Protocol for Eight-Hour Ozone Modeling of the Houston/Galveston/Brazoria Area

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List of Acronyms

AQP – Air Quality Planning
ARD – Acid Rain Data
Auto – GC – Automated Gas Chromatograph
BCs – Boundary Conditions
BPA – Beaumont-Port Arthur
CAIR2 – Clean Air Interstate Rule, Phase 2
CAMx – Comprehensive Air Model with Extensions
CBIV – Carbon Bond Mechanism, Version 4
CB05 – Carbon Bond Mechanism, Version 05
CENRAP/RPO – Central Region Air Program/Regional Planning Organization
CO – Carbon Monoxide
DERC – Discrete Emission Reduction Credit
DFW – Dallas-Fort Worth (nonattainment area)
DV – Design Value
EGAS – Economic Growth Analysis System
EGU – Electrical Generating Unit
EI – Emissions Inventory
EPA – United States Environmental Protection Agency
EPS3 – Emissions Processing System, Version 3
ERG – Eastern Research Group
ESAD – Emission Specific Attainment Demonstration
ETA-PBL – ETA Weather Model Planetary Boundary Layer Numerical Algorithm
FDDA – Four Dimensional Data Assimilation
GEOS – CHEM – Goddard Earth Observing Systems Chemistry Model
GloBEIS – Global Biosphere Emissions and Interactions System
HARC – Houston Advanced Research Center
HECT – HRVOC Emissions Cap and Trade
HC – Hydrocarbon
HGB – Houston-Galveston-Brazoria
H-GAC – Houston-Galveston Area Council
HRVOC – Highly Reactive Volatile Organic Compound
HSC – Houston Ship Channel
IPM – Integrated Planning Model
KM – Kilometer
KVs – Vertical Exchange Coefficient
LU/LC – Land-use Land-cover
MECT – Mass Emissions Cap and Trade
MM5 – Fifth Generation Meteorological Model
NAAQS – National Ambient Air Quality Standard
NASA – National Aeronautics and Space Administration
NCEP – National Centers for Environmental Prediction
NEI – National Emissions Inventory

NMIM – National Mobile Inventory Model
NOAA – National Oceanic and Atmospheric Administration
NOAH – NCEP - Oregon State Univ. - Air Force - Hydrological Research Laboratory
NO_X – Nitrogen Oxides
NO_Y – Nitrogen Species
O_3 – Ozone
OSD – Ozone Season Day
PAR – Photosynthetically Active Solar Radiation
PPB – Parts per Billion
PPB-C – Parts per Billion Carbon
PPBv – Parts per Billion by Volume
PSCFv2 – Potential Source Contribution Factor, version 2
REMI – Regional Economic Models, Inc.
RRF – Relative Response Factor
SI – Special [emissions] Inventory
SIP – State Implementation Plan
STARS – State of Texas Air Reporting System
STT – Sea Surface Temperature
TCEQ – Texas Commission on Environmental Quality
TexAER – Texas Air Emissions Repository
TexAQS II – Second [2006] Texas Air Quality Study
TNMHC – Total Non-Methane HydroCarbon
TPD – Tons Per Day
TTI – Texas Transportation Institute
TxDOT – Texas Department of Transportation
UT-CSR – University of Texas Center for Space Research

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1 SUMMARY

This protocol presents procedures the Texas Commission on Environmental Quality (TCEQ) is using or plans to use to model ozone in the Houston/Galveston/Brazoria (HGB) area with the Comprehensive Air Quality Model with Extensions (CAMx), an acceptable photochemical model (see Table 13.1; U.S. EPA, 2007). The focus of this modeling is to support attainment demonstration analyses for the eight-hour ozone standard using a future year of 2018. The modeling will use base case episodes from 2005 and 2006, including the 2006 Texas Air Quality Study (TexAQS II) intensive field monitoring period from August 1 through October 15, 2006. Modeling an extensive number of days will help ensure that control strategies (adopted or proposed) will be effective over the most prevalent meteorological conditions associated with the formation of unhealthy levels of ozone in the HGB nonattainment area. This modeling analysis will rely heavily upon data collected during both the TexAQS 2000 and TexAQS II and will incorporate recent scientific advancements as appropriate. The TexAQS II is yielding an immense set of air quality, meteorological, and emissions data which will significantly advance the science of ozone air pollution in Texas and elsewhere. The modeling provides a means of integrating all the disparate elements of both TexAQS studies, as well as recent advances in meteorological modeling, the emissions inventory, and the conceptual understanding of eight-hour ozone, into a holistic three-dimensional picture of the HGB airshed. This conceptual understanding will aid the study of the interplay of the many factors that drive formation of ozone in Houston.

The objective of this modeling protocol is to maintain and enhance the technical credibility of the study by establishing in advance agreed-upon procedures for conducting a successful modeling project. A second but potentially even more important objective of this modeling is to continue advancing the understanding of the many complex processes and interactions that cause ozone standard exceedances along the upper Texas coast. Section 2 of the protocol describes the study design, including the background, Texas air quality studies, managerial organizational structure, and schedule. Section 3 presents salient issues (e.g., episode selection) from the conceptual model for ozone formation in the HGB airshed, which provides a qualitative description of the region's ozone photochemistry and the many factors that collectively result in exceedances of the ozone standard. The remainder of the protocol describes the structure of the modeling system, the development of needed model databases, the plans for model performance evaluation, the procedures to determine whether proposed control strategies are sufficient to show attainment of the eight-hour ozone standard, and the procedures for documenting the study results.

This protocol reflects the current plans of the TCEQ modeling staff but may be modified to account for new science, better modeling tools, changes in resources, or other events. This protocol should be considered a living document, which changes as necessary to reflect the current plans of the TCEQ in coordination with EPA Region 6 and stakeholders via the Southeast Texas Photochemical Modeling Technical Committee (SETPMTC).

Current plans are to submit a State Implementation Plan (SIP) revision based on this modeling to EPA by April 15, 2010. The purpose of SIP revision is to satisfy requirements for an eight-hour ozone attainment demonstration.

2 MODELING/ANALYSIS STUDY DESIGN

This modeling protocol describes the procedures that will be used in the development of new ozone modeling for the HGB nonattainment area ozone SIP revision. These procedures generally conform to the recommendations set forth in the EPA document:
"Guidance on the Use of Models and Other Analyses for Demonstrating Attainment of Air Quality Goals for Ozone, $PM_{2.5}$, and Regional Haze, EPA-454/B-07-002. U.S. Environmental Protection Agency, Office of Air Quality Planning and Standards, Research Triangle Park, NC 27711. April 2007" (U.S. EPA, 2007).

As per the EPA guidance, this protocol 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 evaluation and interpretation of model results;
- procedures for using the model to determine whether proposed control strategies are sufficient to ensure attainment of the National Ambient Air Quality Standard (NAAQS); and
- documentation to be submitted to the regional EPA office for review.

2.1 Background

The 1990 Federal Clean Air Act (FCAA) Amendments established five classifications for ozone nonattainment areas based on the magnitude of the monitored one-hour ozone design values and established dates by which each classified area should attain the NAAQS. Based on the monitored one-hour ozone design value at that time, the HGB Consolidated Metropolitan Statistical Area (Brazoria, Chambers, Fort Bend, Galveston, Harris, Liberty, Montgomery, and Waller Counties) was classified severe-17, with an attainment date of 2007. Dating back to 1990, there have been six SIP revisions with supporting photochemical modeling addressing the one-hour ozone NAAQS. The most recent HGB SIP revision, submitted in December 2004, was approved by EPA on September 6, 2006.

With the change in the form of the ozone NAAQS from a one-hour standard to an eight-hour standard, in April 2004, EPA classified the HGB area (Figure 1: *Southeast Texas Gulf Coast Region*) as a moderate ozone nonattainment area with an attainment date of June 15, 2010. Ozone SIP revisions addressing the eight-hour ozone standard were due June 15, 2007. Ozone modeling conducted by the TCEQ for the SIP revision demonstrated that it was not possible to attain the eight-hour NAAQS in the HGB area by the prescribed attainment date.

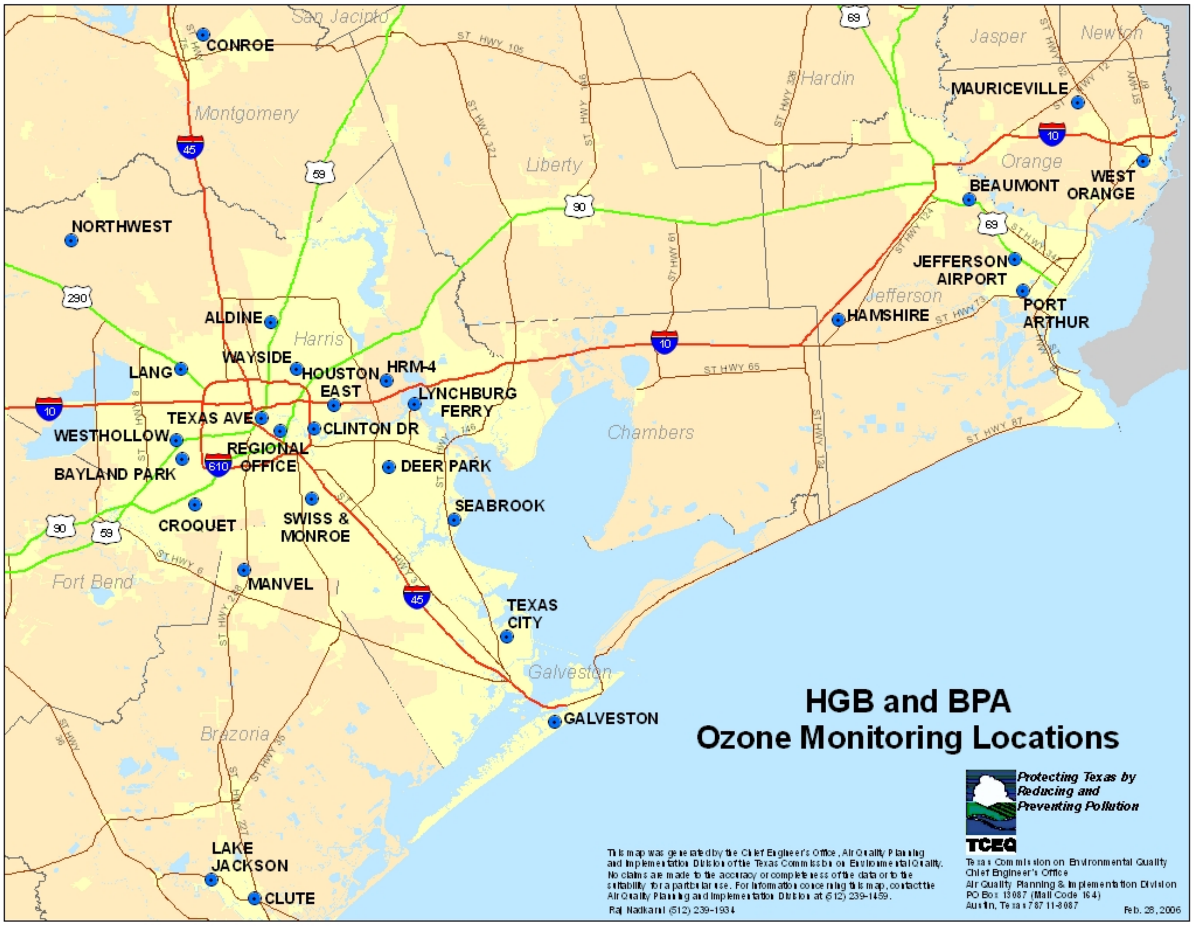

Figure 1: Southeast Texas Gulf Coast Region

Therefore, the ozone SIP revision submitted to EPA on June 15, 2007, included a request to reclassify the HGB area to severe, with an attainment date of June 15, 2019. Because the attainment date is early in the 2019 ozone season, the EPA has prescribed that the modeling attainment test be applied to the previous ozone season. Thus, 2018 is the attainment year used in this analysis.

The modeling presented in this protocol will focus on the modeling of new episodes from 2005 and 2006.

Table 1: *2006 to 2008 Eight-Hour Ozone Design Values for Pertinent HGB Monitoring Sites* lists the 2006 to 2008 eight-hour ozone design values, as well as the average of these design values, for monitoring sites in the HGB nonattainment area. The average of the 2006, 2007 and 2008 design values is the 2006 baseline design value (DV_B) used in the modeling attainment test. The area-wide highest eight-hour ozone DV_B is 96.7 ppb and occurs at the Bayland Park (BAYP, CAMS53) monitor, which is located on the west side of the Houston urban core.

Table 1: 2006 to 2008 Eight-Hour Ozone Design Values (ppb) for Pertinent HGB Monitoring Sites

Monitor Designation	CODE	2006 DV	2007 DV	2008 DV	DV_B
Houston East (C1)	HOEA	83	78	80	80.3
Aldine (C8)	HALC	88	84	83	85.0
Channelview (C15)	HCHV	85	83	80	82.7
NW Harris Co (C26)	HNWA	91	91	85	89.0
Galveston AP (C34)	GALV	83	81	82	82.0
Deer Park (C35)	DRPK	96	93	87	92.0
Seabrook (C45)	SBFP	90	86	80	85.3
Bayland Park (C53)	BAYP	**103**	**96**	**91**	**96.7**
Conroe (C78)	CNR2	85	84	80	83.0
Houston Rg-Off. (C81)	HROC	84	81	74	79.7
Manvel Croix (C84)	MACP	96	91	85	90.7
Clinton (C403)	C35C	85	79	73	79.0
Houston Wayside (C405)	HWAA	78	76	75	76.3
Houston Monroe (C406)	HSMA	99	91	81	90.3
Houston Lang (C408)	HLAA	80	77	76	77.7
Croquet (C409)	HCQA	94	87	80	87.0
Shell Westhollow (C410)	SHWH	96	92	89	92.3
Houston Tx-Av (C411)	HTCA	84	78	76	79.3
HRM3 (C603)	H03H	88	84	80	84.0
Wallisville Rd (C617)	WALV	93	93	90	92.0
Danciger C618	DNCG	83	80	78	80.3
Mustang Bayou (C619)	MSTG	89	84	81	84.7
Texas City (C620)	TXCT	90	84	79	84.3
Lynchburg (C1015)	LYNF	89	82	74	81.7
Lake Jackson (C1016)	LKJK	79	76	76	77.0

Analyses of ambient air quality data collected during TexAQS 2000, as well as the more recent TexAQS II, suggest that ozone formation in the HGB area stems from a combination of two types of emissions and conducive meteorological conditions. The first is the routine emissions of a large industrial base located in an urban core with point source, area source, on-road and non-road emissions typical of a city of over five million people. These emissions are characterized as base emissions and occur on any given day in the HGB area. Ozone forms steadily as the air mass in the airshed ages.

