compressed slightly compared with MEGAN.



Figure 40: Tile Plots of Biogenic Isoprene Emissions for June 1, 2012: (L) CB6 Emissions Generated Using MEGAN, (R) CB05 Emissions Generated Using BEIS; Note different scales on diurnal profile plots.

1.2.4 Emissions of Halogen Compounds

Halogen chemistry was added to the CB6 chemical mechanism by Ramboll Environ under contract to the TCEQ in 2014 to address model over-prediction of ozone advected onshore from the Gulf of Mexico. The CB6 chemical mechanism that includes this option is named CB6h. Emissions of the various halogen compounds used by this mechanism are generated by running the SEASALT preprocessor, which takes land use and WRF-generated meteorology as inputs. Tile plots are generated for each day, domain, and halogen compound modeled, and these are examined visually to check for inconsistencies, obvious errors or omissions, and other visible anomalies in the modeling. Figure 41: *August 5, 2012 Emissions of (L) Iodomethane (CH3I) on the 4 km Domain; and (R) Sea* Salt Chloride (SSCL) on the 36 km Domain shows example tile plots of two halogen species used by the CB6h mechanism displayed on different domains.

If the halogen chemistry option is used, a second merge combining the halogen compounds with the merged low-level emissions file described above is generated for input to CAMx.



Figure 41: August 5, 2012 Emissions of (L) Iodomethane (CH3I) on the 4 km Domain; and (R) Sea Salt Chloride (SSCL) on the 36 km Domain

1.2.5 Merged Low-Level Emissions

Prior to input to CAMx, low-level emissions are merged into a single CAMx-ready input file using the MRGUAM processor of EPS3. Like PIGEMS, MRGUAM produces voluminous reports detailing the merging operation. The TCEQ runs scripts to extract summaries of the merge that ensure all files are accounted for and merged successfully. Figure 42: *Summary of Merge of Low-Level Emissions files for June 8, 2012 on the 12 km Domain* shows a merge of low-level anthropogenic emissions for a summer (i.e. non-school) Friday for the 12 km domain. To expedite processing, biogenic emissions, which change daily, are not included in this merge but are added to the low-level file in a separate, final merge to create day-specific CAMx-ready low-level emission files. Figure 43: *Summary of Merge of Anthropogenic and Biogenic Emissions for Four Days in May, 2012* shows a sample of the final merge for four days (Friday through Sunday) in May 2012 when school was in session.

