MODELING PROTOCOL

Ozone Modeling
for the Northeast Texas
Early Action Compact

Prepared for
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1. INTRODUCTION

This document describes the procedures that will be used in modeling an August 1999 ozone episode for Northeast Texas. A modeling protocol is needed whenever ozone modeling is carried out for the purpose of developing emission reduction strategies that may be included in a State Implementation Plan (SIP). The requirements for a modeling protocol are described in two Environmental Protection Agency (EPA) reports:

> Draft Guidance on the Use of Models and Other Analyses in Attainment Demonstrations for the 8-Hour Ozone NAAQS. EPA-454/R-99-004. EPA Office of Air Quality Planning and Standards, Research Triangle Park, NC 27711. May 1999.
>
> Guideline for Regulatory Application of the Urban Airshed Model, EPA-450/4-91-013, U.S. Environmental Protection Agency Office of Air Quality Planning and Standards, Research Triangle Park, NC 27711. July 1991.

BACKGROUND

The Texas Commission on Environmental Quality (TCEQ) operates three Continuous Air Monitoring Stations (CAMS) in the Tyler/Longview/Marshall (TLM) area of Northeast Texas at Longview (CAMS19), Tyler (CAMS82) and Karnack (CAMS85). The stations shown in Figure 1-1, monitor compliance with the National Ambient Air Quality Standard (NAAQS) for ozone. NETAC also operates a research monitoring site currently located near Waskom and reporting as CAMS612.

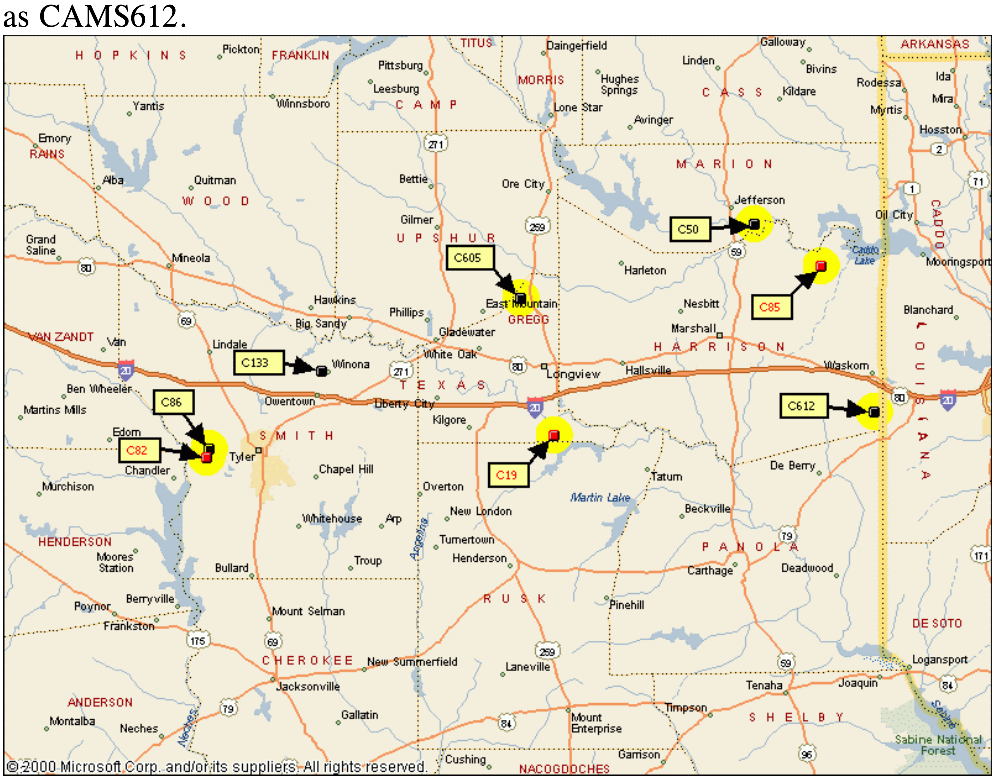

Figure 1-1. Air quality monitoring sites in Northeast Texas.

The Environmental Protection Agency (EPA) can require areas that do not comply with the ozone NAAQS to develop an emissions reduction plan, also called an ozone control strategy. Ozone control strategies are developed and tested using computer models. This protocol specifies the procedures that will be used in ozone modeling in Northeast Texas.

The US Environmental Protection Agency (EPA) currently has a 1-hour ozone National Ambient Air Quality Standard (NAAQS) that is not to exceed 0.12 ppm (124 ppb) with an expected exceedance rate of no more than once per year over three consecutive years (i.e., with complete data capture compliance with the 1-hour ozone NAAQS requires that the fourth highest daily maximum 1-hour ozone concentration in three years at every ozone monitor in the area be less than or equal to 0.12 ppm). Areas that violate the 1-hour ozone NAAQS are classified as ozone nonattainment areas. Ozone nonattainment areas must develop an ozone emissions control plan and demonstrate that they will attain the ozone NAAQS by the date specified in the Clean Air Act Amendments (CAAA) in a State Implementation Plan (SIP). The SIP ozone attainment demonstration is usually accomplished using air quality modeling.

In 1997, EPA promulgated a new ozone NAAQS that is potentially much more stringent than the old 1-hour standard. The new form is based on ozone measurements averaged over eight hours; violations of the 8-hour ozone standard occur when the fourth highest 8-hour ozone concentration each year, averaged over three consecutive years, at an individual monitor exceeds 0.08 ppm (84 ppb). The actual nonattainment designations are likely to be based on ambient measurements taken during the three years between 2001-2003. Regions that are currently designated as nonattainment of the 1-hour ozone NAAQS must still attain this standard (i.e., have three consecutive years over which the fourth highest hourly ozone concentrations at all monitors are 124 ppb or less). Once an ozone nonattainment region attains the 1-hour ozone NAAQS, then the 1-hour standard can be revoked by EPA and the area would be required to meet only the 8-hour standard.