The second type of emissions is characterized as intermittent releases (emission events, e.g., maintenance activities, startups or shutdowns) of pollutants such as highly reactive volatile organic compound (HRVOC). Ozone forms rapidly when these concentrated HRVOC emission releases occur in the immediate presence of NO_X. Emission events can increase the magnitude of one-hour ozone peaks compared to those typically resulting from base emissions alone. While these concentrated emission releases can occur in any industrial area, the density of chemical and refining facilities makes their occurrence more likely in the HGB area. The contribution of these two emission types to ozone formation enhances the magnitude of the ozone concentrations in the HGB area.

The photochemical modeling supporting the one-hour ozone SIP revision (approved September 2006) included a dual control strategy, addressing the base emissions of routine emissions and the intermittent releases of HRVOC (emission events). With the change in the ozone NAAQS from a one-hour standard to an eight-hour standard, the one-hour modeling results were also analyzed for the eight-hour ozone standard. In accordance with Section 110 of the 1990 FCAAA, this latter analysis demonstrated that the proposed revisions to the SIP for the one-hour standard would not interfere with attainment of and reasonable further progress towards the eight-hour ozone standard. The June 2007 SIP revision, which addressed the eight-hour ozone standard, included rule revisions to implement additional emission reductions (e.g., low emission diesel fuel for marine sources, VOC emission reductions from storage vessels and degassing operations).

2.2 Texas Air Quality Studies, 2000 and 2006

From August 15 to September 15, 2000, approximately 250 investigators from more than 35 organizations joined the TCEQ in the TexAQS 2000 to carry out field research to improve the technical understanding of the factors affecting ozone and fine particle concentrations in the eastern half of Texas. TexAQS 2000 was based in Houston, and its work concentrated on the Houston region. TexAQS 2000 collected extensive data useful for supporting photochemical modeling of episodes that occurred during the study period. As a result of major findings from TexAQS 2000, the number of auto-GC monitors, particularly in the HGB area, was increased from three to 12. The majority of the new auto-GCs, which began operation in 2003, are industry-sponsored, and agreements have been developed with industry to extend their operation beyond 2009. The addition of the auto-GC data is expected to greatly enhance the modeling of episodes from 2005 and 2006.

TexAQS II was an 18 month project initiated in the latter part of the summer of 2005 concluding with a field intensive monitoring period from August 1 to October 15, 2006. Similar to TexAQS 2000, TexAQS II was funded, designed and implemented by numerous federal, state and private entities. To facilitate the timely integration of the TexAQS II findings into the eight-hour ozone SIP process, a Rapid Science Synthesis (RSS) component was included as a part of the TexAQS II study. The RSS is composed of teams of researchers assigned sets of specific science/technical questions pertinent to understanding and modeling ozone in the HGB area. The RSS results are expected to greatly enhance the modeling of episodes from 2005 and 2006. More information about TexAQS II is available at
http://www.tceq.state.tx.us/implementation/air/airmod/texaqs-files/TexAQS_II.html#2006data.

2.3 Technical and Policy Organizations

Several organizations provide input pertaining to the modeling and analysis.

2.3.1 Texas Environmental Research Consortium (TERC)

TERC was formed in 2001 and is composed of representatives from state government, Harris County, the City of Houston, academia, business, environmental and health professionals, and the Texas Clean Air Working Group (http://www.tercairquality.org/). The goal of TERC is to advance leading edge air quality science so that policymakers and regulatory agencies can make sound decisions when developing and implementing air quality legislation. In pursuit of this goal, the TERC Science Advisory Committee (SAC) has identified issues in several areas that require additional support:

- Scientific issues related to air emissions, chemistry, meteorology and modeling;
- Policy issues;
- Human Exposure issues;
- Methods for assessing progress; and
- Information dissemination.

The Houston Advanced Research Center (HARC) acts as the research management organization for TERC, contracting with researchers to provide additional support in the above identified areas (http://www.harc.edu/). HARC through TERC provides support of scientific research pertinent to SIP-related modeling for the HGB area. To the extent practicable and timely, TERC-sponsored scientific research results will be used in the current SIP modeling.

2.3.2 Southeast Texas Photochemical Modeling Technical Committee

The SETPMTC serves in an advisory role for the technical aspects of applying photochemical modeling and improving the science. The TCEQ meets bimonthly with SETPMTC members to review modeling progress. Meeting material (e.g., agendas, technical presentations) can be found at http://www.tceq.state.tx.us/implementation/air/airmod/committee/pmtc_set.html and the membership of this committee can be found at http://www.tceq.state.tx.us/implementation/air/airmod/committee/pmtc_set_members.html.

2.3.3 Modeling/Analysis Policy Group

The TCEQ meets periodically with the Regional Air Quality Planning Committee (RAQPC) to discuss relevant regulatory policy issues. RAQPC provides oversight and review of photochemical modeling as related to development of the SIP and policy implications. RAQPC is composed of representatives from local governments, business/industry, environmental groups, and the public and works directly with TCEQ and EPA on regulatory policy issues. RAQPC is coordinated by the Houston-Galveston Area Council (H-GAC), the metropolitan planning organization for the HGB area. The membership of this committee can be found at http://www.h-gac.com/taq/airquality/raqpc/default.aspx.

2.4 Management Structure and Modeling/Analysis Schedule

The Air Modeling and Data Analysis (AMDA) section has the responsibility for planning and conducting the eight-hour ozone SIP modeling. AMDA is part of the Air Quality Division of the Chief Engineer’s Office (CEO) of the TCEQ. The CEO organization chart is shown in Figure 2: *Management Organization Chart*.

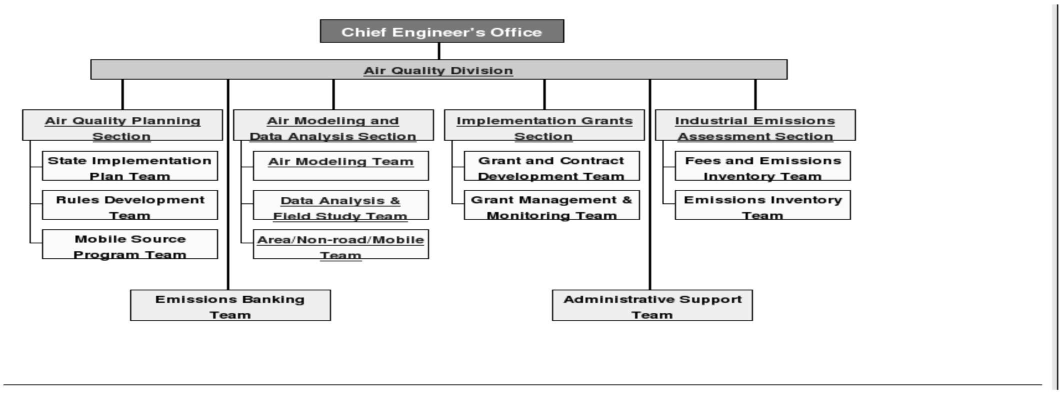

Figure 2: Management Organization Chart

Table 2: *Schedule of 2005 and 2006 Episode Modeling Activities for HGB* and Table 3: *Schedule of Attainment Modeling Activities for HGB* list the activities for this eight-hour modeling analysis and projected completion dates for the 2005 and 2006 episodes, respectively. Detailed discussions of most of these activities can be found later in this document.

Table 2: Schedule of 2005 and 2006 Episode Modeling Activities for HGB

2005 Modeling Episodes	
Conduct base case modeling and complete current baseline modeling • Conduct meteorological modeling • Conduct emissions modeling and processing • Conduct model performance evaluations	October 2006 – June 2008
2006 Modeling Episodes	
Conduct base case modeling and complete current baseline modeling • Conduct meteorological modeling • Conduct emissions modeling and processing • Conduct model performance evaluations	December 2006 - August 2008

Table 3: Schedule of Attainment Modeling Activities for HGB

Attainment Modeling	
Conduct Baseline Modeling • Develop 2006 baseline emissions • Conduct 2006 baseline modeling	September 2008 – January 2009
Conduct future baseline modeling with current controls and project future design values • Develop 2018 future baseline emissions with applicable growth and current controls • Project future design values • Conduct VOC/NO_X matrix modeling (estimating additional emission reductions) Conduct attainment modeling with current and proposed controls • Develop emission control modeling files • Conduct modeling sensitivity runs • Conduct attainment modeling with selected controls	September 2008 -- March 2009

3 CONCEPTUAL MODEL OF OZONE FORMATION IN THE HGB AIRSHED

A conceptual model describes the major factors affecting ozone formation and their interrelationships. The primary purpose of the conceptual model is to provide a basis for qualitative model performance evaluation, that is, to determine whether the model replicates major features described in the conceptual model. In addition, the conceptual model can be a guide to selecting modeling episodes.

In general, ozone forms in the Houston-Galveston-Brazoria (HGB) area as a result of complex interactions between coastal meteorology, emissions of ozone precursors and atmospheric chemistry. In the HGB area, each of these three factors is complex in its own right. The coastal meteorology of the HGB area during ozone events is dominated by the land/sea/bay breeze circulations and how they interact with larger-scale synoptic forcing, such as the typical summertime high pressure over the Gulf of Mexico. The VOC emissions from industrial facilities in Houston can vary in magnitude from day to day, and the mixtures of VOCs emitted can vary greatly from facility to facility. In addition, there is a wealth of biogenic emitted VOCs in and around the HGB area. The NO_X emissions in Houston originate from the typical point, area, and on-road and non-road mobile sources found in most large cities, but they are supplemented by large point source emissions from industrial and petrochemical sources, international and local shipping, and emissions from port activities, which are collocated with sources emitting reactive VOCs. The atmospheric chemistry in HGB is complex because of the unique mixture of VOCs that are emitted in the industrial areas, which can combine with the relatively common mixture of ozone precursors emitted in the urban areas.

Of these major factors (i.e., meteorology, emissions and chemistry), the meteorology has the predominant influence on whether an ozone exceedance day (i.e., eight-hour ozone $\geq$ 85 ppb) occurs. This is in part because of its variability, for example, assuming a particular emissions level, high ozone is more likely to occur on a hot sunny day with stagnant winds than on rainy or windy days, because under the former situation, conditions are conducive to ozone formation and accumulation. The meteorological conditions resulting from the interaction of the effects from local scale land sea breeze and synoptic scale high pressure over the Gulf of Mexico are most frequently associated with ozone exceedances in the HGB area.

On days with a very light synoptic scale influence, the local scale land sea breeze dominates, creating coastal oscillation effects due to the temperature gradient between the land and the water. As the land heats during the day, the air rises inducing a sea breeze (onshore flow). At night as the land cools below the temperature of the water, the winds reverse resulting in a land breeze (offshore flow). The land breeze, occurring as it does in the late night and early morning hours, carries ozone precursors out over Galveston Bay and the Gulf of Mexico. As the sun heats up the land, it also initiates photochemistry, such that when the wind reverses to an onshore flow, ozone laden air is carried over the HGB area.

On days when the synoptic scale and local scale effects balance one another, conditions are even more conducive for ozone formation and accumulation because the balance of forces can create an extended period of stagnation. The location and strength of the synoptic scale high pressure determines when and where stagnation occurs. High ozone tends to occur if the emissions that pool during the period of stagnation are exposed to strong sunlight before they can disperse (Nielsen-Gammon et al., 2005; Banta et al., 2006). The presence of Galveston Bay influences the coastal oscillation because the temperature gradient between the bay and the land can result in a bay breeze, which usually arrives in the city each day before the gulf breeze (Banta et al., 2006; Darby, 2006; Nielsen-Gammon et al., 2005) .

A compilation of surface wind data from the TCEQ monitoring network during eight-hour ozone exceedance days during August and September, 1998 through 2005 (Figure 3: *Hodogram of Hourly Resultant Winds; Eight-Hour Exceedance Days, Aug. – Sept. 1998 – 2006*) shows a diurnal clockwise rotational veering wind pattern associated with eight-hour ozone exceedance days. This wind pattern is consistent with the interaction of the effects from local scale land sea breeze and synoptic scale high pressure over the Gulf of Mexico, which result in the late night and early morning land breeze switching to a bay and gulf breeze in the late morning to early nighttime.