message date: 16Jan13		
USERIN file :/ei/final/userin_files/userin.cb6p.20120608.tx_12km.anthro_merge		
Output UAM file :lo_ei.anthro.cb6p.fri.tx_12km.b112.r3f_summer		
Component Files	NOx_in	NOx_out
/ei/onroad/dfw/2012/grdem/tx_12km/lo_mv.grdem.cb6p.tx_12km.mvs14_hpms.dfw_10co_2012_sum_fri.14Dec10	183.5846	183.5846
/ei/onroad/dfw/2012/grdem/tx_12km/lo_mv.grdem.cb6p.tx_12km.mvs14_offn.dfw_10co_2012_sum_fri.14Dec10	28.1254	28.1254
/ei/onroad/dfm/2012/grdem/xx12km/lo mv.grdem.ob6p.tx12km.mv514_idle.dfw_10co_2012_sum_fri.14Dec10	7.1001	7.1001 10.6201
/ei/onroad/dfw/2012/grdem/tx_12km/lo_mv.grdem.cb6p.tx_12km.mvs14_hpms.hh_2co_2012_sum_fri.14Dec10 /ei/onroad/dfw/2012/grdem/tx_12km/lo_mv.grdem.cb6p.tx_12km.mvs14_offn.hh_2co_2012_sum_fri.14Dec10	10.6201 0.9186	0.9186
/ei/oncod/dfm/2012/grdem/vx_12km/lo_mv.grdem.cbGp.tx_12km.mv91_dle.hh_2co_2012_sum_fri.14Dec10	0.2193	0.2193
/ei/onroad/hgb/2012/grdem/tx_12km/lo_mv.grdem.cb6p.tx_12km.mvs14_hpms.hgb_8co_2012_sum_fri.14Dec10	139.0024	139.0024
/ei/onroad/hgb/2012/grdem/tx_12km/lo_mv.grdem.cb6p.tx_12km.mvs14_offn.hgb_8co_2012_sum_fri.14Dec10	26.1008	26.1008
/ei/onroad/hgb/2012/grdem/tx 12km/lo mv.grdem.cb6p.tx 12km.mvs14 idle.hgb 8cc 2012 sum fri.14Dec10 /ei/onroad/hgb/2012/grdem/tx 12km/lo mv.grdem.cb6p.tx 12km.mvs14 idle.hgb 8cc 2012 sum fri.14Dec10	5.9738 413.1002	5.9738 413.1002
/ei/onroad/tex/2012/grdem/tx_12km/lo_mv.grdem.cb6p.tx_12km.mvs14_hpms.etx_90co_2012_sum_fri.14Dec10 /ei/onroad/tex/2012/grdem/tx_12km/lo_mv.grdem.cb6p.tx_12km.mvs14_offn.etx_90co_2012_sum_fri.14Dec10	44.5342	44.5342
/ei/onroad/tex/2012/grdem/tx_12km/lo_mv.grdem.cb6p.tx_12km.mvs14_idle.etx_90co_2012_sum_fri.14Dec10	12.5635	12.5635
/ei/onroad/tex/2012/grdem/tx_12km/lo_mv.grdem.cb6p.tx_12km.mvs14_hpms.wtx_144co_2012_sum_fri.14Dec10	312.9261	312.9261
/ei/onroad/tex/2012/grdem/tx_12km/lo_mv.grdem.cb6p.tx_12km.mvs14_offn.wtx_144co_2012_sum_fri.14Dec10	27.8379	27.8379
/ei/onroad/tex/2012/grdem/tx_12km/lo_mv.grdem.cb6p.tx_12km.mvs14_idle.wtx_144co_2012_sum_fri.14Dec10 /ei/onroad/usa/2012/grdem/tx_12km/lo_mv.grdem.cb6p.tx_12km.mvs14_dflt.notx_ctz_2012_sum_fri.14Dec15	15.0171 1210.6140	15.0171 1210.6140
/ei/oncoad/usa/2012/grdem/tx 12km/10 mv.grdem.cbp.tx 12km.mvs14 uitv.notz_cts_cts_stristintictoets/ /ei/oncoad/usa/2012/grdem/tx 12km/10 mv.grdem.cbp.tx 12km.mvs14 ditt.notz tx mt 2012 sum fri.14Dec15	155.1471	155.1471
/ei/point/rpo_eps3/grdem/tx_osd/lo_pt.grdem.cb6p.120606.tx_121m.tx_osd_bc112d.mamp.hgb Bco.14Jun25	6.4644	6.4644
/ei/point/rpo_eps3/grdem/tx_osd/lo_pt.grdem.cb6p.120606.tx_12km.tx_osd_bc112d.mamp_dfw_10co.14Jun25	5.7183	5.7183
/ei/point/rpo eps3/grdem/tx osd/lo pt.grdem.cb6p.120606.tx 12km.tx osd bc112d.mamp.no.h.d.18co.14Jun25	72.0367	72.0367
/ei/point/rpo_eps3/grdem/reg_osd/lo_pt.grdem.cb6p.120608.tx_12km.ar_osd_b2011b.14Apr15 /ei/point/rpo_eps3/grdem/reg_osd/lo_pt.grdem.cb6p.120608.tx_12km.la_osd_b2011b.14Apr15	5.6836 23.8249	5.6836 23.8249