On May 14, 1999, the D.C. District Court declared that EPA exceeded their authority in setting the 8-hour ozone standard and remanded it back to EPA. EPA appealed the decision to the US Supreme Court who in February 2001 upheld the new 8-hour ozone standard and remanded implementation issues back to the lower court. The lower court issued a ruling in March 2002 than required EPA to develop a new 8-hour ozone implementation approach and EPA plans to propose such an implementation rulemaking soon. Although EPA has not officially proposed a new implementation schedule, states have been asked to provide the EPA with a list of recommended 8-hour ozone nonattainment areas and boundaries by mid-2003. EPA is then expected to make 8-hour ozone nonattainment designations by April 2004 based on 2001-2003 ambient air quality data.

OZONE ATTAINMENT STATUS OF NORTHEAST TEXAS

In recent years ozone levels measured at Longview have exceeded the levels of both the 1-hour and 8-hour standards, and ozone levels measured at Tyler have exceeded the level of the 8-hour standard. In 1996, the TLM area became a Flexible Attainment Region (FAR) and a mechanism for developing strategies to attain the 1-hour ozone standard was implemented under a Memorandum of Agreement (Flexible Attainment Region Memorandum of Agreement, September 16, 1996). The TLM area has received funding from the Texas legislature to address ozone air quality issues. These resources have funded studies through the East Texas Council of Governments (ETCOG) under the technical and policy direction of the North East Texas Air Care (NETAC) organization. In 1999, ENVIRON completed an ozone modeling study for two 1-hour ozone episodes that included future year modeling for 2007 and the evaluation of future year emission reduction strategies. In 2002, the TCEQ submitted a State Implementation Plans (SIP) for Northeast Texas that was based on NETAC studies and included local emissions reductions measures and demonstrated attainment of the 1-hour ozone standard by 2007. At the end of 2002, NETAC embarked upon a process called an “Early Action Compact” (EAC) for developing 8-hour ozone control strategies. The EAC process is discussed below. The purpose of this modeling protocol is to guide ozone modeling for the Northeast Texas EAC.

EARLY ACTION COMPACT (EAC)

The TCEQ worked with the US EPA and stakeholders to develop the “Early Action Compact” (EAC) Protocol. The basic principals of the EAC Protocol are as follows:

- Early emission reductions to attain the 8-hour ozone standard;
- Local control, with broad-based public input;
- State support to ensure technical integrity of the early action plan;
- Early action plan incorporated into the SIP;
- Effective date of nonattainment designation and/or designation requirements is deferred (as long as all EAC terms and milestones are met);
- Safeguards to return to a traditional SIP requirements if EAC terms and/or milestones are not met.

In order to qualify for an EAC, an area must currently be attaining the 1-hour ozone standard. If a current 1-hour ozone attainment area has 8-hour ozone whose values that are approaching or exceeding the 8-hour ozone standard, the area may opt-in to the EAC in lieu of possibly being declared an 8-hour nonattainment area in 2004. There are several significant impacts from being declared an ozone nonattainment area:

- Transportation conformity budgets must be met or highway funds may be cut off;
- Major new or modified construction in the nonattainment area must offset its emissions to build in the area; and
- The area’s economic growth is restricted.

There are several steps in the EAC:

<u>Step#1: The Compact</u>

- Details how the EAC Plan will be developed;
- Lays out enforceable milestones with specific deadlines that must be met or 8-hour ozone planning reverts back to the traditional nonattainment area designation approach; and
- Must be signed and submitted to EPA by December 31, 2002.

Step#2: EAC Plan Development

- Components of the EAC Plan include:
  - Emissions Inventory
  - Modeling
  - Control Strategy that Demonstrates Attainment by 2007
  - Attainment Maintenance Analysis for Planning Growth to 2012
- The EAC Plan to be included in a SIP that must be submitted to EPA by December 31, 2004;
- Any adopted rules must be implemented by December 31, 2004 (target is attainment of the 8-hour ozone standard by 2007 relying on three years of monitored ozone data from 2005-2007); and
- Must address emissions growth until at least 2012.

EPA's commitment and safeguards for the EAC are as follows:

- If the area is meeting its EAC milestones at the time of 8-hour ozone nonattainment designations and is violating the 8-hour ozone standard:
  - Effective date of attainment designation and/or designation requirements is deferred.
- If the area attains the 8-hour ozone standard in 2007:
  - The area is re-designated as attainment and there are no further requirements.
- If the area fails to meet the milestones of the EAC then:
  - The area forfeits participation in the EAC.
  - The area enters into the traditional 8-hour ozone implementation process.
  - There are no delays or favorable treatment.
- If the area fails to attain the 8-hour ozone standard in 2007 (i.e., violates the 8-hour ozone standard based on 2005-2007 observed air quality data)
  - The Area is immediately designated as an 8-hour ozone nonattainment.
  - SIP revision due from State by December 31, 2008.
  - No delay in attainment date.

The key milestone dates in the Northeast Texas EAC are shown in Table 1-1.

Table 1-1. Key milestone dates for the Northeast Texas Early Action Compact (EAC).