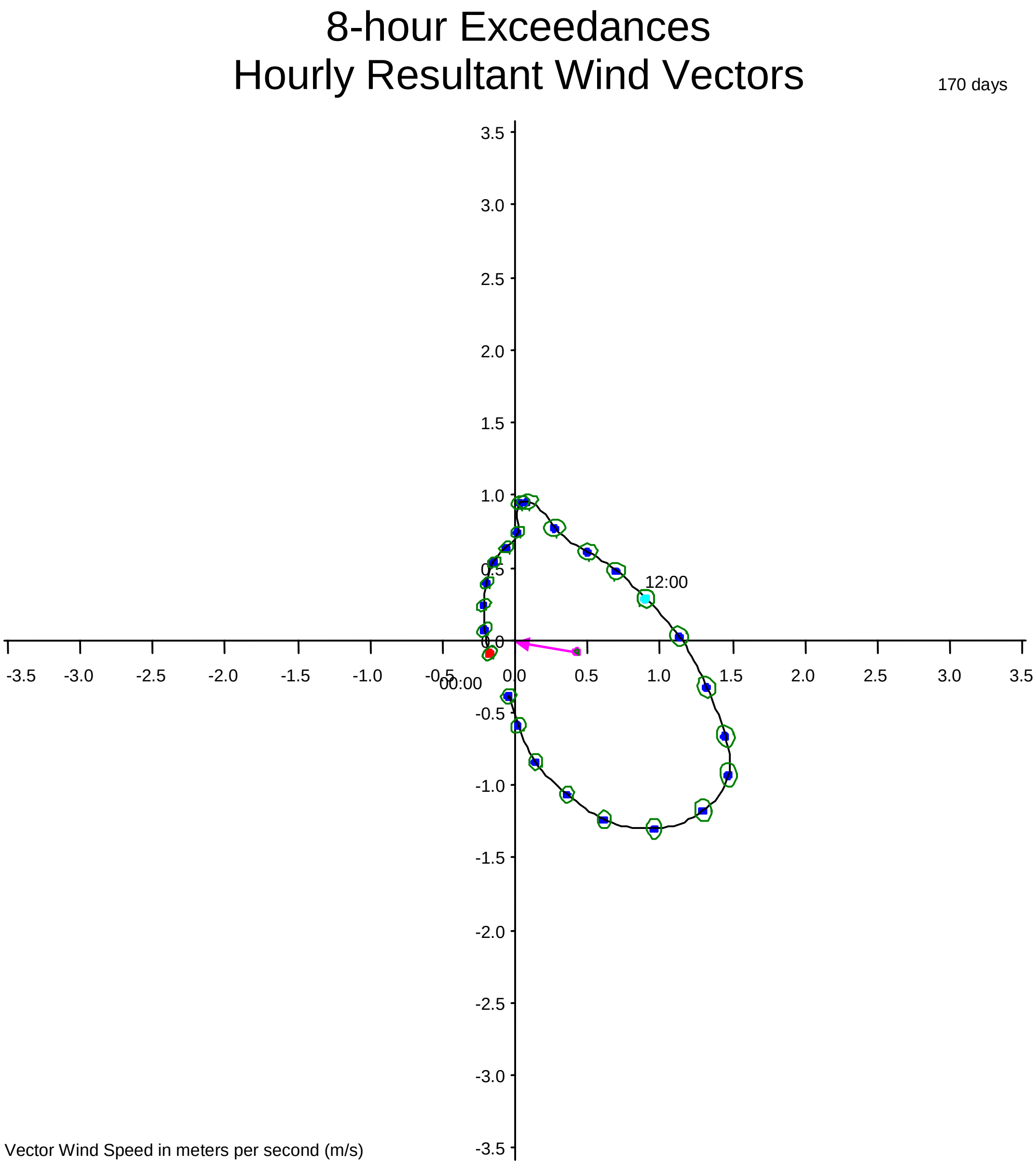

Figure 3: Hodogram of Hourly Resultant Winds; Eight-Hour Exceedance Days, 2000 – 2006

Although the diurnal clockwise rotational veering wind pattern is most often associated with eight-hour ozone exceedance days, there are a couple of other surface wind patterns associated with eight-hour ozone exceedance days, although they occur less frequently. The second most frequent surface wind pattern associated with eight-hour ozone exceedance days is called a "Flow Reversal." The flow reversal pattern is also consistent with the interaction of the effects from local scale land sea breeze and synoptic scale high pressure over the Gulf of Mexico. However, in this pattern, the switch from a land breeze to a sea breeze happens over a much shorter period of time.

Another surface wind pattern occasionally associated with eight-hour ozone exceedance days, which is not consistent with the land/sea breeze phenomenon, is characterized by light but consistent winds with northerly and easterly components. This surface wind pattern is consistent with the easterly migration through the northern plains (mid-latitudes) of synoptic scale high pressure systems that can transport air with a relatively high ozone background concentration into the HGB area.

The TexAQS 2000 and TexAQS II studies have provided extensive data and information on the interactions between coastal meteorology, emissions of ozone precursors and atmospheric chemistry that result in ozone formation in the HGB area. The TCEQ uses these findings in a continuing process to improve the conceptual model of ozone formation in the HGB area. Appendix A: *Houston-Galveston-Brazoria Nonattainment Area Ozone Conceptual Model* and Appendix B: *Final Rapid Science Synthesis Report* provide SIP-relevant findings from the TexAQS 2000 and TexAQS II studies and describes the major factors affecting ozone formation and their interrelationships. For example, these findings indicate that on a number of the days with some of the highest daily maximum ozone concentrations measured at monitors to the southwest and west of the Houston city core, elevated concentrations of ozone precursors (e.g., NO_X, HRVOC) from the Houston Ship Channel, suitably mixed and irradiated, are transported by the clockwise rotational veering wind pattern.

4 SELECTION OF EPISODES

The TexAQS 2000 episode was well suited to SIP modeling for the one-hour ozone NAAQS and the initial eight-hour NAAQS analysis. However, there are several advantages to selecting new episodes for eight-hour ozone SIP modeling. Many regulatory and demographic changes have occurred since 2000, which mean there will be more confidence in analyses based on more recent episodes. In addition, episodes from 2005 and 2006 can take advantage of the TexAQS II data and findings, especially during the August 1 - October 15, 2006, intensive field campaign. Selecting a number of episodes is useful because with a large number of days it is more likely that the frequency of days associated with various ozone-conducive wind patterns will be consistent with the conceptual model. In addition, the eight-hour attainment test benefits from including a large number of days with modeled peak ozone concentrations near each monitor's design value. Using several episodes from 2005 and 2006 also complies with the primary criteria set forth in EPA's eight-hour ozone modeling guidance for selecting ozone episodes for eight-hour ozone attainment demonstration modeling (U.S. EPA, 2007):

1. Select a mix of episodes reflecting a variety of meteorological conditions that frequently correspond with observed eight-hour daily maximum ozone concentrations greater than 84 ppb at different monitoring sites;

2. Select periods during which observed eight-hour ozone concentrations are close to the eight-hour ozone Design Value at each key monitor;

3. Select periods for which extensive air quality/meteorological databases exist; and

4. Model a sufficient number of days so that the modeled attainment test can be applied at all of the ozone monitoring sites that are in violation of the NAAQS.

Because the period of the TexAQS II field intensive provides an extraordinarily rich data base on which to evaluate hypotheses and validate modeling results, episodes have been selected from this period. However, due to the paucity of ozone exceedance days which occurred during the TexAQS II field intensive, ozone exceedance days that occurred earlier in 2006 and during 2005 were also identified as candidate episodes. With consensus from the SETPMTC, the TCEQ has selected three episodes from 2005, and one episode from 2006 prior to the TexAQS II field intensive period. Table 4: *Selected Episodes* summarizes the dates of the selected episodes.

Table 4: Selected Episodes

Period of Episode	Number of Exceedance days
5/19/05 – 6/3/05	8
6/15/05 – 6/30/05	9
7/26/05 – 8/8/05	8
5/31/06 – 6/15/06	12
8/1/06 – 10/15/06	15*

* Not all the exceedance days may be used.

EPA guidance recommends at least 10 days with an eight-hour ozone concentration at or above 85 ppb threshold in the Relative Response Factor (RRF) calculation for each nonattainment monitoring site. Although the guidance indicates that the threshold can be reduced to 70 ppb in order to get at least 10 days, the model response to emission reductions may diminish for lower modeled concentrations (Figure 4.1, U.S. EPA, 2007). The TCEQ will work with the EPA, Region 6 to select the appropriate days to use in the RRF calculation for each monitor without unrealistically dampening model response to future emission reductions by basing the calculation on unrepresentatively low values.

Table 5: *Possible RRF Applicable Days at Various Minimum Threshold Ozone Concentrations (ppb) for 2005/2006 Nonattainment Monitors* shows the number of days with monitored concentrations at or above various thresholds for each of the HGB nonattainment monitors. Although the RRF is based on modeled rather than monitored days, the summary of monitored ozone concentrations suggests that at a 70 ppb threshold, there will likely be at least 10 modeled days for the RRF calculation at each monitor, with the possible exception of Clinton (C35C, CAMS 403).

Table 5: Possible RRF Applicable Days at Various Minimum Threshold Ozone Concentrations (ppb) for 2005/2006 Nonattainment Monitors

Monitor Designation	CODE	Days ≥ 70	Days ≥ 80	Days ≥ 85
Houston East (C1)	HOEA	19	9	7
Aldine (C8)	HALC	29	8	5
Channelview (C15)	HCHV	21	5	5
NW Harris Co (C26)	HNWA	34	21	13
Galveston AP (C34)	GALV	14	5	3
Deer Park (C35)	DRPK	34	15	10
Seabrook (C45)	SBFP	31	15	8
Bayland Park (C53)	BAYP	34	19	14
Conroe (C78)	CONR	20	7	5
Houston Rg-Off. (C81)	HROC	26	10	9
Manvel Croix (C84)	MACP	38	19	16
Clinton (C403)	C35C	9	4	1
Houston Monroe (C406)	HSMA	28	14	10
Croquet (C409)	HCQA	23	12	8
Shell Westhollow (C410)	SHWH	27	19	12
Houston Tx-Av (C411)	HTCA	18	5	1
HRM3 (C603)	H03H	30	17	6
Wallisville Rd (C617)	WALV	35	16	12
Mustang Bayou (C619)	MSTG	21	11	4
Tx-City (C620)	TXCT	26	9	5
Lynchburg (C1015)	LYNF	30	9	8

5 MODELS AND MODELING INPUTS

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 emissions models selected need to interface effectively.

5.1 Model Selection

5.1.1 Selection of Air Quality Model

To ensure that a modeling study can be successfully used as technical support for an attainment demonstration SIP, 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 be convinced of the suitability of the model. The following three prerequisites were identified for selecting the air quality model to be used in the HGB attainment demonstration:

- Must have a reasonably current, peer-reviewed, scientific formulation.
- Must be available at no or low cost to stakeholders.
- 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 CAMx. The model is based on well-established treatments of advection, diffusion, deposition, and chemistry. Another important feature is that NO_X emissions from large point sources can be treated with the plume-in-grid submodel that 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 at http://www.camx.com. In addition, the TCEQ has many years of experience with CAMx. CAMx was used for the modeling conducted in the DFW and BPA nonattainment areas, as well as for modeling being conducted in other areas of Texas (e.g., San Antonio).

The TCEQ plans to use CAMx, Version 4.53 which includes a number of upgrades and new features. Some of the upgrades and features the TCEQ plans to use in this application include:

Parallel Processing - Multi-processor support is now fully included in CAMx,

Piecewise Parabolic Method (PPM) advection solver – The PPM solver may include less numerical diffusion and may be easier to accommodate future improvements to horizontal mixing with than the Smolarkiewicz solver,

CMC fast chemistry solvers for CB05 - The CMC solver provides a ten-fold speedup in the chemistry solution and is compatible with the updated CB05 mechanism, and

Flexi-nesting option - Flexi-Nesting allows nested grids to be introduced during a simulation (at a restart) and allows CAMx to interpolate any or all of the input data for a nested grid from parent grids.

In addition, the TCEQ plans to use some of the probing tools supported by CAMx4.53 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. Process analysis 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 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 noncontrollable precursor. APCA would only attribute ozone production to biogenic emissions when ozone formation is due to the interaction of biogenic 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.

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

5.1.2 Selection of Meteorological Model

Currently the two most common state-of-the-science prognostic meteorological models used to provide input to an air quality model are the Regional Atmospheric Modeling System (RAMS) and the Penn State University/National Center for Atmospheric Research (PSU/NCAR) Fifth Generation Mesoscale Model (MM5). The Weather Research and Forecasting Model (WRF) is beginning to be used in modeling for research and may soon be ready for SIP modeling. Both the RAMS and MM5 meteorological models are based on the full set of primitive dynamic equations that govern atmospheric motions and thus are equally suitable for generating inputs to an air quality model. The TCEQ has selected the MM5 model primarily because it is being used for several other air quality modeling projects within Texas (e.g., TexAQS II real-time modeling, and use by Texas universities, Central Regional Air Planning Association (CENRAP), and near-nonattainment areas). Further, the TCEQ has years of experience in applying MM5 to historical ozone episodes, and it is publicly available, which allows stakeholders to use and modify the model free of charge.

The TCEQ plans to use the latest version of MM5 (version 3.7.3). This model is supported by a broad user community including the EPA, CENRAP, 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. Application of MM5 for a given episode requires the specification of initial and boundary conditions, as well as model parameterizations. These parameterizations include specification of surface parameters such as soil moisture and emissivities, a planetary boundary layer (PBL) scheme, and cumulus parameterizations. In addition, the TCEQ will be using the four dimensional data assimilation (FDDA) capabilities to conduct both analysis and observation nudging.