/ei/poins/rpo_eps/graem/reg_osd/io_pt.graem.coop.rvoud.xx_ltxm.rk_osd_ps/ulio_tapris /ei/poins/rpo_eps/graem/reg_osd/io_pt.graem.cobp.120608.tx_l2km.ok_osd_p2011b.14Apris	47.2828	47.2828
/ei/point/rpo_eps3/grdem/reg_osd/lo_pt.grdem.cb6p.120608.tx_12km.no_westarlaoktx_osd_b2011b.14kpr15	14.3100	14.3100
/ei/point/rpo_eps3/grdem/os/lo_pt.grdem.cb6p.110601.tx_12km.gwei2011a.15Feb18	26.9563	26.9563
/ei/nonroad/grdem/tx_12km/lo_nr.grdem.cb6n.wkd.tx_12km.NONROAD_12_b14_hgb8co.158ep09	50.7868	50.7868
/ei/nonroad/grdem/tx_12km/lo_nr_grdem.cb6n.vkd.tx_12km.WONROAD 12_b14_dfw10co.153ep09 /ei/nonroad/grdem/tx_12km/lo_nr_grdem.cb6n.vkd.tx_12km_WONROAD 12_b14_dfw10co.153ep09	64.5132 161.0184	64.5132 161.0184
/ei/nonroad/grdem/tx_12km/lo_nr.grdem.cb6n.wkd.tx_12km.NONROAD_12_b14_etx92co.153ep09 /ei/nonroad/grdem/tx_12km/lo_nr.grdem.cb6n.wkd.tx_12km.NONROAD_12_b14_wtx144co.153ep09	172.4068	172.4068
/ei/offroad/grdem/tx 12km/lo nr.grdem.cb6p.wkd.tx 12km.OFFR12 b10 switcher hgb8co.15Dec14	3.0862	3.0862
/ei/offroad/grdem/tx_12km/lo_nr.grdem.cb6p.wkd.tx_12km.OFFR12_b10_switcher_dfw10co.15Dec14	2.9727	2.9727
/ei/offroad/grdem/tx_12km/lo_nr.grdem.cb6p.wkd.tx_12km.OFFR12_b10_switcher_tx236co.15Dec14	7.0421	7.0421
/ei/offroad/grdem/tx_12km/lo_nr.grdem.cb6p.wkd.tx_12km.OFFR12_b10_linehaul_c1_hgb8co.15Dec15 /ei/offroad/grdem/tx_12km/lo_nr.grdem.cb6p.wkd.tx_12km.OFFR12_b10_linehaul_c2_hgb8co.15Dec15	11.9670 0.2911	11.9670 0.2911
/ei/offrod/grdem/xz_likm/lo_nr.grdem.cbop.wd.tx_likm.OFFR12_bl0_linehaul_c1_dfv10c.15Dec15	11.7332	11.7332
/ei/offroad/grdem/tx 12km/lo nr.grdem.cb6p.wkd.tx 12km.OFFR12 b10 linehaul c2 dfw10co.15Dec15	0.3666	0.3666
/ei/offroad/grdem/tx_12km/lo_nr.grdem.cb6p.wkd.tx_12km.OFFR12_b10_linehaul_c1_tx236co.15Dec15	99.6599	99.6599
/ei/offroad/grdem/tx 12km/lo nr.grdem.cb6p.wkd.tx 12km.OFFR12 b10 linehaul c2 tx236co.15Dec15	3.8905	3.8905 6.6989
/ei/nonroad/grdem/tx_12km/lo_nr.grdem.cb6p.wkd.tx_12km.NONROAD_12_b13_Drill_Rigs_Bt3pK_dfw10co.14Nov12 /ei/nonroad/grdem/tx_12km/lo_nr.grdem.cb6p.wkd.tx_12km.NONROAD_12_b13_Drill_Rigs_Bt3_no_dfw10co.14Nov12	2.8467	2.8467
/ei/norroad/grden/tx_121m/lo_nr.grdem.cbcp.wkd.tx_121m.NONROAD_12_b13_Drill_Rigs_tx_other_hgb8co.14Nov12	0.8097	0.8097
/ei/nonroad/grdem/tx_12km/lo_nr.grdem.cb6p.wkd.tx_12km.NONROAD_12_b13_Drill_Rigs_tx_other_no_hgb8co.14Nov12	8.5926	8.5926
/ei/nonroad/grdem/tx_12km/lo_nr.grdem.cb6p.wkd.tx_12km.NONROAD_12_b13_Drill_Rigs_EF3.14Nov12	45.1340	45.1340
/ei/nonroad/grdem/tx_12km/lo_nr.grdem.cb6p.wkd.tx_12km.NONROAD_12_b13_Drill_Rigs_HS.14Nov12	3.8845	3.8845
/ei/nonroad/grdem/tx_12km/lo_nr.grdem.cb6p.wkd.tx_12km.NONROAD_12_b13_Drill_Rigs_PB.14Nov12 /ei/offroad/grdem/tx_12km/lo_nr.grdem.cb6p.wkd.tx_12km.airports12_b9_hgb_8co.15Sep08	27.1092 6.2097	27.1092 6.2097