Date	Item
December 31, 2002	Signed EAC agreement
June 16, 2003	Identify/describe potential local emission reduction strategies
November 30, 2003	Initial modeling emission inventory completed Conceptual model completed Base case (1999) modeling completed
December 31, 2003	Future year (2007) emission inventory completed Emission inventory comparison for 1999 and 2007 Future case modeling completed
January 31, 2004	Schedule for developing further episodes completed Local emission reduction strategies selected One or more control cases modeled for 2007 Attainment maintenance analysis (to 2012) completed Submit preliminary Clean Air Action Plan (CAAP) to TCEQ and EPA

Date	Item
March 31, 2004	Final revisions to 2007 control case modeling completed Final revisions to local emission reduction strategies completed Final attainment maintenance analysis completed Submit final CAAP to TCEQ and EPA
December 31, 2004	State submits SIP incorporating the CAAP to EPA
December 31, 2005	Local emission reduction strategies implemented no later than this date
December 31, 2007	Attainment of the 8-hour ozone standard

RELATED STUDIES IN NORTHEAST TEXAS

The Northeast Texas area has received biennial funding from the Texas legislature to address ozone air quality issues through the "near non-attainment areas" program. These resources have funded studies through the East Texas Council of Governments (ETCOG) under the technical and policy direction of the Northeast Texas Air Care (NETAC) organization. The activities conducted in each biennium are briefly summarized below.

> **FY 96/97**: ETCOG sponsored studies in to provide a better understanding of the conditions leading to high ozone concentrations. These studies examined the emissions inventory for the area as well as carrying out ambient monitoring.
>
> **FY 98/99**: Previous studies were extended through additional emission inventory development and ambient monitoring activities, plus the development of computer models to describe ozone formation in the TLM area. The TLM 1996 emission inventory developed was submitted by the TCEQ to EPA's National Emission Trends (NET96) database. Ozone models were developed for two episode periods (June 18-23, 1995 and July 14-18, 1997) that were selected because they had high 1-hour ozone levels (they also had high 8-hour ozone levels). A control strategy was developed that demonstrated attainment of the 1-hour ozone standard in 2007.
>
> **FY 00/01:** Studies continued ambient monitoring through the collection of VOC samples and the operation of a research ozone-monitoring site near Longview. The local emission inventory was improved and updated to 1999 for submission to EPA's NET99 database. A new ozone model was developed for an August 1999 ozone episode. This episode was selected after completing a conceptual model for the conditions that lead to high 8-hour ozone levels.
>
> **FY 02/03:** Ambient monitoring is continuing with the collection of VOC samples at Longview and the operation of a research ozone-monitoring site near Waskom. An aircraft monitoring study was completed in August/September 2002 to investigate the contributions of local emissions and regional ozone transport. The local emission inventory is being improved and updated to 2002 for submission to EPA's National Emission Inventory (NEI) database. Ozone modeling and control strategy activities are focused on supporting the EAC and meeting EAC milestones in 2003/2004.

Full descriptions of the completed studies are contained in the following reports available from the ETCOG.

Ambient Monitoring

Air Quality in East Texas. Findings for the 1995-1997 Biennium from the University of Texas. Prepared by the University of Texas at Austin, Department of Chemical Engineering and Center for Energy Studies, Austin 78712. October 1997.

Final Report for Project Number UTA98-0371 between the East Texas Council of Governments and the University of Texas at Austin through Environ Corporation. Prepared by the University of Texas at Austin, Department of Chemical Engineering and Center for Energy and Environmental Resources, Austin 78712. December 1999.

Air Quality Monitoring in East Texas During Year 2000. Prepared by Air Quality Solutions, Inc., 1301 S IH-35 Suite 107, Austin, TX 78741. January 26, 2001.

Air Quality Monitoring in East Texas, 2001 Final Report. Prepared by Air Quality Solutions, Inc., 1301 S IH-35 Suite 107, Austin, TX 78741. April 2002.

Air Quality Monitoring in East Texas, 2002 Final Report. Prepared by Air Quality Solutions, Inc., 1301 S IH-35 Suite 107, Austin, TX 78741. April 2003.

Emission Inventories

Tyler/Longview/Marshall Flexible Attainment Region Emission Inventory. Ozone Precursors, VOC and NOx 1995 Emissions. Prepared by Pollution Solutions, 3000 Taku Road, Cedar Park, TX 78613. May 1997.

Tyler/Longview/Marshall Flexible Attainment Region Emission Inventory. Ozone Precursors, VOC and NOx 1996 Emissions. Prepared by Pollution Solutions, 3000 Taku Road, Cedar Park, TX 78613. 1998.

A Biogenic Emission Inventory for the Tyler/Longview/Marshall Area Based on Local Data. Prepared by ENVIRON International Corporation, 101 Rowland Way, Novato, CA 94945. March 1999.

Tyler/Longview/Marshall Flexible Attainment Region Emission Inventory. Ozone Precursors, VOC and NOx 1999 Emissions. Prepared by Pollution Solutions, 3000 Taku Road, Cedar Park, TX 78613. June 2001.

Air Quality Modeling

Ozone Modeling Protocol for the Tyler/Longview/Marshall Area. Prepared by ENVIRON International Corporation, 101 Rowland Way, Novato, CA 94945. 22 April 1998.

Selection of Episodes for East Texas Photochemical Model Development. Prepared by ENVIRON International Corporation, 101 Rowland Way, Novato, CA 94945. 7 October 1998.

Ozone Modeling for the Tyler-Longview-Marshall Area of East Texas. Prepared by ENVIRON International Corporation, 101 Rowland Way, Novato, CA 94945. 12 November 1999. Revised 3 August 2001.

Conceptual Model for 8-Hour Ozone in East Texas and Episode Selection for New Photochemical Modeling. Prepared by ENVIRON International Corporation, 101 Rowland Way, Novato, CA 94945. 12 September 2000.