The most recent application of MM5 by the TCEQ was for the extended TexAQS 2000 episode (August 15 to September 6, 2000). For this application a suitable set of parameterizations was determined, which included the NOAH (National Centers for Environmental Prediction - Oregon State University - Air Force Weather Agency - Hydrological Research Laboratory) land surface model with emissivity modifications provided by a National Aeronautics and Space Agency (NASA) Surface and Atmospheric Radiation Budget study (http://www-surf.larc.nasa.gov/surf/pages/emiss.html); the Eta PBL scheme with the turbulent kinetic energy (TKE) option; and the Grell cumulus parameterization (coarse domains). Analysis FDDA nudging will be applied to the larger (greater than 4 km) gridded domains using the Eta Data Assimilation System (EDAS) reanalysis wind fields, which are derived from a national observational wind monitoring network. Observational FDDA nudging will be applied to the smaller (4 km) gridded domains using data derived from radar profiler measurements, much of which was collected as part of the TexAQS II study. The TCEQ plans to initiate MM5 modeling of the 2005 and 2006 episodes, including the intensive monitoring period of TexAQS II, using these parameterizations and using FDDA with available reanalysis and observational data. However, an application of a complex meteorological model like MM5 may likely require changes to the parameterizations to determine a suitable set for specific episodes.

5.1.3 Selection of Emissions Modeling System

Typically, raw emissions inventory databases provide point, area, on- and non-road mobile, and biogenic sources of emission estimates of criteria pollutants, including NO_X and VOC, on an annual, seasonal, daily or, in rare cases, hourly basis. The processing of raw emissions datasets to air quality model-ready inputs is accomplished through the use of emissions models. These emissions models temporally distribute, spatially allocate, and chemically speciate the emissions to the resolution and chemical mechanism used by the air quality model.

The three most common emissions modeling systems used to process anthropogenic emissions into the gridded, hourly resolved, and chemically speciated emissions needed for an air quality model are version 3 of the Emissions Processing System (EPS3), the 2000 Emissions Modeling System (EMS2000), and the Sparse Matrix Operator Kernel Emissions (SMOKE). TCEQ has selected the EPS3 primarily because it is being used for several other air quality modeling projects within Texas, it is easily modified to accommodate the complexity of emissions sources and highly detailed emissions information required for the HGB area, and TCEQ modeling staff have years of experience in using EPS to process the rather unique emissions in the HGB area. Additionally, the EMS2000 requires a SAS licensing fee, which could limit stakeholder usage, and SMOKE lacks flexibility to accommodate the highly resolved link-based on-road mobile source emissions reflecting the hour of day, day of week, vehicle-type distributed vehicle miles traveled (VMT), diurnal speed distribution and bi-directional traffic.

For biogenic emissions, TCEQ selected version 3.1 of the Global Biosphere Emissions and Interactions System (GloBEIS) biogenics emissions model (Guenther et al., 2002; Yarwood et al., 2001; Yarwood et al., 2000; Guenther et al., 1999) rather than the SMOKE-BEIS, BEIS-3, or MEGAN models, because it can incorporate local land cover data developed specifically for Texas (Feldman et al., 2007), solar radiation data derived from GOES satellite imagery, and temperature data derived from kriged observational data. GloBEIS also has built-in quality assurance functions.

5.2 Modeling Domains

5.2.1 CAMx Modeling Domains

Figure 4: *CAMx Modeling Domains* depict the modeling domains used in CAMx. The horizontal configuration of the CAMx modeling domains consist of a 2 km x 2 km grid encompassing a major portion of the HGB nonattainment counties (red box) nested within a 4 km x 4 km grid encompassing both the HGB and BPA ozone nonattainment counties (blue box), nested within a 12 km x 12 km grid covering the eastern part of Texas (green box), nested within the outer 36 km x 36 km grid (black box). The 36 x 36 km outer domain was selected to minimize the effect of boundary conditions on predicted ozone concentrations.

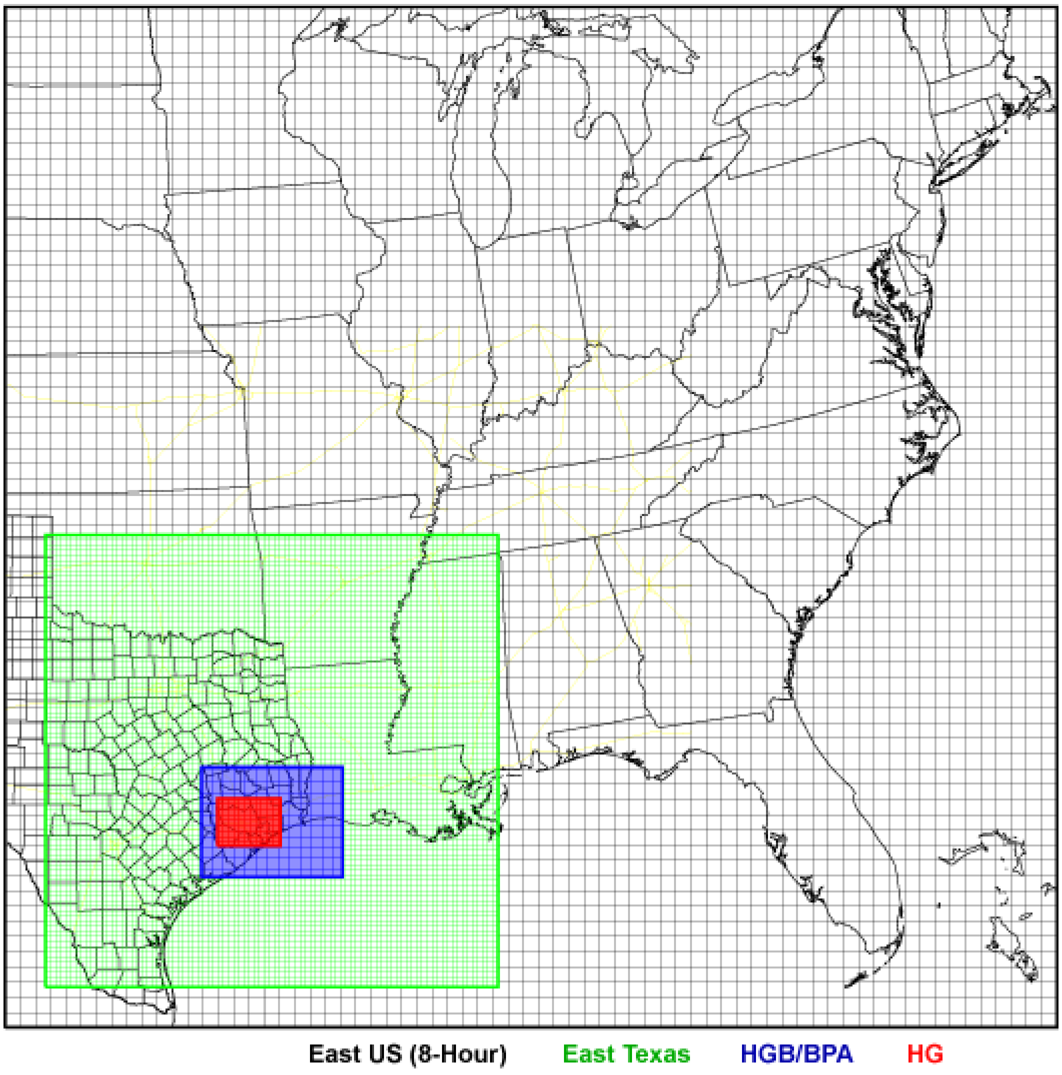

Figure 4: CAMx Modeling Domains

All grids are projected in a Lambert Conformal Projection (LCP) with origin at 100 degrees W and 40 degrees N, and aligned with the grid developed by the EPA for nationwide modeling for regional haze and particulate matter. Choosing a grid system compatible with an existing large-scale grid system serves several functions, including providing ready-made regional inventory data which can be used directly, allowing the TCEQ's modeling to be integrated into regional modeling projects, and promoting consistency among various regional and urban modeling applications in the central United States. Table 6: *CAMx Modeling Domain Definition for the Eight-Hour Modeling Analysis* lists the grid dimensions for the CAMx domain and subgrids for the eight-hour modeling analysis.

Table 6: CAMx Modeling Domain Definition for the Eight-Hour Modeling Analysis

Grid Name	Grid Cell Size	Dimensions (grid cells)	Lower left-hand corner[1]	Upper right-hand corner[1]
Coarse Grid	36 × 36 km	69 × 67	(-108, -1584)	(2376, 828)
Intermediate Grid	12 × 12 km	89 × 89	(-12, -1488)	(1056, -420)
Fine Grid	4 × 4 km	83 × 65	(356, -1228)	(688, -968)
HGB Sub-Grid	2 × 2 km	74 × 56	(394, -1154)	(542,-1042)

[1] Grid corners are in kilometers (easting, northing) relative to grid origin at 100° W and 40°N

Sensitivity analyses performed by the TCEQ and others for the one-hour ozone SIP (December 2004) have suggested that a finer resolution subdomain within the 4 km x 4 km HGB-BPA domain, would be useful in order to resolve the narrow industrial plumes emanating from the Ship Channel and surrounding areas. The modeled chemistry within the narrow plumes seems to behave differently at different domain resolutions. A finer resolution may allow the modeled chemistry to better replicate the ambient chemical reactions. The TCEQ plans to conduct modeling analyses with the 2 km x 2 km subdomain. A 2 km x 2 km subdomain is being planned because the parameterizations in both the CAMx and MM5 models are not designed for subdomains with grid resolutions much below 2 km.

The vertical configuration of the CAMx modeling domains consist of a varying 28-layer structure used with the 4 km x 4 km horizontal domain and a varying 17-layered structure used with the 12 km x 12 km and 36 km x 36 km horizontal domains. The unique meteorology induced by the land/sea/bay effects and the unique mixture of industrial sources, which release pollutants across a wide range of elevations, indicate the need for more vertical layers, particularly near ground level, with the 4 km x 4 km domain. Table 7: *CAMx Vertical Layer Structure for Fine Grid* and Table 8: *CAMx Vertical Layer Structure for Intermediate and Coarse Grids* show the vertical structuring of the 28-layered and 17-layered configurations, respectively.

The emissions modeling system, including EPS3 and GloBEIS, uses the same horizontal and vertical domains as CAMx, although, the non-point source emissions categories within the 4 km x 4 km domain are developed at a 2 km x 2 km resolution. Additionally, the on-road mobile source emissions within the 36 km x 36 km domain are developed at a 12 km x 12 km resolution.

Table 7: CAMx Vertical Layer Structure for Fine Grid

CAMx Layer	MM5 Layer	Top (m AGL)	Center (m AGL)	Thickness (m)
28	38	15179.1	13637.9	3082.5
27	36	12096.6	10631.6	2930.0
26	32	9166.6	8063.8	2205.7
25	29	6960.9	6398.4	1125.0
24	27	5835.9	5367	937
23	25	4898	4502.2	791.6
22	23	4106.4	3739.9	733
21	21	3373.5	3199.9	347.2
20	20	3026.3	2858.3	335.9
19	19	2690.4	2528.3	324.3
18	18	2366.1	2234.7	262.8
17	17	2103.3	1975.2	256.2
16	16	1847.2	1722.2	256.3
15	15	1597.3	1475.3	249.9
14	14	1353.4	1281.6	243.9
13	13	1209.8	1139	143.6
12	12	1068.2	998.3	141.6
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	609.5	564.9	89.3
7	7	520.2	476.0	88.5
6	6	431.7	387.8	87.8
5	5	343.9	300.4	87.0
4	4	256.9	213.7	86.3
3	3	170.5	127.7	85.6
2	2	84.9	59.4	51.0
1	1	33.9	16.9	33.9

Note: AGL - Above ground level.

Table 8: CAMx Vertical Layer Structure for Intermediate and Coarse Grids

CAMx Layer	MM5 Layer	Top (m AGL)	Center (m AGL)	Thickness (m)
17	38	15179.1	12172.9	6012.5
16	32	9166.6	7501.3	3330.7
15	27	5835.9	4970.9	1730
14	23	4105.9	3565.9	1080
13	20	3025.9	2564.5	922.9
12	17	2103	1728.1	749.8
11	14	1353.2	1210.6	285.2
10	12	1068.2	929.3	277.5
9	10	790.6	700.0	181.0
8	8	609.5	564.9	89.3
7	7	520.2	476.0	88.5
6	6	431.7	387.8	87.8
5	5	343.9	300.4	87.0
4	4	256.9	213.7	86.3
3	3	170.5	127.7	85.6
2	2	84.9	59.4	51.0
1	1	33.9	16.9	33.9

Note: AGL - Above ground level.

A feature pertinent to the modeling domains arising from the application of RRFs is the modeling grid cell array to use near a monitor to calculate the RRF. EPA's guidance suggests a 7 x 7 grid cell array for domains with grid cell sizes of 4 km x 4 km and for grid cell sizes less than 4 km, that the EPA regional office should be consulted as to the appropriate array size. Figure 5: *Near Monitoring Site Grid Cell Array Size* shows a map of the 2 km x 2 km subdomain nested in a portion of the 4 km x 4 km fine grid domain depicting the monitors, and the extent of 7 x 7, 5 x 5 and 3 x 3 grid cell arrays based on the 2 km grid. The TCEQ initially plans to use the 7 x 7 grid cell array to calculate the RRF for each monitor. If time permits, the TCEQ may conduct an analysis to determine whether a smaller grid cell array may be more appropriate for some monitors.