/ei/officad/gdem/tx 12km/lo nr.gdem.cbcp.rkd.tx 12km.airports12 b9 dfw 10co.1538p08	10.6110	10.6110
/ei/offroad/grdem/tx 12km/lo nr.grdem.cb6p.wkd.tx 12km.airports12 b9 tx 236co.15Sep08	3.5467	3.5467
/ei/offroad/grdem/tx_12km/lo_nr.grdem.cb6p.wkd.tx_12km.OFFR12_b8a_att_ships.133ep05	7.9450	7.9450
/ei/area/grdem/oilgasp/tx_12km/lo_ar.grdem.cb6p.wkd.tx_12km.area12d_oilgasp.BtSpK_dfw10co.15May05	19.3284	19.3284
/ei/area/grdem/oilgasp/tx_12km/lo_ar.grdem.cb6p.wkd.tx_12km.area12d_oilgasp.BtS_no_dfw10co.15May05 /ei/area/grdem/oilgasp/tx_12km/lo_ar.grdem.cb6p.wkd.tx_12km.area12d_oilgasp.tx_other_hgb8co.15May05	22.3370 2.0901	22.3370 2.0901
/e//area/grdem/oigdap/vs_intm/io_ar.grdem.cbcp.wkd.vs_interail_oigdap.ts_otme_modect.iomayoo /ei/area/grdem/oigdap/vs_12km/lo_ar.grdem.cb6p.wkd.vs_intax areail_oigdap.ts_otme_modect.iomayoo	145.8607	145.8607
/ei/area/grdem/oilgasp/tx_12hm/lo_ar.grdem.cb6p.wkd.tx_12km.area12d_oilgasp.HS_15May05	56.5518	56.5518
/ei/area/grdem/oilgasp/tx_12km/lo_ar.grdem.cb6p.wkd.tx_12km.area12d_oilgasp.EF3.15May05	186.0022	186.0022
/ei/area/grdem/oilgasp/tx_12km/lo_ar.grdem.cb6p.wkd.tx_12km.area12d_oilgasp.FB.15May05	104.3447	104.3447
/ei/area/grdem/oilgasp/tx_12km/lo_ar.grdem.cb6p.wkd.tx_12km.oilgasp2012_nei2011v1_noTX.130ct21 /ei/area/grdem/oilgasp/tx_12km/lo_ar.grdem.cb6p.wkd.tx_12km.offshore_oilgasp08.13Feb20	501.5931 0.7928	501.5931 0.7928
/ei/area/groem/oilgaap/sx_ii/m/lo_ar.groem.corp.wkd.sx_ii/m.orisnore_logbowl/iseo20 /ei/area/groem/area/sx_i2/m/lo_ar.groem.cofp.wkd.sx_i2/m.area12_v1_hgb8co.13Nov26	25.7895	25.7895
/ei/area/grdem/area/tx_12km/lo_ar.grdem.cb6p.wkd.tx_12km.area12_v1_dfw10co.13Nov26	29.6566	29.6566
/ei/area/grdem/area/tx_12km/lo_ar.grdem.cb6p.wkd.tx_12km.area12_v1_tx236co.13Nov26	62.0468	62.0468
/ei/nonroad/grdem/tx_12km/lo_nr_grdem.cb6p.wkd.tx_12km.nmim08a.2012_noTX.12Sep11	359.1385	359.1385
/ei/offroad/grdem/tx_12km/lo_nr.grdem.cb6p.wkd.tx_12km.by2012_nei2011v1_noTX_loco.130ct01 /ei/offroad/grdem/tx_12km/lo_nr.grdem.cb6p.wkd.tx_12km.fy12_nei2008v2_noTX_switchers.13Jun05	207.0049 15.5371	207.0049 15.5371
/ei/ofrroad/graam/x_liim/io_nr.graam.cbop.wka.tx_liim.tyiz_meiu000vz_noix_matchers.isuunuo /ei/ofrroad/graam/xx_liim/io_nr.graam.cb6p.wka.tx_liim.by2012_nei2000v2_noIX_harbor_vessel_inport_limited.133ep04	44.8730	44.8730
/ei/offroad/grdem/tx 12km/lo nr.grdem.cb6p.wkd.tx 12km.by2012 nei2008v2a noTX harbor vessel underway limited.13Sep04	112.7354	112.7354
/ei/offroad/grdem/tx_12km/lo_nr.grdem.cb6p.wkd.tx_12km.by12a_nei2008v2_noTX_airports.133ep10	16.3397	16.3397
/ei/area/grdem/area/tx_12km/lo_ar.grdem.cb6p.wkd.tx_12km.area2012_nei2011v1_noTX.13Oct10	239.2375	239.2375
/ei/offroad/grdem/tx_12km/lo_nr.grdem.cb6p.wkd.tx_12km.GWEInonplatform2011noCMV.15Jun11 ./mexico/lo_ei.anthro.cb6p.fri.tx_12km.b2012d.mexico_summer	697.9346 374.9864	697.9346 374.9864
.,		
NOx Total (tons/day)	6732.9658	6732.9658