Ozone Modeling Protocol for FY 2000/2001 Projects in the Tyler/Longview/Marshall Area of East Texas. Prepared by ENVIRON International Corporation, 101 Rowland Way, Novato, CA 94945. 9 January 2001

Meteorological Modeling and Performance Evaluation of the August 13-22, 1999 Ozone Episode. Prepared by ENVIRON International Corporation, 101 Rowland Way, Novato, CA 94945. 7 August 2002

Revised Meteorological Modeling and Performance Evaluation of the August 13-22, 1999 Ozone Episode. Prepared by ENVIRON International Corporation, 101 Rowland Way, Novato, CA 94945. 27 January 2003.

Modeling an August 1999 Ozone Episode in Northeast Texas. Prepared by ENVIRON International Corporation, 101 Rowland Way, Novato, CA 94945. 5 May 2003.

RELATED STUDIES IN OTHER AREAS

The TCEQ is modeling the August 13-22, 1999 period to develop ozone control strategies for the Dallas/Fort-Worth (DFW) area. The modeling protocol for the DFW area was developed jointly by the TCEQ and ENVIRON:

Development of a Photochemical Modeling Database to Address 1-Hour and 8-Hour Ozone Attainment in the Dallas/Fort Worth Area. Prepared by ENVIRON International Corporation, 101 Rowland Way, Novato, CA 94945 and the Texas Commission on Environmental Quality, 12118 Park 35 Circle, Austin, Texas 78753. 22 May 2003.

The DFW and Northeast Texas modeling share the same 36 km and 12 km grids but have different 4 km grids. Both studies have similar emission inventories and are based on similar meteorological modeling with MM5. ENVIRON is completing the DFW base case modeling and performance evaluation by August 2003 and the TCEQ will continue with future year modeling and control strategy evaluation for DFW.

The Oklahoma Department of Environmental Quality (ODEQ) is modeling the August 13-25, 1999 period to develop ozone control strategies for the Oklahoma City and Tulsa areas. The modeling protocol for the ODEQ modeling was developed by ENVIRON:

> Development of a Photochemical Modeling Database to Address 8-Hour Ozone Attainment in the Tulsa and Oklahoma City Areas. Prepared by ENVIRON International Corporation, 101 Rowland Way, Novato, CA 94945 for the ODEQ, 707 North Robinson, Oklahoma City, Okalahoma 73105-3483. 31 December 2002.

ODEQ is modeling a slightly longer period than Northeast Texas and DFW. The ODEQ modeling uses the same 36 km grid as the Texas modeling studies, but has different 12 km and 4 km grids. The ODEQ and Texas studies have similar regional emission inventories and are based on similar meteorological modeling with MM5.

STUDY OBJECTIVES

The purpose of this modeling will be to extend previous work by updating the emissions inventories (for point, area, mobile, and biogenic sources), carrying out additional ambient monitoring, and bringing all the information together through the development and application of a photochemical ozone modeling system. This will:

- Provide a better understanding of conditions leading to elevated 8-hour ozone concentrations in Northeast Texas.
- Evaluate the likelihood of future exceedances of the ozone NAAQS in the area.
- Develop emissions reduction strategies to assure that the area does not exceed the ozone NAAQS in the future.
- Provide the technical analyses and documentation required for the EAC Clean Air Action Plan (CAAP) and future SIP revisions.

STUDY PARTICIPANTS

The modeling for this study is being performed by ENVIRON International Corporation (ENVIRON) under contract to the East Texas Council of Governments (ETCOG). The key personnel at ENVIRON who are directing and performing the study are identified below along with their contact information:

Dr. Greg Yarwood	Project Manager and Ozone Modeling	415/899-0704	gyarwood@environcorp.com
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The contacts at the East Texas Council of Governments (ETCOG) are:

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Kilgore, TX 75662
Phone (903) 984-8641
Fax (903) 983-1440

NETAC TECHNICAL ADVISORY COMMITTEE

The North East Texas Air Care (NETAC) Technical Advisory Committee will oversee all activities carried out during the course of the study. This committee includes representatives from the EPA and TCEQ as well as local governments, industries and environmental groups. The current members of the NETAC Technical Advisory Committee are as follows:

Mayor Murray Moore, City of Longview
Jim Mathews, NETAC Attorney, Mathews and Freeland
Robert Ray, Assistant City Attorney, City of Longview
Sharon Wellman, Eastman Chemical Company
Greg Morgan, Projects Coordinator, City of Tyler
Janet Cook, Asst. City Manager, City of Marshall
Erik Snyder, EPA Region 6
Michael Morton, EPA-Region 6
Mike Magee, SIP Coordinator, TCEQ-Austin
James Red, TCEQ-Austin
Charles Murray, TCEQ-Region 5 Air Program
L. Dale Rhoades, LaGloria Oil & Gas Company
Kelly Spencer, AEP/SWEPCO
Howard Ground, Manager Air Quality, AEP/SWEPCO
Dick Robertson, TXU Air Quality Manager
David Duncan, TXU
Dwight K. Shellman, Jr., Caddo Lake Institute, Inc.
Ramon Alvarez, Ph.D., Environmental Defense Fund
Eric Albritton, Attorney

Henry C. Bradbury, Environmental Solution

Members of the NETAC Technical Advisory Committee can be contacted through the ETCOG.

2. EPISODE SELECTION

A conceptual model of ozone formation in Northeast Texas was prepared and used as the basis for an episode selection analysis (ENVIRON, 2000). The episode selection methodology and conclusions are summarized below.

Ozone data for Northeast Texas monitors from 1995 through 1999 were reviewed along with meteorological data such as back-trajectories and daily weather maps. Episodes suitable for developing a new regional scale model for 8-hour ozone in Northeast Texas were identified by the following criteria:

- Choose periods from 1997 to 1999 since this matches the current design value period, the existing modeling includes an older episode from 1995, and there are more air quality data in recent years because of the Jefferson CAMS and NETAC studies.