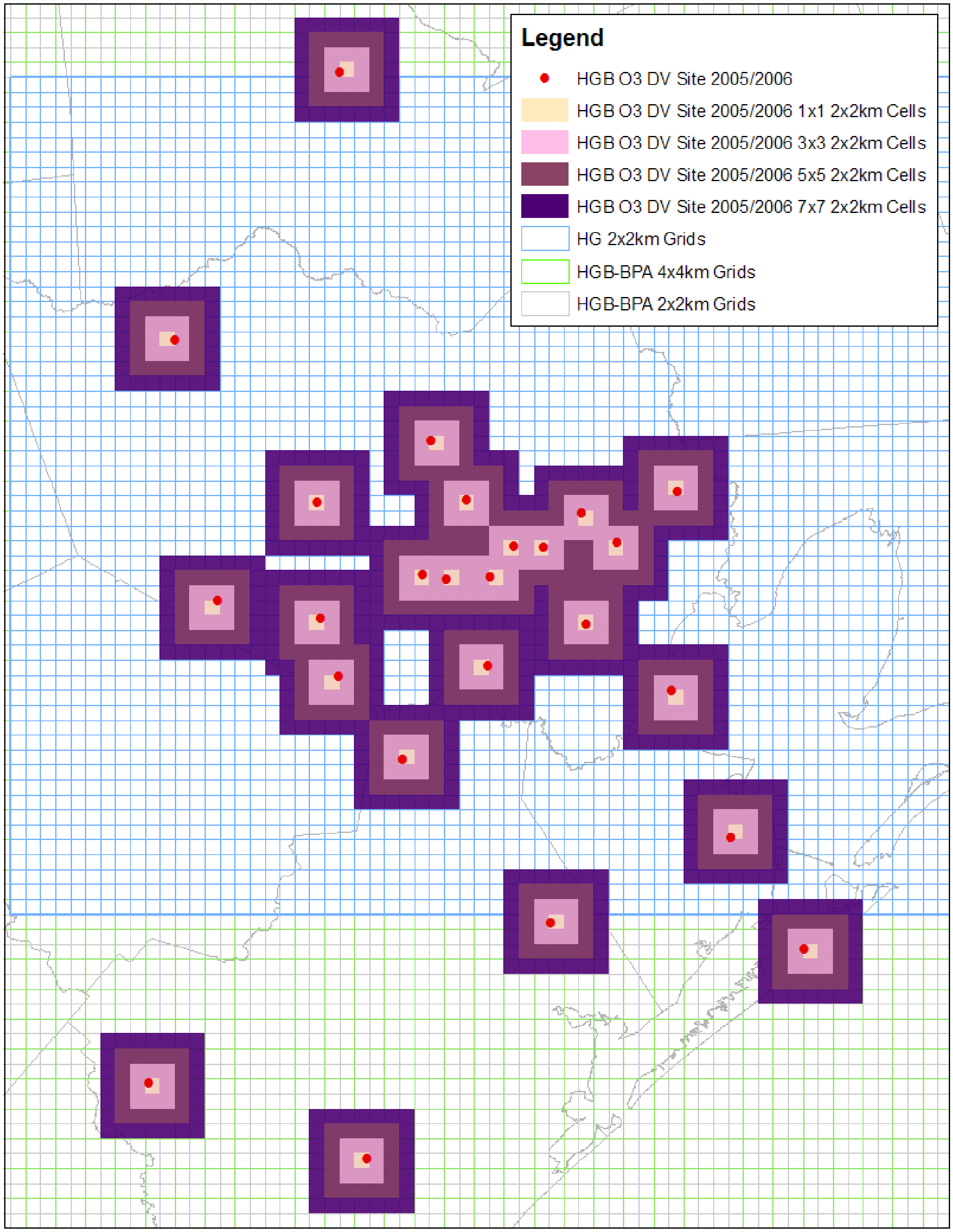

Figure 5: Near Monitoring Site Grid Cell Array Sizes

5.2.2 MM5 Modeling Domains

The horizontal configuration of the MM5 modeling domains consist of a 4 km x 4 km grid encompassing the east Texas and western Louisiana (Figure 6: *MM5 Modeling Domains*, red box), nested within a 12 km x 12 km grid covering all of Texas (green box), nested within a 36 km x 36 km grid covering the eastern three-fourths of the United States (blue box), nested within a 108 km x 108 km domain covering most of the northern hemisphere (black box). Each of the CAMx domains of comparable resolution embeds in the MM5 domains as required to allow for the incorporation of the necessary boundary conditions from MM5 into CAMx, with the exception of the 36 km x 36 km MM5 domain. The MM5 36 km x 36 km modeling domain does not extend eastward enough to embed the eastern boundary of the 36 km x 36 km CAMx modeling domain. To address this situation, Environ developed software to use the adjacent 108 km grid cells and disaggregate them down to 36 km grid cells to extend the 36 km x 36 km domain eastward enough to embed the 36 km x 36 km CAMx modeling domain. Since the eastern boundary of the 36 km x 36 km CAMx modeling domain is quite distant from the HGB area, this adjustment is expected to have a minimal effect, if any, on predicted ozone concentrations. Also shown in Figure 6: *MM5 Modeling Domains* is a 2 km x 2 km subdomain for the HGB area. The TCEQ does not plan to routinely run the MM5 model with the 2 km x 2 km subdomain. However, MM5 modeling with the 2 km x 2 km subdomain may be used with the CAMx 2 km x 2 km subdomain for a model sensitivity analysis. Table 9: *MM5 Modeling Domain Definition for the Eight-Hour Modeling Analysis* lists the horizontal grid configurations for the MM5 modeling domains.

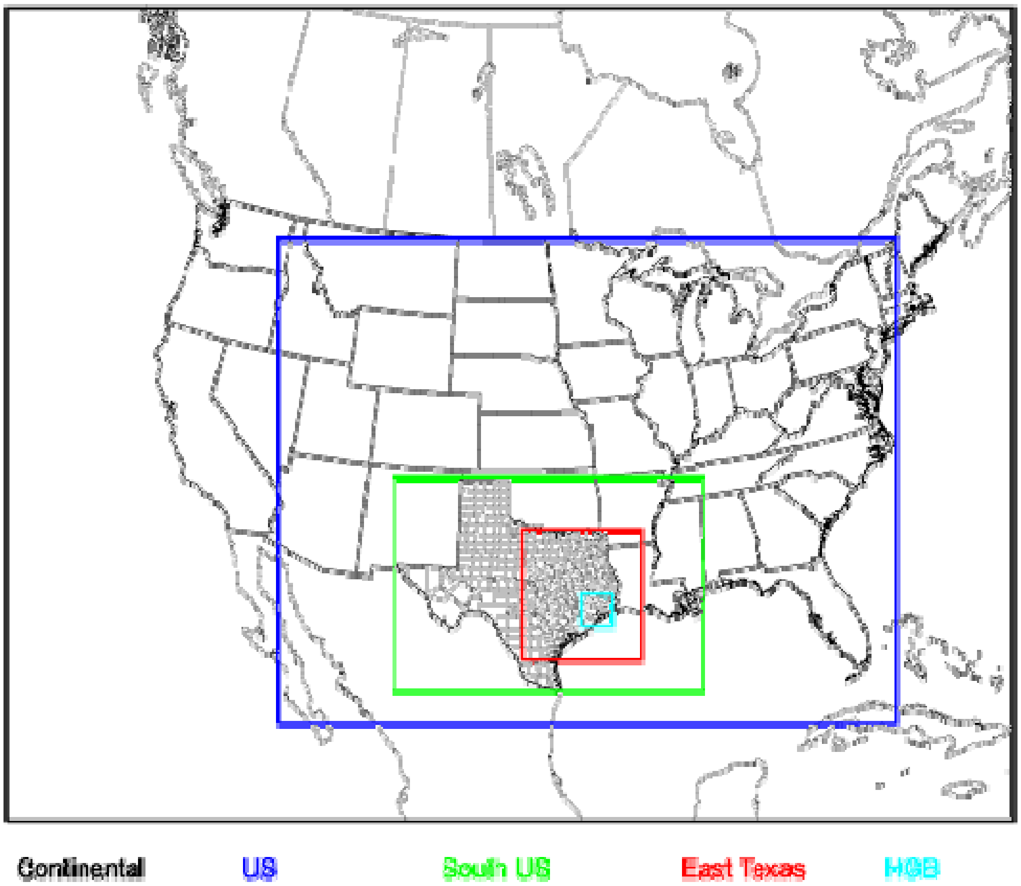

Figure 6: MM5 Modeling Domains

Table 9: MM5 Modeling Domain Definition for the Eight-Hour Modeling Analysis

Grid	Dimensions (grid cells)	Lower left-hand corner[2]	Upper right-hand corner[2]
108 × 108 km.	53 x 43	(-2808, -2268)	(2808, 2268)
36 × 36 km.	97 x 76	(-1296, -1728)	(2160, 972)
12 × 12 km.	145 x 100	(-648, -1548)	(1080, -360)
4 × 4 km.	166 x 184	(72, -1380)	(732,-648)
2 × 2 km.	91 x 91	(396, -1188)	(576, -1008)

[2] Grid corners are in kilometers (easting, northing) relative to grid origin at 100° W and 40°N

The vertical configuration of the MM5 modeling domains, listed in Table 10: *MM5 Vertical Layer Structure*, consists of a varying 43-layer structure used with all the horizontal domains.

Table 10: MM5 Vertical Layer Structure

Layer	Sigma	Layer Top (m AGL)	Center (m AGL)	Thickness (m)
43	0.000	20806.8	20362.1	889.6
42	0.010	19917.3	19341.4	1151.7
41	0.025	18765.6	18117.9	1295.3
40	0.045	17470.3	16918.8	1103.1
39	0.065	16367.2	15773.2	1188.1
38	0.090	15179.1	14662.7	1032.8
37	0.115	14146.3	13602.4	1087.8
36	0.145	13058.5	12577.6	961.9
35	0.175	12096.6	11596.6	1000.0
34	0.210	11096.7	10587.9	1017.5
33	0.250	10079.1	9622.9	912.6
32	0.290	9166.6	8752.3	828.6
31	0.330	8338.0	7958.1	759.8
30	0.370	7578.2	7269.5	617.3
29	0.405	6960.9	6671.3	579.2
28	0.440	6381.7	6108.8	545.8
27	0.475	5835.9	5577.7	516.3
26	0.510	5319.5	5108.7	421.6
25	0.540	4898.0	4695.9	404.0
24	0.570	4493.9	4299.9	388.0
23	0.600	4105.9	3919.3	373.3
22	0.630	3732.7	3552.8	359.7
21	0.660	3373.0	3199.5	347.1
20	0.690	3025.9	2858.2	335.5
19	0.720	2690.4	2528.1	324.6
18	0.750	2365.8	2234.4	262.8
17	0.775	2103.0	1974.9	256.1
16	0.800	1846.9	1721.9	249.8
15	0.825	1597.0	1475.1	243.9
14	0.850	1353.2	1281.4	143.6
13	0.865	1209.6	1138.8	141.6
12	0.880	1068.0	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

Note: AGL - Above ground level.

5.3 Modeling Inputs and Outputs

Since the outputs from the MM5 model and the emission modeling system are inputs to the CAMx model, the modeling inputs and outputs for the MM5 model and the emission modeling system will be presented before the inputs and outputs for the CAMx model.

5.3.1 MM5 Modeling Inputs and Outputs

The MM5 requires inputs for specifying surface parameters, which determine surface characteristics for the mesoscale forcing. Initially the TCEQ plans to use the NOAH land surface model (LSM) to provide the necessary surface parameters, with the exception of the NOAH LSM emissivities, which will be modified according to a NASA study (http://www.surf.larc.nasa.gov/surf/pages/emiss.html). The University of Houston (UH) is continuing to make enhancements to the surface characteristics input to MM5 by incorporating the recently collected University of Texas Center for Space Research (UT-CSR) land use and land cover (LU/LC) data along with the Texas Forest Service (TFS) LU/LC data. The TCEQ plans to test MM5 with this new LU/LC data when it becomes operational.

UH is also developing a routine for producing hourly time-varying sea surface temperatures (SST) that can be input to MM5. Initially, the TCEQ will use episode specific daily averaged SST, but plans to test MM5 with hourly SST data when the UH routine becomes operational.

When MM5 is used to simulate historical episodes, FDDA is typically used to nudge the model predictions toward observed meteorological parameters. The use of FDDA notably improves the MM5 replication of multi-day episodes and has become the standard approach in SIP modeling. The TCEQ plans to use two types of FDDA in the application of MM5. The first, typically referred to as analysis nudging, uses the EDAS reanalysis wind fields on the 108, 36 and 12 km domains. The second, typically referred to as observational nudging, uses radar profiler wind data on the 4 and 2 km domains.

Aside from data input to MM5, there are a variety of parameterizations of the physical processes in MM5 that must be selected. In particular, there are several schemes for simulating the planetary boundary layer (PBL). Initially, the TCEQ will be using the Eta-TKE PBL scheme, as this seems to provide the most accurate PBL heights in the coastal area of Houston. As time permits, TCEQ plans to test MM5 using other combinations of physics options.

Where possible the output parameters from the MM5 model are compared to monitored data to evaluate the model’s performance. In particular, the TCEQ uses a statistical package designed to interface with MM5 that evaluates four model parameters: wind speed, wind direction, temperature and humidity. This statistical package generates standardized tables and graphics for bias, root mean square error, and index of agreement for each of the four meteorological parameters.

5.3.2 Emissions Processing System Inputs and Outputs

For stationary sources (i.e., point and area sources), routine emission inventories constitute the major inputs to the emissions modeling system. For mobile sources and biogenic sources emissions are derived from emission models of their own. For example, link-based, on-road mobile source emissions are derived from a travel demand model coupled with the EPA MOBILE6.2 emission factor model, non-road mobile source emissions are derived from the EPA NMIM mobile source model, and biogenic emissions are derived from the GloBEIS model. With the exception of the biogenic emissions, for which the GloBEIS model outputs CAMx model-ready emissions, the emissions for the other source categories will be processed using EPS3 to generate CAMx model-ready emissions that are day-specific, gridded, speciated and temporally (hourly) allocated. The TCEQ plans to use a variety of graphical techniques (e.g., emission density plots) to quality assure (QA) the modeling emissions. Emission density plots

(EDPs) used for QA purposes will be developed for each of the major emission source categories (e.g., point, on-road), as well as some sub-categories (e.g., tanks, locomotives), at pertinent grid resolutions (e.g., 2 km for on-road within the eight-county HGB area, 4 km and 12 km for MMS Gulf emissions). Since emissions for most source categories are ozone season day (OSD) with adjustments for weekend days, EDPs used for QA puposes will focus primarily on weekdays. For those sub-categories with higher temporal resolution (e.g., EGUs, tank landing), EDPs will be developed as needed to compare and contrast differences.