Figure 42: Summary of Merge of Low-Level Emissions files for June 8, 2012 on the 12 km Domain



Figure 43: Summary of Merge of Anthropogenic and Biogenic Emissions for Four Days in May, 2012

CHAPTER 2: METEOROLOGICAL MODELING QA/QC

The WRF modeling system comprises several modules, including the WRF Preprocessing System (WPS), Real (vertical balancing of variables from pressure to sigma levels), ndown (nestdown), and various other modules that create inputs for the WRF model. WRF is executed in a two-way nested configuration commensurate with the WRF modeling domains.

Application of the WRF modeling system for a given episode requires specification of initial and boundary conditions, as well as model parameterizations as inputs to the various modules. Some of the inputs to the modules require pre-processing of raw meteorologically related data. The initial and boundary conditions are derived from global scale modeling performed by the National Centers for Environmental Prediction (NCEP). The NCEP conducts rigorous QA/QC of the global analysis fields before they are publicly released. The specifications for WRF include the surface parameters such as soil moisture, a planetary boundary layer (PBL) scheme, and cumulus parameterizations. Updates and quality assurance of new land use/land cover data and vegetative parameters have been incorporated with the assistance of National Oceanic and Atmospheric Administration interactive data language (IDL) scripting.

In addition, the TCEQ is using the four dimensional data assimilation capabilities of the WRF modeling system to conduct both analysis and observational nudging. The analysis data are also derived from pre-processing routines. The analysis nudging uses the NCEP Eta Data Assimilation System (EDAS) reanalysis wind fields on the 108, 36 and 12 km domains. The NCEP also conducts rigorous QA/QC on the EDAS reanalysis wind fields prior to public release. The TCEQ has built the observational nudging files from radar profiler wind data on the 4 km domain using a combination of SAS programs and Perl scripts. The output from the radar profiler pre-processing routine is

graphically inspected to ensure the wind data are reasonable. Desirable features include:

- Realistic vertical profiles of wind speed and wind direction; and
- Realistic diurnal pattern in the change of wind speed and wind direction.

Running the WRF modeling system requires verification through the namelist.input file that switches and options have been correctly selected. In addition, the surface characteristic parameters, e.g., soil moisture, are graphically inspected after running WPS, Real, and ndown to ensure they continue to be reasonable. To document quality assurance activities, a log file is created for the processing sequence of each of the preprocessors and WRF modeling system modules. This log file contains the name and location of the input and output files, the date the files were processed, and a brief description of the processing results. A sample of the log file for a WRF run is shown in Figure 44: *Sample Log File for a TCEQ WRF Run for June 2012*.

pdated on Novembe	r 24, 2015		
Select another log	record		
	Run Nam	e: 201206.wrf361.i2.87.2	8lyr
	Log Entry a	nd Quality Control (Log II	D: 416)
Run Staff	Khalid Al-Wali	Run Date	May 30, 2015
QA Staff	Khalid Al-Wali	QA Date	June 2, 2015
		Run Information	
Project Name	HGBMCR	Episode	June 1 - 30, 2012
Model	WRF 3.6.1	Domains	4km
	C	escription and Note	
Compilation File	configure.wrf [view]		
Model Setup File	C:\fakepath\namelist.input.RPO.2012-se	ason.ndown-3.pxa.YSU.W	/SM6.3dsfcC.cyclone.gq_sfc_0.2012.05.31.0 [view]
Other	This scenario includes 87 vertical levels Meteorological data used - NCEP NAM 40 No cumulus convective scheme Madis Obs Nudging profiler data 3D analysis nudging and hrly surface ana YSU scheme PBL (boundary-layer) Monin-Obukhov scheme (surface-layer) Pleim-Xiu Land Surface Model - soil mois sf_urban_physics set to 1 (which does no WRF with 87 levels CAMx with default 28	KM (grid 212) Ilysis nudging ture initialized from Ana ot impact model output if	

The raw WRF output is used to generate a set of time series and scatter plots that are primarily used to assess the model's performance, but examination of these plots can also reveal potential errors or inconsistencies in the model formulation. Figure 45: Time-Series Plots of Wind Speed and Direction, Temperature, *and Absolute Humidity Averaged across All Sites in the DFW Nonattainment Area for June 2012; Each panel shows (top) observed and modeled* values, (center) model bias, and (bottom) absolute error shows June 2012 hourly meteorological predictions, observations, and deviations averaged across the DFW area for a WRF run, and Figure 46: *Scatter Plots of Modeled vs.*

Observed (upper left) Wind Speed; (upper right) Wind Direction; (lower left) Temperature; and (lower right) Absolute Humidity; Day (red) and night (blue) values are color-coded, and error rates for specified thresholds are provided for each plot Figure 46: Scatter Plots of Modeled vs. Observed (upper left) Wind Speed; (upper right) Wind Direction; (lower left) Temperature; and (lower right) Absolute Humidity; Day (red) and night (blue) values are color-coded, and error rates for specified thresholds are provided for each plotshows a set of scatter plots comparing modeled and observed values of the same parameters, this time showing every hour in June 2012 for a single site, Houston Aldine (CAMS 8).