- Choose a multi-day period with 3 or more "high ozone" days as defined below.

- Choose a period with high ozone at both Longview and Tyler. Based on the EPA guidance and current design values, high ozone is considered to be an 8-hour value of 85 - 101 ppb at Tyler, and 90 - 110 ppb at Longview.

- Choose a period with representative meteorological conditions (preferably stagnation with transport at the beginning or end of the period).

- Availability of supporting meteorological data, in particular data from the NCEP EDAS model, is a strong advantage. EDAS data are available since 1997 but there are occasional missing days or blackout periods.

- Availability of special air-quality data such as Baylor Aircraft flights and NETAC monitoring studies.

- An August or September episode may be preferable as this complements the existing June and July episodes, but this factor is secondary to having representative meteorology.

A search through 1997 to 1999 using these selection criteria listed above identified four candidate episodes:

1. August 26 to Sept 4, 1998
2. August 2 to August 7, 1999
3. August 15 to August 22, 1999
4. September 15 to September 20, 1999

The ozone data for these periods are summarized in Table 2-1 along with the maximum temperatures at Longview.

Table 2-1. Maximum ozone levels and temperatures for four candidate modeling episodes.

Date	Longview Maximum Temperature	Max 8-hour Ozone (ppb)				Max 1-hour Ozone (ppb)			
		Longview	Tyler	Jefferson	Big Woods	Longview	Tyler	Jefferson	Big Woods
8/26/98	97	85	68	59		108	74	65	
8/27/98	99	104	84	64		118	93	66	
8/28/98	101	114	87	76		129	95	81	
8/29/98	99	96	83	54		123	92	55	
8/30/98	95	73	85	51		79	104	59	
8/31/98	92	82	78	50		88	87	54	
9/1/98	96	73	73	50		78	79	53	
9/2/98	97	86	99	67		89	108	70	
9/3/98	99	107	91	76		125	99	81	
9/4/98	101	96	90	76		107	103	82	
8/2/99	96	95	61	60		108	68	66	
8/3/99	95	84	89	77		94	110	83	
8/4/99	95	91	88	79		132	102	83	
8/5/99	95	114	120	76		124	127	87	
8/6/99	95	missing	97	81		41	118	86	
8/7/99	97	missing	91	98		missing	102	115	
8/15/99	93	66	73	55		73	95	60	
8/16/99	95	105	92	71		124	109	74	
8/17/99	96	110	97	90		134	105	94	
8/18/99	99	88	74	91		91	78	98	
8/19/99	102	91	85	81		101	91	87	
8/20/99	97	80	86	70		90	99	72	
8/21/99	95	87	92	67		95	107	71	
8/22/99	96	91	77	82		107	78	87	
9/15/99	85	75	85	64	70	85	107	71	73
9/16/99	86	79	82	76	72	89	90	82	77
9/17/99	83	75	86	69	69	86	97	79	76
9/18/99	86	86	91	83	78	88	103	99	84
9/19/99	90	97	91	84	96	117	102	92	105
9/20/99	92	110	99	88	89	138	105	91	100

The August 2-8, 1999 period was eliminated because ozone data for Longview were missing on August 6 and 7 (see Table 2-1) severely restricting the usefulness of this period for control strategy development.

The August/September 1998 period was given the lowest priority among the remaining three candidates for the following reasons:

- Important supporting meteorological data (the NCEP EDAS analyses) are missing for most of this period.

- The meteorology includes several very stagnant days characterized by very "spikey" ozone readings at Longview (August 27 and 28). These days are very similar to the episodes already modeled for 1-hour ozone.

In selecting between the remaining two candidate periods, the August 1999 episode was given the highest priority for modeling since the September 1999 episode appears atypical and may be difficult to model for Northeast Texas. To be specific:

- The meteorology during the September 1999 episode appears to be unusual for high ozone episodes in Northeast Texas.
  - Temperatures were unusually cool for an ozone episode. Maximum temperatures at Longview were mostly in the mid 80's rather than the high 90's (see Table 3).
  - Upper level winds were from the west and unusually strong at 5000 m.
  - Widespread daily rainfall occurred in North Texas and Oklahoma. Archived NEXRAD data show rainfall in the area between Dallas to Shreveport on 4 of the 5 days.
  - We do not recommend choosing an atypical ozone episode as the cornerstone of 8-hour ozone control strategy development efforts.

- Some of the unusual meteorological factors mentioned above are also likely to make this a difficult period to model successfully for Northeast Texas. There is a greater risk of the September 1999 episode performing poorly in Northeast Texas than the August 1999 episode.

- The August 1999 episode provides more high ozone days to use for control strategy evaluation than the September 1999 episode (see Table 2-1).

SELECTED EPISODE: AUGUST 13-22, 1999

The period August 15 – August 22, 1999 was selected for 8-hour ozone modeling in Northeast Texas. When spin-up days are added, this means modeling August 13 – August 22, 1999

The hourly ozone data recorded at the Northeast Texas CAMS during this period are shown in Figure 2-1. High ozone levels were recorded at all three locations, with especially high levels recorded at Longview on August 16 and 17.