5.3.2.1 Point Source Emissions

Point source modeling emissions will be derived from a number of inventories, such as regional inventories (e.g., 2002 CENRAP, National Emissions Inventory (NEI), Acid Rain Database (ARD), Gulf Wide Emissions Inventory (GWEI), Mexico NEI, Canada), state inventories (e.g, the State of Texas Air Reporting System (STARS), adjacent state inventories) and local inventories (e.g., 2006 TexAQS II Hourly Special Inventory (SI), Tank Landing Loss (TLL) special inventory). In addition, for the current modeling effort, the TCEQ plans to assess the feasibility of using information from the Consolidated Compliance and Enforcement Data System (CCEDS) to identify and quantify significant emission events.

For regions outside of Texas, the TCEQ plans to use emissions data from either the 2002 CENRAP or the 2002 NEI, adjusted for growth and controls to 2005 and 2006, with substituted hourly Acid Rain Data (ARD) emissions, the 2005 GWEI, and Phase 3 of the 1999 Mexico NEI emissions as input to EPS3. However for the three states bordering Texas (Louisiana, Oklahoma and Arkansas), the TCEQ will acquire their state-specific 2005 point source inventories, except for Louisiana, which considers 2004 a more representative year (non-Katrina). For regions inside of Texas, the TCEQ will use data from 2005 and 2006 STARS substituted with hourly ARD emissions, where appropriate, 2005 TexAER, the TexAQS II SI emissions, TLL emissions, and if feasible, CCEDS-derived emissions as input to EPS3.

Since the top of the first modeling layer in the CAMx domains is 33.9 meters, the TCEQ plans to use a plume height cutoff of 30 meters to discriminate between elevated and low level points. The TCEQ also plans to use the Plume-in-Grid (PiG) feature of EPS3 for selected point sources (e.g., large power plants). The PiG feature of EPS3 includes a threshold emission value, for which the TCEQ plans to use 5 tpd, and a collocation radius by geographic region (e.g., state/county) or CAMx modeling domain, for which the TCEQ plans to use 1.0 meter for all domains.

For the HGB area, the TexAQS II study findings indicate that HRVOC emissions continue to be greater than currently reported in STARS. Therefore, the TCEQ is working to reconcile the HRVOC emissions with emission rates inferred from ambient concentration data as appropriate. The TCEQ plans to use the potential source contribution factor (PSCF) analysis to reconcile the HRVOC emissions with the ambient HRVOC concentrations measured at auto-GCs. The TCEQ will provide EPA with the documentation of the PSCF analysis. Further emissions reconciliation based on TexAQS II analyses may be considered, if the TexAQS II analyses are available in a timely manner. The reconciled HRVOC emissions will be processed through EPS3.

For the 2006 baseline non-ARD point sources (including all sources in GWEI, Canada and Mexico), the TCEQ plans to use the same ozone season day emissions used in the 2006 base cases, except for the fires and the tank landings. The TCEQ does not plan to include fires in the 2006 baseline as fire emissions cannot be estimated for the 2018 future year. For the 2006 baseline tank landing emissions, the TCEQ plans to use the average of the tank landing emissions for those 2006 episode days with non-zero emissions. For the 2006 baseline ARD sources (EGUs), the TCEQ plans to estimate the emissions using the average of the 2006 third quarter hourly ARD emissions. In addition, the TCEQ plans to use the same 2006 PSCF emissions reconciliation used in the 2006 base case in the 2006 baseline.

For the 2018 future year point sources, the TCEQ plans to develop the emissions differently for the various regions of the modeling domain. For the states outside of Texas, the TCEQ plans to base the future year point sources on the emissions inventory developed for the 2018 CENRAP regional haze modeling. However, for the electrical generating units (EGUs) in the 2018 CENRAP point source inventory, the TCEQ plans to use the EPA CAIR Phase 2 (CAIR2) allowances. Even though the legal challenge to CAIR has resulted in the rule being remanded (not vacated), the TCEQ expects that emission limits on EGUs in 2018 will likely be comparable to the CAIR2 allowances.

For the attainment areas within Texas, the TCEQ plans to use CAIR2 allocations for EGUs, as already described. The EGU emissions will include consideration of new EGUs which have received an operating permit from the TCEQ and may start operation after 2006. For all the other point sources (i.e., non-EGUs) within the attainment areas of Texas, the TCEQ will apply growth (e.g., Texas REMI-EGAS) and controls (e.g., East Texas Engine Rule) as appropriate.

For point sources within the DFW and BPA nonattainment areas, the TCEQ will use emissions consistent with their latest SIP revisions. For the HGB nonattainment area, the TCEQ will use the MECT and HECT allocations as applicable to the pertinent point sources. For non-MECT or non-HECT point sources within the HGB nonattainment area, the TCEQ will apply growth (e.g., REMI-EGAS) and controls (e.g., tank degassing) as appropriate.

The TCEQ commissioned a survey to identify point sources within Texas whose future emissions may be altered as a result of compliance with consent decrees, Board orders, or as a result of emission off-sets. The TCEQ will review the survey results and if possible, include results in the 2018 emission estimates.

5.3.2.2 Area Source Emissions

Area source modeling emissions are also derived from a number of inventories, such as the regional inventories from CENRAP, NEI and the GWEI, and state inventories, such as TexAER. In addition, the Northeast Texas 2005 gas compressor inventory will be included.

For regions outside of Texas, the TCEQ plans to use area source emissions data from the 2002 CENRAP, 2005 GWEI and 2000 Canadian inventories. The 2002 CENRAP area source emissions will be adjusted using EGAS for growth to 2005 and 2006. Newer emissions (i.e., post 2000) are not available for Canada, and neither are reliable growth factors. Particular to the

2005 GWEI, the non-road emissions are included as area sources. For regions inside of Texas, the TCEQ will use data from the 2005 TexAER data base and the Northeast Texas 2005 gas compressor inventory. The 2005 TexAER includes the flash emissions associated with the Oil and Gas Production area source category. 2005 TexAER and Northeast Texas 2005 gas compressor emissions will be grown to 2006 using the Texas-specific REMI-EGAS growth factors for the 2006 base case episodes. Emissions data from these inventories will be processed with EPS3 to generate CAMx model ready emissions that are day-specific, gridded, speciated and temporally (hourly) allocated.

For the 2006 baseline area sources, the TCEQ plans to use the same emissions as used in the 2006 base cases.

For the 2018 future year area source emissions outside of Texas, the TCEQ plans to use the 2002 NEI with the latest EGAS growth factors. For the future year area source emissions within Texas, the TCEQ plans to apply the Texas-specific REMI-EGAS growth factors to the 2005 TexAER emissions data base and the Northeast Texas 2005 gas compressor inventory, as appropriate.

5.3.2.3 Non-Road Source Emissions

Non-road mobile source modeling emissions are also derived from a number of inventories, such as the CENRAP, NEI and TexAER inventories. With the exception of marine, aircraft and locomotive emissions, which will be referred to as “off-road” emissions, the initial non-road emissions will be determined using the EPA NMIM mobile source emissions model.

For regions outside of Texas, the TCEQ will use the non-road emissions data from the EPA NMIM for 2005 and 2006. As described above, the 2005 GWEI non-road and off-road emissions are included in the area source category. For regions inside of Texas, the TCEQ plans to use the Texas specific non-road emissions model (TexN) developed under contract by ERG for 2005 and 2006. The off-road emissions will be developed using data from the 2005 TexAER data base. Emissions data will be processed with EPS3 to generate CAMx model ready emissions that are day-specific, gridded, speciated and temporally (hourly) allocated. In addition, for equipment using heavy-duty diesel engines, EPS3 emissions will be post-processed to adjust for episode-specific temperature and humidity.

Within the HGB and BPA areas, emissions from ships will be modeled as point sources since many have tall stacks and/or sufficient plume rise to exceed the 30 meter plume height cut-off. These sources are modeled by placing pseudo-stacks along shipping lanes, such as the Houston Ship Channel and Intracoastal Waterway. Similarly, emissions from wildfires and controlled burning generate smoke plumes that can rise thousands of feet and will be modeled as pseudo point sources. The TCEQ plans to contract with Environ to modify EPS3 to reasonably allocate fire emissions in the vertical layers.

For the 2006 baseline non-road sources (including the off-road categories), the TCEQ plans to use the same emissions as used in the 2006 base cases.

For the 2018 future year non-road mobile source emissions for states outside Texas, the TCEQ plans to use the EPA NMIM model for all applicable categories. For the future year off-road emissions for states outside Texas, the TCEQ plans to use the 2002 NEI with the latest EGAS growth factors and the national locomotive and marine engines controls. For regions within Texas, the TCEQ plans to use the TexN model for non-road emissions, and for the off-road emissions, the TCEQ plans to use the 2005 TexAER with the Texas-specific REMI-EGAS growth factors and locomotive and marine engines national controls.

5.3.2.4 On-Road Mobile Source Emissions

On-road mobile source emissions inventories will be developed for the HGB and BPA areas, the remaining counties within Texas, and the states outside of Texas. For the regions within Texas, the Texas Transportation Institute (TTI), under contract to the TCEQ, will develop the on-road mobile source emissions. For the region outside of Texas, the TCEQ will use the EPA NMIM to develop emissions for each of the states within the modeling domain. The spatial and temporal resolution of the emissions will decrease with distance from the HGB/BPA areas.

For the HGB and BPA areas, TTI will obtain link-based travel demand modeling (TDM) output from H-GAC and the Texas Department of Transportation (TxDOT), respectively. The TDM output includes VMT and speed parameters estimated by roadway link. TTI will use automatic traffic recorder (ATR) data available from TxDOT to adjust the TDM output to create hourly Weekday, Friday, Saturday, and Sunday “day type” VMT estimates for both school and summer (i.e., non-School) “season types.” Vehicle classification data, also available from TxDOT, will be used by TTI to allocate the VMT among the 28 available MOBILE6.2 “vehicle classes” for each roadway link.

TTI will estimate average hourly operating speeds on each roadway link for each combination of day and season type. County specific MOBILE6.2 model inputs will account for differences in meteorological parameters, local age distribution, and use of TxLED, RFG, Low RVP and I/M testing. MOBILE6.2 emission rates in grams per mile will be estimated for speeds ranging from 2.5 to 65 miles per hour (mph) for the various “roadway categories.” Link-based VMT and speed-based emission rate are multiplied to develop the link-based hourly emissions for each of the day and season types for the 2005 and 2006 episode periods and a 2018 future year. For the 2006 baseline, the TCEQ plans to use the 2006 summer season type emissions, the same as used for summer days in the 2006 base cases. This is consistent with the summer season type emissions used for the 2018 future year.

For the Texas counties outside the HGB and BPA region, TTI will use traffic data collected by TxDOT (e.g., ATR) for the Highway Performance Monitoring System (HPMS). This data is used to estimate typical summer season, county-wide, hourly, day-type VMT and speeds on 19 roadway categories for the 28 available MOBILE6.2 vehicle classes. County-specific MOBILE6.2 model inputs will account for differences in meteorological parameters, local age distribution, use of TxLED, RFG, Low RVP and I/M testing. MOBILE6.2 speed-based emission rates are multiplied by the county-wide VMT to develop the hourly emissions for the 2005 and 2006 episode periods, and a 2018 future year. For the 2006 baseline, the TCEQ plans to use the same on-road emissions as used in the 2006 base cases. No school season adjustment will be used since these county-wide emissions are both relatively small and they are located relatively far from the HGB and BPA region.

For the region outside Texas, the TCEQ will use the EPA NMIM to develop emissions for 12 vehicle types on 12 roadway categories. Since the national VMT data provided with NMIM are only for 1999 and 2002, the TCEQ will rely on the Highway Statistics Series of data available from the Federal Highway Administration (FHWA) to project VMT beyond 2002. Ratios from the TTI-developed Texas on-road emissions will be used to adjust the summer weekday emissions output from NMIM to 2005, 2006 and 2018. These weekday emissions will then be scaled to create Friday, Saturday, and Sunday emissions using corresponding ratios in the TTI-developed Texas emissions. For the 2006 baseline, the TCEQ plans to use the same on-road emissions as used in the 2006 base cases.

The on-road emissions from each of the different regions will be processed with EPS3 to generate day-type specific CAMx model ready emissions that are gridded, temporally allocated by hour, and speciated for the CB05 mechanism. Since the Texas on-road emissions received from TTI are already provided by hour, EPS3 processing will preserve the hourly distribution of the emissions.

For the HGB and BPA region, the link-based emissions will be spatially allocated to the appropriate grid cells according to the TDM geographic coordinates defining the links. In accordance with EPA guidance, 3.4 percent of the emissions from vehicle classes HDDV8a and HDDV8b will be extracted and processed as heavy-duty diesel truck idling emissions. Spatial allocation of these idling emissions will be based on available parking places at known truck stop locations, while temporal allocation will be based on the inverse distribution of hourly HDDV8a and HDDV8b VMT. No heavy-duty diesel truck idling emissions will be developed for the other two regions (i.e., Texas non HGB and BPA counties and states outside Texas). For these regions, the heavy-duty diesel truck idling emissions are expected to be too small and too distant to warrant development.

For the region consisting of the remaining counties in Texas, the HPMS-based on-road emissions will be spatially allocated by appropriate roadway categories (e.g., interstates, state highways, arterials), while emissions from minor roadways and local streets will be allocated spatially by a human population surrogate.

As indicated previously, after the Texas on-road EPS3 processing is complete, hourly emission profiles for each of the day-types will be created and applied to the non-Texas emissions derived with the EPA NMIM. In addition, a spatial allocation, similar to that used for the Texas non HGB and BPA region (i.e., roadway categories and population) will be used for the non-Texas region.