Figure 45: Time-Series Plots of Wind Speed and Direction, Temperature, and Absolute Humidity Averaged across All Sites in the DFW Nonattainment Area for June 2012; Each panel shows (top) observed and modeled values, (center) model bias, and (bottom) absolute error



Figure 46: Scatter Plots of Modeled vs. Observed (upper left) **Wind Speed;** (upper right) **Wind Direction;** (lower left) **Temperature; and** (lower right) **Absolute Humidity;** Day (red) and night (blue) values are color-coded, and error rates for specified thresholds are provided for each plot

After the WRF modeling has been completed, the output must be converted to a format that can be read by CAMx. This is accomplished by applying the WRFCAMx preprocessor to the raw WRF output. A large number of graphics displaying the WRFCAMx output is produced for each run, and these are used to both ensure successful completion of the process and to evaluate performance of the processed meteorological data to be input to CAMx. Three of the available time series are shown in Figure 47: *Selected Time Series for WRFCAMx Output at the Hinton Street Monitor*: (top) Observed and Modeled 10 m Wind Vectors; (middle) Observed and Modeled 2 m Temperature; and (bottom) Modeled Vertical Diffusivity (KV) and Planetary Boundary Layer (PBL) Depth (no observed PBL depth is available for this site) for the Hinton

Street site; in addition to 10 m wind vectors, 2 m temperatures, and vertical diffusivity (K_v) with planetary boundary layer (PBL) depth (shown), time series plots are also created automatically for 17 m winds and temperatures (center of first model layer), skin temperature, and layer 1 absolute humidity. Hourly wind maps are produced (see example plot in Figure 48: *Sample Wind Vector Plot for 4 km Domain, 03:00 CST, June 2, 2012*), providing a visual representation of layer 1 modeled wind fields overlaid with observations.



Figure 47: Selected Time Series for WRFCAMx Output at the Hinton Street Monitor: (top) **Observed and Modeled 10 m Wind Vectors;** (middle) **Observed and Modeled 2 m Temperature; and** (bottom) **Modeled Vertical Diffusivity (K**_v**) and Planetary Boundary Layer (PBL) Depth** (no observed PBL depth is available for this site)



Figure 48: Sample Wind Vector Plot for 4 km Domain, 03:00 CST, June 2, 2012

CHAPTER 3: INITIAL AND BOUNDARY CONDITIONS

Initial conditions (concentration data at the beginning of the simulation) and boundary conditions (time-varying concentrations alongside the outermost grid cells of the 36 km domain and (optionally) the top of the modeling domain) are generated by global models developed by contractors and provided to the TCEQ. The TCEQ receives global model output from the Goddard Earth Observing System model with Chemistry (<u>GEOS-Chem</u>) from the Goddard Earth Observing System model with Chemistry (<u>GEOS-Chem</u>) from the contractor, and the initial and boundary conditions are extracted using software supplied by the contractor. This process involves mapping the chemical species from the global model to CB6 and mapping the large global model grid cells onto the CAMx 36 km domain. The extraction runs are monitored to ensure successful completion and to check for any errors or warnings, and graphical displays are produced to allow visible inspection of the CAMx inputs as described below.

Initial conditions are extracted for the first hour of the CAMx simulation only. Figure 49: *Initial Concentrations of Ozone (L) and Olefins (R) at 0:00* on May 16, 2012 shows initial concentrations of ozone and the CB6 OLE (olefins) extracted for CAMx runs starting at 0:00 on May 16, 2012. The coarse grid cells of the global model are easily seen in the picture. Figure 50: *CAMx Lateral Boundary Conditions for June 23, 2013, 0:00 to 3:00* shows an example plot of lateral boundary conditions for 0:00 to 3:00 on June 23, 2012. Concentrations are represented by "curtain" plots showing the values for each vertical layer along the domain wall for the three-hour period (GEOS-Chem output was provided in three-hour intervals).