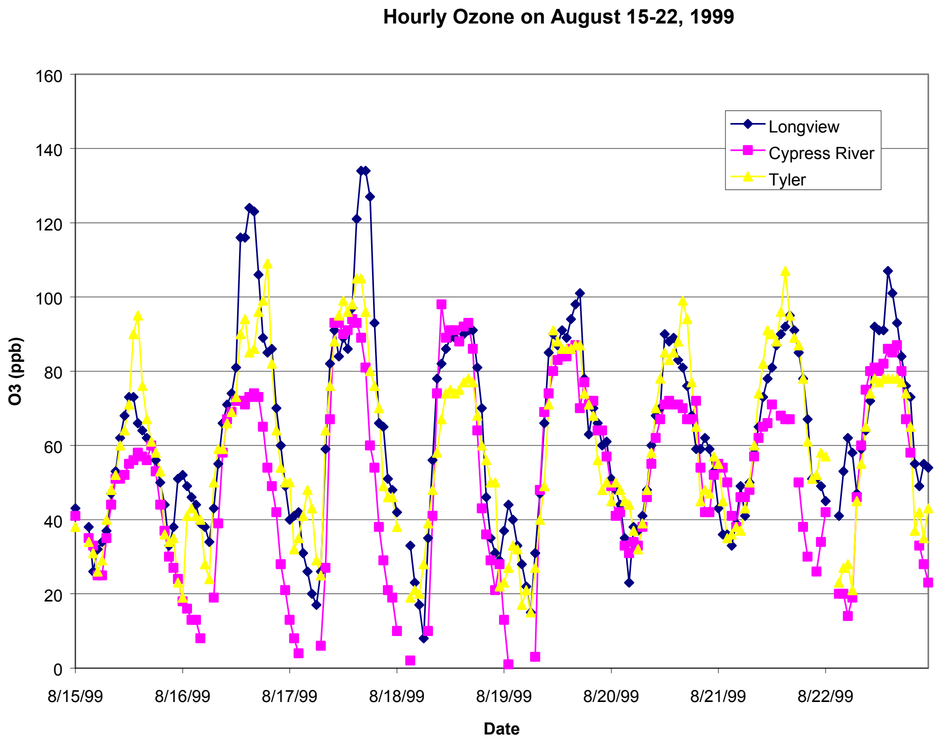


Figure 2-1. 1-hour average ozone levels at Northeast Texas CAMS for August 15-22, 1999.

3. MODEL SELECTION

This section introduces the models selected for use in the Northeast Texas Modeling Study and provides literature references to studies where the selected models have been evaluated and tested. The modeling methodology outlined in this protocol follows EPA's guidance for 1-hr regulatory modeling (EPA, 1996) as well as the current guidance for 8-hr modeling (EPA, 1999) in ozone attainment demonstrations.

The models selected for this study include:

- The Fifth Generation PSU/NCAR Mesoscale Model (MM5, version 3.4) meteorological model (Dudhia, 1993)
- Version 2x of the Emissions Processing System (EPS2x)
- The Comprehensive Air quality Model with extensions (CAMx, version 4.02) photochemical grid model (ENVIRON, 2003a)

METEOROLOGICAL MODELS

Currently, the two most commonly used state-of-the-science prognostic meteorological models are:

- The Regional Atmospheric Modeling System (RAMS, version 4.3)
- The Fifth Generation PSU/NCAR mesoscale model (MM5, version 3.4).

A number of recent studies have compared the theoretical formulations and operational features of these models (see, for example, Mass and Kuo, 1998; Seaman, 1995, 1997; Pielke and Pearce, 1994). Other studies have evaluated their performance capabilities under a range of atmospheric conditions (e.g., Hanna et. al., 1998; Seaman et al., 1992, 1995, 1996; Tesche and McNally, 1993a-f; McNally and Tesche, 1996, 1998). Also, several studies actually present model performance evaluation results for the RAMS and MM5 models for the 1995 OTAG episode (Tesche and McNally, 1996; Tesche et. al., 1997). These studies reveal that MM5 and RAMS have very similar technical specifications and capabilities and can generate comparable performance in the hands of experienced practitioners.

RAMS

RAMS was originally developed at Colorado State University and is now a proprietary (but widely available) model that is continuously upgraded and maintained by Atmet. Similar to the MM5, the foundation of this model has evolved over a 20-year period. The current version of the RAMS model represents the blending of the Colorado State University Mesoscale Model (CSUMM), commonly referred to as the Pielke model (Pielke, 1974), and a non-hydrostatic cloud physics model (Cotton et al., 1982; Tripoli and Cotton, 1982). The SAIMM and CSUMM-FDDA (McNally, 1990) models are modest extensions of the early CSUMM code. RAMS has been used for several air quality studies, including the Lake Michigan Ozone Study, the OTAG modeling, regional ozone modeling for the state of Texas, and air quality modeling in El Paso.

RAMS is a limited-area prognostic meteorological model based on the full set of primitive dynamic equations govern atmospheric motions (Walko and Tremback, 1991). The equation set is non-hydrostatic with prognostic equations for wind components, temperature, moisture, and pressure. Optional parameterizations exist for turbulent diffusion; solar and terrestrial radiation; moist processes including the formation and interaction of clouds and precipitation; sensible and latent heat exchange between the atmosphere, multiple soil layers, and a vegetation canopy; the kinematic effects of terrain; and cumulus convection (Tremback et al., 1985). RAMS optionally incorporates a four-dimensional data assimilation (FDDA) package that nudges predictive fields toward gridded balanced objective analyses derived from meteorological measurements. This ability is particularly useful for historical air quality applications to minimize meteorological model error, or “drift”, in reproducing the conditions of the modeled episode.

In principal, the RAMS domain and grid cell sizes can encompass a broad range of scales, from microscale phenomena such as tornadoes and boundary layer eddies to large-scale synoptic systems. Two-way interactive grid nesting in RAMS allows local fine mesh grids to resolve compact atmospheric systems such as thunderstorms, while simultaneously modeling the large-scale environment of the systems on a coarser grid.