Table 11: *Summary of the Development of On-Road Mobile Sources Emissions* summarizes pertinent features of the planned development of on-road mobile emissions in the different regions of the modeling domain as described above.

Table 11: Summary of the Development of On-Road Mobile Sources Emissions

On-Road Inventory Development Parameter	Texas Metropolitan Areas	Texas Rural Areas	Non-Texas States/Counties
VMT Source	Travel Demand Models (TDMs)	HPMS Data Sets	NMIM Database
VMT Resolution	Roadway “Links” From TDM	19 Roadway Categories	12 Roadway Categories
Season Types	School and Summer (i.e., non-School)	Summer Only	Summer Only
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	MOBILE6.2 Default
Spatial Resolution	Excellent	Very Good	Good
Temporal Resolution	Excellent	Very Good	Good
MOBILE6.2 Vehicle Classes	28	28	12
Temperature/Humidity Diesel NO_X Correction	Yes	Yes	No
“18-Wheeler” Idling Emissions Separation	Yes	No	No

5.3.2.5 Biogenic Emissions

The TCEQ selected the GloBEIS model because it can incorporate detailed locality specific land-use data and solar radiation data from GOES satellite imagery. The GloBEIS model also has built-in QA reporting functions. The land cover and vegetation data bases used for input to GloBEIS derived from the following sources:

UT-CSR land cover database (Feldman et al., 2007) - This data base was developed from classification of recent Landsat 7 data, Shuttle Radar Topography Mission and National Elevation datasets to identify wetlands, and USDA Common Land Unit (CLU) data to identify agricultural land.

TCEQ Texas vegetation database (Wiedinmyer et al., 2001) - This database was derived from Texas Parks and Wildlife vegetation data, urban land use data from Braden, Collie, and Turner

Consulting, agricultural statistics from the National Agricultural Statistics Survey, and field surveys carried out during 1999.

Biogenic Emissions Landuse Data, version 3 (BELD3; Kinnee et al., 1997) - A vegetation database for the entire North American continent, prepared specifically for creating biogenic emissions inventories.

Mexican land use and vegetation database (Mendoza-Dominguez et al., 2000) - The database was created by researchers at the University of Monterrey and Georgia Tech.

For southeast Texas (i.e., the 4 km x 4 km domain), the new UT-CSR land cover and vegetation data will be used. For all other regions within Texas, the Wiedinmyer et al. data will be used. The BELD3 database will be used only for the regions outside of Texas, with the exception of Mexico, where the Mexican land use and vegetation database will be used.

Photosynthetically-active solar radiation (PAR) data for the biogenic emissions modeling will be obtained from the website operated by the Global Energy and Water Cycle Experiment (GEWEX) Continental International Project (GCIP) and GEWEX Americas Prediction Project (GAPP) http://metosrv2.umd.edu/~srb/gcip/cgi-bin/historic.cgi?auth=no. The data can be downloaded at half-degree resolution and will be reprocessed to match the TCEQ modeling grids. These data are derived from hourly GOES satellite imagery of cloud cover, which have been processed with a solar irradiation model (Pinker and Laszlo, 1992).

For all regions modeled, the TCEQ plans to prepare the hourly temperature fields using kriging algorithms in the SAS software. Variograms will be fitted for each hour, so that each hour will be interpolated with a variogram that fits its inherent degree of variation. Temperature data will be obtained from weather stations throughout the United States, including data from the National Weather Service, the EPA AIRS air quality database, the National Buoy Data Center, the Texas A&M Crop Weather Program, the Louisiana Agricultural Information Service, and the Texas Coastal Oceanographic Observation Network. The data from each of these sources has been quality-assured by the organizations that run the monitoring networks and will be further checked for anomalies by the TCEQ.

After each biogenic emissions modeling file is created, two additional files will be created to assist in quality assurance. An emissions summary file, showing hourly domain-wide total emissions of isoprene, monoterpenes, other VOCs, NOx, and CO, is created to allow quick comparison of different days. A model configuration file is also created listing the input files used to create the emissions file. The model configuration file shows the GloBEIS model settings. These files will be archived with the emissions files.

Since the biogenic emissions are associated with meteorological features, The TCEQ plans to use the same episode-specific emissions for the 2006 baseline and 2018 future air quality modeling.

5.3.3 CAMx Modeling Inputs and Outputs

5.3.3.1 Modeling Inputs

The outputs from the emissions modeling processors, EPS3 and GloBEIS, and from the MM5 meteorological model 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.

Initially the TCEQ plans to use the same initial, lateral boundary and top concentrations prepared by Environ for modeling conducted for the DFW 8-hour SIP (May 2007). Two different conditions were established: clean conditions were used over water, and moderate conditions were used for over land. Table 12: *Concentrations (ppb) Used to Define CAMx Initial and Lateral Boundary Conditions*, lists the pollutant species and the corresponding concentrations for the clean and moderate conditions. For the initial conditions, the moderate concentration levels were used below 1700 meters and the clean concentration levels at 1700 meters and aloft. Since at least two "spin-up" days are modeled at the beginning of each episode, the influence of the initial conditions on the third day is typically very minimal. For the lateral boundary conditions, the clean concentration levels were used over water, and the moderate concentration levels were use over land below 1700 meters (Figure 7: *Lateral Boundary Condition Assignments Below 1700 meters*), and the clean concentration levels were used at 1700 meters and aloft. The clean concentration level was used for the boundary conditions at the top of the modeling domain.

Table 12: Concentrations (ppb) Used to Define CAMx Initial and Lateral Boundary Conditions

Species	**Moderate**	**Clean**
O3	40	40
CO	200	100
NO	0.1	0.1
NO2	1	1
HNO3	3	1
HNO2	0.001	0.001
ALD2	0.555	0.05
ETH	0.51	0.15
HCHO	2.1	0.05
OLE	0.3	0.05
PAR	14.9	7.6
TOL	0.18	0.0786
XYL	0.0975	0.0688
ISOP	0.1	0.001
PAN	0.1	0.1
H2O2	3	1
MEOH	0.001	0.001
ETOH	0.001	0.001

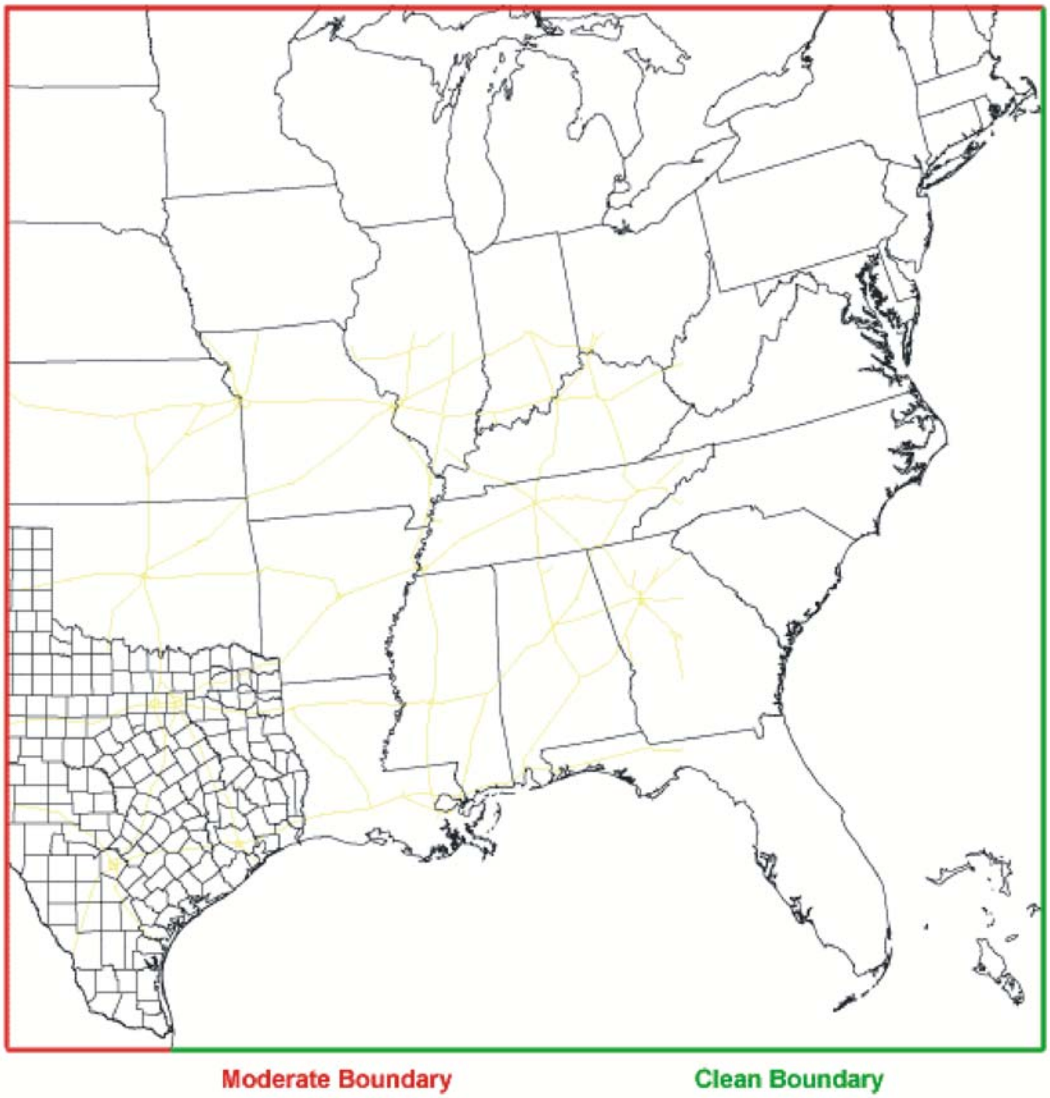

Figure 7: Lateral Boundary Condition Assignments Below 1700 meters

The TCEQ is also working with NASA and the Jet Propulsion Laboratory (JPL) to derive episode-specific boundary conditions from global air quality models such as the Model for Ozone and Related chemical Tracers (MOZART) global air quality model. The TCEQ plans to use these episode-specific boundary conditions if they can be developed in a timely manner.

Gridded land-use data characterizing surface features, 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 eleven land use categories, as defined by the USGS land-use land-cover (LULC) database. Initially, the TCEQ plans to use the land-use file developed for previous SIP modeling (e.g., DFW 2007 SIP), which was derived from the most recent USGS LULC database. The TCEQ is working with Texas A&M University on a project to update the land use file for the 2 km domain and portions of the 4 km domain, in the vicinity of HGB, using more highly resolved LULC data collected by the TFS and the UT-CSR.

A chemistry parameters file, a photolysis rates file and an albedo/haze/ozone file are also input to CAMx. These files are inter-related and specific for the selected chemical mechanism, CB05, and as a result must be coordinated to function together. The TCEQ will use episode-specific satellite data from the Total Ozone Mapping Spectrometer (TOMS) to prepare the photolysis rates and the albedo/haze/ozone files.

5.3.3.2 Modeling Outputs

CAMx outputs CB05 species in molar concentration units of parts per million by volume (ppmv). Some of the CB05 species are actual chemical species and include ozone, nitric oxide, nitrogen dioxide, carbon monoxide, ethane, ethene, formaldehyde and acetaldehyde. 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 and source apportionment results. Process analysis, including chemical process analysis (CPA) and integrated process rate (IPR) analysis, provides in depth details of ozone formation, showing the various physical and chemical processes that determine the modeled ozone concentrations at specified locations and times. Process analysis modeling output is typically used as a part of the performance evaluation. Source apportionment, such as Ozone Source Apportionment Technology (OSAT) and Anthropogenic Precursor Culpability Assessment (APCA), determines 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 the High-Order Direct Decoupled Method (HDDM), respectively. The DDM or HDDM calculate CAMx's sensitivity to changes in inputs directly as the model is executed and can be used to evaluate performance as well as the future year modeling.

5.4 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. Appendix B provides a detailed QA/QC plan developed by the TCEQ to be used during modeling, which is consistent with EPA guidance to ensure the scientific soundness and defensibility of the modeling.

6 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 NO_X and VOC. The model's ability to correctly replicate this relationship is necessary to have confidence in the model's prediction of the response of ozone to various control measures.

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

The TCEQ plans to incorporate the recommended eight-hour performance measures into its evaluations but will continue to focus primarily on one-hour performance analyses, especially in the HGB area. The high resolution meteorological and emissions features characteristic of the area 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.

The TCEQ also plans to evaluate the model performance at some of the more rural monitors within Texas beyond the HGB area. Since the modeling resolution is more coarse in the rural areas (e.g., 12 km grid), the performance evaluations the TCEQ plans to use will be predominantly based on graphical measures.

6.1 Operational Evaluations

6.1.1 Statistical Measures

Statistical measures provide a quantitative evaluation of model performance. At a minimum, TCEQ plans to use the following recommended statistics (EPA, April 2007) in evaluating performance of the base case modeling.

Unpaired Peak Accuracy (UPA) - This statistic compares the difference between the maximum modeled ozone concentration and the highest monitored ozone concentration found over all hours and over all monitoring stations for each day simulated. This comparison will be made for both one- and eight-hour peak ozone concentrations.

In the past EPA recommended an acceptable range for the UPA of ± 15-20% for one-hour ozone. For eight-hour ozone, EPA has not included the UPA as a recommended statistical measure. However, this statistic will be computed to ensure that the model is generating sufficiently high ozone peaks on each day of the simulation.