Layer 1 OLE Concentration of Initial Conditions Environ's GEOS-CHEM (a0) for rpo_36km domain (base 2012)



Figure 49: Initial Concentrations of Ozone (L) and Olefins (R) at 0:00 on May 16, 2012



O3 Concentration of Lateral Boundary Conditions Envrion's GEOS-CHEM for rpo_36km domain (2018 with 2012 met)



CHAPTER 4: OTHER CAMX INPUT FILES

Besides emissions and meteorological inputs, CAMx requires the following inputs:

- Chemistry Parameters The chemistry parameter files are supplied with CAMx and are specific to the chemical mechanism used; the appropriate file for the mechanism used (CB6) is specified in the run script. It is not edited and no QA is required (CAMx will terminate if this file is not specified).
- Ozone Column An ozone column file must be created for each day modeled, but this file can be built once and then used for subsequent runs unless the grid definition (including vertical layer structure) is modified. This file is created from archived satellite ozone measurements using a utility supplied with CAMx called O3MAP. Because this process is essentially automatic except for supplying the grid definition, QA of these files is accomplished simply by verifying successful completion of O3MAP and subsequent processing with CAMx.
- Photolysis Rates Like the Ozone column file, the photolysis rate files are generated by a program (TUV) developed and supplied by the National Center for Atmospheric Research (NCAR) and requires only minimal user input, specifically the output from the O3MAP program. As is the case with O3MAP, QA of these files is accomplished simply by verifying successful completion of O3MAP and subsequent processing with CAMx.
- Landuse File The Landuse file contains information on land surface characteristics that are important to atmospheric physicochemical processes such as surface reflectance (albedo) and deposition of atmospheric constituents like ozone. Land cover data are assigned to one of 26 classes used by the <u>Zhang</u> <u>dry deposition scheme</u>, although not all classes are used in the current application. In addition to the Zhang parameters, the landuse file contains the Leaf Area Index, a satellite product related to the density of foliage that is important in estimating dry deposition to foliage, and also an optional elevation file.

As these data are assembled into a single file, QA is accomplished through checking each process for errors. After the landuse file has been successfully assembled, additional QA is accomplished by examining graphical displays of the various components on each domain, as illustrated in Figure 51: *Three Components of the CAMx Landuse File*: (Top) Zhang Landuse Category 7, Deciduous Broadleaf Trees on the 4 km Domain; (Center) July 2012 Leaf Area Index on the 12 km Domain, and (Bottom) Surface Elevation on the 36 km Domain.



Figure 51: Three Components of the CAMx Landuse File: (Top) **Zhang Landuse Category 7, Deciduous Broadleaf Trees on the 4 km Domain;** (Center) **July 2012 Leaf Area Index on the 12 km Domain, and** (Bottom) **Surface Elevation on the 36 km Domain**

CHAPTER 5: CAMX EXECUTION

The TCEQ performs many simulations to test model performance, include revised inputs, and evaluate alternative model configurations. Each run is cataloged and a

detailed log entry describing the inputs and options chosen for that run is created. Figure 52: *Sample CAMx Run Log* shows a log entry from a recent CAMx run. At the bottom of the log entry is an option to view the job control file which defines the input files and specifies execution options. Job control files are kept in order to verify exactly what inputs and parameters went into the run.

Each run is checked for successful completion. Occasionally a run will halt due to network problems, power failures, or for reasons that are not entirely clear. CAMx maintains a restart file, which can be used to initialize the model at the end of the last successfully completed day. This feature is especially valuable for model runs of several episode weeks or longer.

As each day completes a number of output files are generated. When the entire run completes, these output files are read into a series of graphical and statistical analysis routines which are used to assess model performance and compare one run with another. Each run is analyzed, and any anomalies are noted. This serves as the final QA/QC step for each model run.

Air Quality Modeling Log Viewer

Updated on 2016-01-21

Select another log record

	Log Entry	and Quality Control	(Log ID: 1760)
Run Staff	Jim MacKay	Date	November 20, 2015
QC Staff	Weining Zhao	Date	November 22, 2015
		Run Information	
Project/Episode	TX: June 1 - 30, 2012		
AQ Model	CAMx 6.2s CB6r2h		
Run Name	bc12_12jun.r3d2_ss.2012_wrf361_p2a_i2_d	l	
Elevated El	bc12.r3d2		
Low-level El	bl12.r3d_ss32		
	Model Performa	ance Evaluation (MPE) Check List [view]
		Description and No	te
Meteorology	 WRF v3.6.1 - 2012_wrf361_p2 (pxa.YSU.KF.WSM pxa = Pleim-Xiu Land Surface Model (soil moister YSU = YSU PBL scheme KF = Kain-Fritsch cumulus WSM5 = WSM5 microphysics 3D-analysis nudging WRF v3.6.1 - 20120_wrf361_i2 (pxa.YSU.WSM6. pxa = Pleim-Xiu Land Surface Model (soil moister YSU = YSU PBL scheme WSM6 = WSM6 microphysics 3dsfc1h = hourly 3D and surface analysis nudging fdda = profiler data FDDA sf_urban_physicas set to 1 WRF2CAMx v4.2 CMAQ Kv and 100m Kv Patch (kv100) for all doi 29 vertical layers with one extra top layer (WR subgrid cloud diagnostic option with stratiform 	ure initalized from an 3dsfc1h.fdda.gqsfc0) ure initalized from an ng mains (_b) F sigma level 41) add	alysis) for tx_4km domain alysis) ed to the current standard layers (_d)
Biogenic El	MEGAN 2012_wrf361_p2.2012_qc108_urbfunc (B - MEGAN v2.10 - land cover: Guenther 2008 30 second data - temperature: WRF output from 2012_wrf361_ - PAR: WRF output through MCIP with 0.45 adju - LAI: 8-day MODIS 2006 LAI data with urban ce	p2 (12/36km) and 20 ustment factor ells filled according to k 17) for Developed O	12_wrf361_i2 (4km) five TCEQ urban land cover classes using a weighted pen Areas=3.3, Developed Low Intensity=2.3, Developed