The model equations are solved horizontally on an Arakawa-C grid structure defined on a rotated Polar-stereographic map projection. The vertical coordinate is a terrain-following sigma-z representation. Typically, RAMS utilizes 30 or so vertical levels with the first grid point about 50 meters above the surface. The top of the model domain is typically around 16-km above sea level. Fine grids nested within this structure may have vertical resolutions as fine as 10 meters; the fine grid's top may be around 4-km above the surface. As many as four levels of grid nesting may be used. Prognostic equations are also used for the soil surface temperature and water content. The number of soil levels employed in RAMS is typically about a dozen in the top meter of soil. A uniform representative soil type is assumed for the full domain.

RAMS is available under license from Atmet. Current licenses fees range from zero for the Federal Government to about $10k with one year of technical support for other groups.

MM5

MM5 is the most technically advanced and widely used public-domain prognostic model. The model is described by Dudhia (1993). MM5 has been widely used for preparing inputs to urban- and regional-scale photochemical air quality models. EPA is using a version of the MM5 as part of the Models3 air quality modeling system.

MM5 was developed at Pennsylvania State University over 20 years ago, and in cooperation with NCAR, has consistently been improved and updated over the last 10 years. Like RAMS, MM5 is based on the full set of non-hydrostatic primitive equations. Optional parameterizations exist for boundary layer schemes; cloud and precipitation physics; heat budgets for multiple soil layers; the kinematic effects of terrain; and cumulus convection. MM5 can also encompass a broad range of scales, from the microscale to synoptic systems. One- or two-way interactive grid nesting is allowed, as well as moveable nests that allow the model to follow weather features such as hurricanes. MM5 also contains a FDDA package, but unlike RAMS, allows for nudging toward gridded analyses or individual observations separately or in combination.

The model equations are solved horizontally on an Arakawa-B grid structure defined on a number of available map projections. The Lambert Conformal projection is currently being used for large-scale air quality applications in the U.S. The vertical coordinate is a terrain-following sigma-p representation. Typically, 20-30 vertical levels are specified, with the first grid point 20-50 meters above the surface, and the top of the model around 16-km above sea level.

MM5 is a publicly available at no cost and with no license restrictions.

Meteorological Model Selection

Either MM5 or RAMS would be technically appropriate for use in an ozone modeling study for Northeast Texas. The MM5 meteorological model was selected because:

- It contains all of the technical attributes required to simulate meteorological conditions associated with 1-hour and 8-hour ozone exceedance events in the Northeast Texas area;
- It is publicly available to all with no license fees or restrictions on use which allows industry and local governments to duplicate the modeling results.
- It is being used by the State of Texas for the development of several other ozone modeling projects including Houston and DFW.

In this work, the latest version of MM5 (version 3.4) will be used.

EMISSIONS MODELING SYSTEMS

There are three main emissions modeling systems that are used to processing anthropogenic emissions into the gridded, hourly resolved, and chemically speciated emissions needed for photochemical modeling.

<u>EPS2</u>: Version 2 of the Emissions Processing System was originally developed as part of the UAM-IV Modeling System (Morris and Myers, 1990). It is Fortran based and was designed to operate on 1990 era computer systems with memory constraints which limited its application to urban-scale modeling domains. More recently EPS has been speeded up and extended to treat regional-scale modeling domains (EPS2x). It is the emissions modeling

system used by the State of Texas for SIP modeling. It is Fortran-based, easy to use, and incorporates a strong quality assurance and reporting capability

EMS95: The Emissions Modeling System (EMS) is a SAS-based emissions processor that was used extensively during OTAG. As it is SAS-based, emissions summary reports can be readily prepared and it has strong quality assurance. The main weakness revolves around SAS that requires an expensive SAS license, requires some expertise in SAS to use, and is slower than the Fortran based models.

SMOKE: The Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system is a Fortran based system that is faster than the other two emissions models. However, the quality assurance (QA) is not integrated into the model as well as the other two systems. Recent experience in the Western Regional Air Partnership (WRAP) where SMOKE was applied by its developers, the QA weakness in SMOKE caused numerous difficulties that would be difficult to overcome when preparing a SIP under a tight schedule.

Emissions Model Selection

In selecting an emissions modeling system for Northeast Texas ozone modeling, the following criteria were considered:

- Ability to incorporate EPA's MOBILE6 and NONROAD emissions estimates into the modeling system.
- Fast processing of emissions to generate model-ready inventories.
- Strong Quality Assurance (QA) and reporting capabilities.
- Free public access and availability without any restrictions on use.
- Compatibility with other previous and ongoing work in related areas.

EPS2x was selected as the emissions modeling system because it was the only model that satisfied all of the criteria above. In particular, EPS2x is currently being used by the TCEQ for all other SIP modeling activities in Texas.

Use of the SMOKE emissions modeling system was considered. However, our experience with SMOKE in modeling for the Western Regional Air Partnership has been that some features are still under development and testing. Further, the Quality Assurance (QA) component in SMOKE is not as advanced as either EMS or EPS. Given the tight deadlines for EAC ozone modeling activities, it was felt prudent to select a fully tested emissions model with strong QA/QC capability.

AIR QUALITY MODELS

Several photochemical air quality models have been developed for ozone modeling and applied to different areas in the U.S. EPA's latest Guidelines for Air Quality Models (EPA, 2003) has no "preferred model," so areas can choose between several "alternative models." The latest EPA ozone modeling guidance lists the following *prerequisites* for an alternative model to be accepted:

1. The model must not be proprietary.
2. It should have received a scientific peer review.
3. It should be applicable to the specific problem on a theoretical basis.
4. It should be used with a database that is adequate to support the application.
5. It should have performed in past applications in such a way that estimates are not likely to be biased low.
6. It should be applied consistently with a protocol on methods and procedures.