Mean Normalized Bias (MNB) - This statistic compares the relative difference between modeled and monitored ozone concentrations, paired in time and space, averaged over all hours and over all monitoring stations. The MNB will be calculated for individual episode days by averaging over all monitoring sites, and individual sites by averaging over all days. The MNB provides a measure of the model’s tendency to over- or under-predict monitored ozone concentrations. A positive bias indicates that the model’s ozone concentrations are too high, and a negative bias indicates the converse. A bias near zero is desirable, although this does not necessarily mean the model is replicating ozone concentrations well since combining large positive and negative relative differences can result in a near-zero MNB.

For one-hour ozone, EPA has recommended a range of ± 5-15%, and calculating the MNB only when the monitored ozone concentration is 60 ppb or greater. For eight-hour ozone, EPA also recommends limiting the calculation of the MNB to monitored ozone concentrations over a minimum threshold of 40 or 60 ppb, but no range is given for consideration of suitable performance. The TCEQ plans to compute the MNB for the one-hour ozone concentrations using a minimum threshold of 60 ppb. However, for the eight-hour ozone concentrations, the TCEQ plans to compute the MNB using the daily maximum eight-hour ozone concentrations.

Mean Normalized Gross Error (MNGE) - This statistic is similar to the MNB, except that the absolute value of the relative differences between modeled and monitored ozone concentrations paired in time and space are averaged over all hours and over all monitoring stations. The MNGE will be calculated for individual episode days by averaging over all monitoring sites and individual sites by averaging over all days. This statistic is representative of the overall deviation between the modeled and monitored concentrations. The MNGE is always greater than or equal to zero.

As for the MNB, the TCEQ will compute the MNGE for the one- and eight-hour ozone concentrations using a minimum threshold of 60 ppb for one-hour and the daily maximum for the eight-hour, respectively. For one-hour ozone concentrations, the recommended range for MNGE is ± 30-35%, but no range is specified for eight-hour.

For both the MNB and MNGE, the TCEQ plans to use a modeled value based on a bi-linear interpolation of the ozone concentrations in the grid cells around a monitor.

These statistical measures will be used primarily for ozone concentrations, although they may be applied to some of the ozone precursors. In addition, the TCEQ may use other statistical measures such as mean fractional bias and mean fractional error as deemed necessary in the performance evaluation.

6.1.2 Graphical Measures

Graphical measures provide a qualitative evaluation of model performance. At a minimum, the TCEQ plans to use the following recommended graphics in evaluating performance of the base case modeling (EPA, April 2007):

Time Series Plots - For monitoring stations in the domain, the hourly monitored and bi-linearly interpolated modeled concentrations can be compared 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 locations.

The TCEQ plans to develop hourly time series plots for ozone and some ozone precursors (e.g., NO_X, VOC) at appropriate sites. Comparing the modeled versus monitored concentrations of precursors can indicate whether the model is correctly replicating the physico-chemical processes by which ozone was actually generated.

Since averaging over several hours smooths the modeled and observed concentrations and obscures important features, TCEQ does not plan to develop time series plots for eight-hour concentrations of ozone or ozone precursors.

Scatter Plots - Scatter plots of hourly monitored and bi-linearly interpolated modeled ozone concentrations will be developed for appropriate monitors for all episode days. This should show overall patterns of under- and/or over-prediction for an entire episode. Comparing between selected monitors should show any geographically related differences in prediction patterns. The TCEQ plans to develop hourly scatter plots for some ozone precursors (e.g., NO_X, VOC) at selected monitors and for all episode days, as well. Quantile/Quantile (Q/Q) plots indicating the rank distribution of the monitored versus modeled ozone concentrations will also be developed and included on the scatter plots.

Peak Ozone Tile Plots - Tile plots of one- and eight-hour daily ozone maxima overlaid with monitored maximum values provide a visual means of assessing where the model predicted peak concentrations compared with observations. TCEQ will develop plots showing the peak daily concentration (one- and eight-hour) simulated in each grid cell.

Ozone Animations - Tile plots of hourly modeled ozone concentrations overlaid with monitored maximum values will be combined into an animated sequence. Animations of ozone precursors (NO_X, VOC) will also be developed as needed. Viewing the sequence of tile plots as an animation provides insight into the model's physico-chemical processes, such as how ozone forms, and how it is transported and dispersed by the model.

Aloft measurements - During the TexAQS II, numerous aircraft flights collected a rich set of aloft ozone, ozone precursor, and reaction product measurements. Additionally, data were collected at the Moody Tower at the University of Houston at an elevation of approximately 70 meters above ground level (AGL). Data from aircraft transects will be compared with model predictions along the flight path. Data collected at the Moody Tower will be compared with model predictions at the appropriate vertical layer using time series plots as described above.

6.2 Diagnostic Evaluations

6.2.1 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 following analyses will be performed to determine the model sensitivity to various model input parameters:

Alternative meteorological characterization - TCEQ will analyze the sensitivity of the predicted ozone and ozone precursors to changes in the meteorological inputs using a variety of parameterizations/characterizations of the meteorological modeling. The use of different parameterizations/characterizations will change various meteorological parameters, such as the wind speed and the vertical mixing coefficients. These analyses may have the added benefit of identifying the best meteorological characterization for use in this modeling application.

Alternative boundary conditions - Because the area of most interest, the fine grid domain about HGB, is far from the lateral boundaries, the sensitivity to boundary conditions has been relatively small in past modeling applications. However, recent modeling conducted for other Texas areas suggests a higher level of sensitivity to the specification of boundary conditions. The TCEQ plans to analyze the sensitivity of the predicted ozone and ozone precursors to changes in the boundary conditions. In particular, the TCEQ plans to work with staff from NASA/Jet Propulsion Laboratory in developing episode specific boundary conditions.

Alternative emissions inventory assumptions - The TexAQS studies have provided substantial evidence that the reported emissions under-estimate some of the ozone precursors. The TCEQ will analyze the sensitivity of the predicted ozone concentrations to changes in the emissions, particularly the HRVOC, as well as the less highly reactive VOCs. The TCEQ is planning to use the PSCF analysis to reconcile HRVOC emissions with the ambient HRVOC concentrations measured at the auto-GCs. A sensitivity of the predicted ozone concentrations with and without the HRVOC reconciliations will be conducted. Additionally, a sensitivity of the predicted ozone concentrations to changes in the emissions of the less highly reactive VOCs will be conducted.

6.2.2 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 which 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 HGB area. Another analysis of this type that the TCEQ may conduct involves comparing the changes in the modeled versus monitored NO_X- or VOC-limitation both geographically and temporally over the HGB area.

Probing Tools - These 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 on the Houston urban core and the highly industrial ship channel. The TCEQ may also conduct source apportionment analyses (e.g., OSAT, APCA, HDDM/DDM) on the base case modeling. The TCEQ plans to conduct source apportionment analyses on the future case modeling, to understand the contribution from various 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 2000 ozone design values (i.e back cast from the 2006 baseline to year 2000). The model-projected year 2000 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 control measures.

7 ATTAINMENT YEAR MODELING AND CORROBORATIVE ANALYSES

The attainment demonstration will consist of the attainment year modeling and the corroborative analyses. The TCEQ plans to conduct attainment year modeling in accordance with the EPA attainment test procedure for eight-hour ozone modeling. Additionally, the TCEQ plans to provide a suite of corroborative analyses providing additional assurance that any control strategy proposed for the HGB area will result in attainment at all monitors.

7.1 Attainment Year Modeling

In accordance with the “severe” eight-hour ozone classification for the HGB area and the EPA modeling guidance, the TCEQ is using 2018 as the future year for attainment modeling. Using the 2018 projected future year emissions, which include growth and current regulatory control measures, the TCEQ will model the future year. As per the EPA guidance, the TCEQ plans to project the 2018 future year design values, DV_F, using the relative response factor, RRF, and the 2006 base year design value, DV_B, at each of the monitors in the HBG area with a 2006 DV_B greater than or equal to 85 ppb.

The TCEQ plans to calculate the RRFs, in accordnce with the EPA guidance, using the average of the 2006 baseline modeled daily maximum eight-hour ozone concentrations above 84 ppb within the 7 x 7 grid cell array about the monitor. Also per the EPA guidance, if there are fewer than 10 days with 2006 baseline modeled daily maximum eight-hour ozone concentrations greater than 84 ppb, then days with modeled concentrations less than or equal to 84 ppb will be used so the average is based on at least ten days.

The TCEQ expects that most, if not all, of the DV_Fs will be below 85 ppb, demonstrating attainment. In the case that not all the DV_Fs are below 85 ppb, the TCEQ plans to conduct sensitivity testing to determine what additional emission reductions may be necessary to demonstrate attainment. In the case that all the DV_Fs are notably below 85 ppb, the TCEQ plans to consult with EPA to determine whether mid-year modeling would be needed to address the "as expeditiously as practicable" provision.

Prior to release of the EPA's Modeled Attainment Test Software (MATS), the TCEQ developed its own procedure for calculating RRFs and future design values. In addition, the TCEQ procedure performs a spatial interpolation, so like MATS, the TCEQ procedure can also be used to analyze unmonitored areas (i.e., an out-of-network test). While conceptually similar to MATS, the TCEQ's procedure was designed specifically to be integrated into the CAMx modeling process. This facilitates the calculation of RRFs and DV_Fs and the spatial interpolation. For example, MATS requires input in Latitude/Longitude, while the TCEQ procedure works directly with the Lambert Conformal Projection (LCP) data used in our post-processing modeling applications. Also, MATS cannot easily handle multi-year base case data; the TCEQ procedure can. Finally, MATS uses a technique called Voronoi Neighbor Averaging (VNA) for spatial interpolation, while the TCEQ approach relies on the more familiar kriging technique. The TCEQ staff have conducted an analysis comparing the RRF and DV_Fs resulting from using MATS and the TCEQ procedure and showed very minimal differences. (Note: The TCEQ has provided EPA with the analysis comparing the RRF and DV_Fs results and will provide the software and documentation on the TCEQ procedure.) Since the ozone monitoring network for the HGB area has a relatively large spatial extent, the TCEQ does not anticipate having to conduct an out-of-network test. However, should an out-of-network test be necessary, the TCEQ plans to use its own procedure.

If needed, to provide directional guidance in identifying control measures that may reduce ozone the most effectively, the TCEQ plans to conduct a number of modeling sensitivities. These sensitivities may include an across-the-board percentage emission reductions matrix, an HDDM analysis and an OSAT/APCA culpability assessment. Using these sensitivity modeling results, specific control measures will be selected. The emissions reductions associated with the specific control measures will be incorporated into the future 2018 modeling and to test their effectiveness, the DV_Fs will be recalculated.

The control strategy will be incorporated into the future 2018 emissions and modeled for the attainment demonstration.

7.2 Corroborative Analyses

As per EPA guidance, the TCEQ plans to conduct additional analyses to corroborate the attainment modeling. The TCEQ's corroborative analysis for the HGB 8-hour ozone SIP will help demonstrate that the processes of ozone formation, accumulation, and transport in the HGB area are now relatively well understood, and therefore the steps needed to make further progress can be discerned. The corroborative analysis will consist of three main sections:

- Discussion of the implications of the modeling results and model performance evaluation, including findings from TexAQS projects and other advanced air quality research studies that have been conducted for the HGB area, and which have contributed greatly to the understanding of Houston's air quality problems;
- Discussion of the trend analyses for ozone and ozone precursor concentrations, including ozone metrics such as the design value, fourth highest daily maximum, ozone gradients, number of exceedance days, and precursor metrics such as annual average, annual 90th percentile and daily peak hourly ambient NO_X concentrations, monthly geometric mean and radar plot geometric mean HRVOC ambient concentrations and monthly geometric mean TNMHC; and
- Discussion of air quality control measures that are not modeled because they cannot be adequately quantified, but are nonetheless expected to yield tangible air quality benefits, such as marine fuel standards for ocean-going vessels, Smartway Transport Partnerships and Blue Skyways Collaboratives, control of flash emissions and energy efficiency measures (e.g. commercial and residential building codes).

The data and analyses presented in the corroborative analysis section will summarize the body of evidence that describes the causes of ozone in Houston.

8 MODELING DOCUMENTATION AND ARCHIVE

8.1 Documentation

EPA recommends that certain types of documentation be provided along with a photochemical modeling attainment demonstration. The TCEQ is committed to supplying the material needed to ensure that the technical support for any SIP revision is understood by all stakeholders. To that purpose, the TCEQ will document the following items in conjunction with the attainment demonstration:

Modeling Protocol - Establishes the scope of the analysis and encourages stakeholder participation in both the study development and the study itself;

Emissions Modeling Appendix - Summarizes the development of the model-ready emissions estimates. This appendix will contain tabular and graphical summaries of the data for the episodic base cases, and the baseline and future years;

Meteorological Modeling Appendix - Summarizes the development of the meteorological parameters used by the photochemical model. This appendix will contain tabular and graphical summaries of the relevant parameters;

Photochemical Modeling Appendix - As discussed in Section 6, an assessment of the suitability of the model to support emissions control policy will be assessed. The findings of that analysis will be discussed comprehensively in the model performance evaluation section of this appendix.

Also, as discussed in Section 6, several diagnostic analyses are planned to determine whether the photochemical modeling results are physically sound;

Description of the Attainment Demonstration Modeling and Weight-of-Evidence (WOE) - This documentation will provide an overall description of the modeling, including the future year modeling with specific control measures, as needed, and WOE arguments based on corroborative analyses, the combination of which suggests attainment will be achieved in a future year; and

External Review - TCEQ will document the review procedures (internal and external) employed in the project. This approach will include instructions provided to interested external parties for accessing the study database, including software utilized as part of the technical analyses.

Note that the above list is not all-inclusive and that additional documentation will likely be developed in the course of fully documenting the modeling activities. Some items may be documented as part of the actual SIP, while others will be provided as Appendices, Attachments, or Supplementary Reports. All relevant documentation will be available electronically, either through the TCEQ web site or by contacting the TCEQ.

8.2 Modeling Archive

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

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