Figure 24: Sample CAMx Run Log (continued on next page)

Point Source El	reg2g AFS listing: bc12jun.reg2p Point Source Emissions in tons/day reg2h AFS listing: bc12jun.reg2h Point Source Emissions in tons/day - elevated fires from FINN reg2i AFS listing: bc12jun.reg2i Point Source Emissions in tons/day reg3: More EGU ramp-up days added fro 15-28/Way2012. bc12jun.reg3 Point Source Emissions in tons/day reg3a: minor update of Gulf sources (June 2011); PM emissions bc12jun.reg3 Point Source Emissions in tons/day reg3a: minor update of Gulf sources (June 2011); PM emissions bc12jun.reg3a Point Source Emissions in tons/day rac - Mexico 2012 based on EPA 2011 Platform v2; Idaho EGUs FIPS fixed bc12.r3c Point Source Emissions in tons/day - Texas and US hourly AMPD (EGU) emissions for 2012; Idaho FIPS fixed. - Texas Ozone Season Day (OSD) from STARS 2012_v4b. - US OSD (except TX) from 2011 NEI/EPA Modeling Platform annual emissions. - Offshore platforms monthly emissions from June 2011 GWEI. - Mexico 2012 interpolation from EPA 2011 Platform v2 with 2008 EI. - Canada 2006 annual National Pollutant Release Inventory (MPRI) and Upsteam Oil and Gas (UOG) inventories from Environment Canada. r3d - fire and ship elevated El using new EPS3 with plume rise distribution override; PiG selection based on 2012 June to Sept (vs just June)	
Area/Non-Road Mobile El	reg2i: fires - elevated wild and agriculture fires reg3: PM emissions r3c: r3d: updated Mexico El	
On-Road Mobile El	reg3: MOVES2014 PM emissions r3c: r3d: updated Mexico El	
Others	CAMx 6.2s (6.20 speedup), CB6 r2h (halogen chemistry) CB6 BC/IC for rpo_36km from Environ's GEOS-CHEM (geos2camx v2.2), no TC LAI: monthly average of 8-day 1km resolution MODIS LAI data ACM2 vertical diffusion = false (use K-theory) ss = sea salt emissions (seasalt v3.2) ramp-up days: 20120516-20120530 (rpo_36km only), 20060531 (all three domains) 3D outputs for tx_4km domain MPI/OPM configuration: 7 MPI nodes and 8 OMP threads per node	
	Job Control File	[view]

Select another log record

Figure 52: Sample CAMx Run Log

CHAPTER 6: GEO-REFERENCED INTERACTIVE MODEL RESULTS EVALUATION AND ANALYSIS PROGRAM (GRIMREAPR)

The GRIMREAPr is a set of analysis tools developed by TCEQ staff to evaluate model results and assess model performance in a geographical frame of reference. In addition to the standard time-series, scatter plots, model performance statistics, etc. that are produced for each model run, the GRIMREAPr provides an interactive visualization environment which allows modelers to view static or animated concentration data for every CB6 species. The view can be zoomed in or out using the

cursor controls and can display differences between model runs and bias at monitoring sites, and displays time series of observed and modeled concentrations on command. GRIMREAPr also provides the capability to overlay the model run with satellite cloud imagery, radar imagery, and HySPLIT back or forward trajectories at user-selected sites. GRIMREAPr is a very powerful tool for analyzing model output and identifying possible errors or deficiencies in the model formulation. A more detailed description of GRIMREAPr with examples is available <u>here</u>.