The following models have been used recently for SIPs:

UAM-IV: Version IV of the Urban Airshed Model (Morris and Myers, 1990) was developed by Systems Applications, Inc., and for many years was EPA's guideline model. However, EPA recently removed this guideline status in its draft revisions to the Modeling Guidance because the UAM-IV is now considered out-dated, although it continues to be used in a few areas mainly using older databases for continuity purposes (e.g., Los Angeles and the California SIP). Available from the EPA at http://www.epa.gov/scram001/.

CALGRID: The CALGRID model was developed by Earth Tech (www.src.com) and was originally funded by the California Air Resources Board (CARB) to improve upon the UAM. CALGRID has been used in the Massachusetts SIP. It is also an outdated model that is not currently being used for any SIP modeling.

UAM-V: Version V of The Urban Airshed Model was developed by Systems Applications International/ICF Consulting and has been used in the Georgia (Atlanta) SIP, by other states, and by the EPA. The public availability and proprietary status are unclear since license terms and availability depend upon who requests the model. A restricted license version of UAM-V is available from the EPA at http://www.epa.gov/scram001/ or the model can be requested from ICF Consulting.

SAQM: The SARMAP Air Quality Model was developed for the CARB and used for the California SIP. SAQM is available on request from the California Air Resources Board (ARB). It has not been used for any ozone SIP work outside of California and will likely be replaced soon in California by one of the newer nested-grid photochemical models (e.g., CMAQ and/or CAMx).

CAMx: The Comprehensive Air Quality Model with extensions was developed by ENVIRON and publicly available at www.camx.com. CAMx was used by the State of Texas for the Houston-Galveston, Beaumont-Port Arthur, and Dallas-Fort Worth ozone attainment demonstration modeling in the Texas SIPs. CAMx is also used by other states for their 1-hour and 8-hour ozone planning and by the EPA for the NOx SIP Call and other rulemakings.

MAQSIP: The Multiscale Air Quality Simulation Platform was developed by the North Carolina Super Computing Center and is publicly available at www.mcnc.org. MAQSIP was used for the North Carolina SIP. It was developed as a prototype for the EPA Models-3/ CMAQ model and is being superceded by Models-3/CMAQ.

CMAQ: The Models-3 Community Multiscale Air Quality (CMAQ) modeling system was developed by EPA as a "one atmosphere" model to address ozone, PM, and visibility issues within one modeling platform. It is only just beginning to be used and has not yet been applied for any SIP modeling.

The technical attributes of several models are compared in Table 3-1.

Table 3-1. Comparison of several widely known ozone air quality models.

Model	**CAMx**	**MODELS-3 CMAQ**	**MAQSIP**	**UAM-IV**	**UAM-V**
Model Developer	ENVIRON	USEPA	MCNC	SAI	SAI
Computational Requirements	Medium	High	High	Medium	Medium
Documentation	Good	Good	Good	Good	Good
Ease of Use	Fair	Poor	Fair	Fair	Fair
Availability	Publicly Available	Publicly Available	Publicly Available	Publicly Available	Restricted
Horizontal Advection	PPM, Bott	PPM, Bott	Bott, Smolarkiewicz	Smolarkiewicz	Smolarkiewicz
Horizontal Diffusion	K-theory Varying Kh	K-theory Constant Kh	K-theory Constant Kh	K-theory Constant Kh	K-theory Varying Kh
Vertical Diffusion	K-theory Input Kv	Bulk and K-theory Internal Kv	Bulk and K-theory Internal Kv	K-theory Internal Kv	K-theory Input Kv
Grid Nesting	2-way, 1-way	1-way	1-way	1-way	2-way, 1-way
Dry Deposition	Yes	Yes	Yes	Yes	Yes
Wet Deposition	Yes	Yes	Yes	No	Yes
Gas-Phase Chemistry	Updated CB4 SAPRC99	Updated CB4 RADM SAPRC99	CB4 RADM	CB4	Updated CB4
Plume-in-Grid	Yes	Yes	No	No	Yes
Source Apportionment	Yes (OSAT, APCA)	No	No	No	No
Process Analysis	Yes	Yes	Yes	No	Yes
DDM Sensitivity Analysis	Yes	No	No	No	No

AIR QUALITY MODEL SELECTION

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

- Two-way grid nesting is essential for regional scale modeling in order to accurately depict local ozone formation in the Northeast Texas area as well as characterizing ozone transport from upwind regions. One-way grid nesting is considered inadequate because emissions are not treated consistently between the coarse and fine grids.

- A plume-in-grid algorithm is required to adequately represent the near source impacts of major NOx sources.

- An updated chemical mechanism is required. The minimum standard is considered the Carbon Bond IV mechanism with updated radical termination reactions and updated isoprene chemistry as used in the OTAG modeling.

- Updated transport algorithms with low numerical diffusion are highly desirable to accurately represent plume impacts of major sources. The PPM or Bott advection schemes are state-of-the-science whereas the Smolarkiewicz scheme is out-dated.

- Free public access and availability without any restrictions on use.

CAMx was selected as the air quality model for this study because it is the only model that satisfies all of the criteria listed above, is publicly available, has previously and is currently being used for several SIPs, and provides several “probing” tools (e.g., source apportionment, process analysis and the direct decoupled sensitivity analysis). For similar reasons, the TCEQ also uses CAMx for all SIP modeling in Texas.

4. MODELING DOMAINS

An important step in the design of an ozone modeling system is specifying the domain and grid system. The CAMx ozone model domain is discussed first since most of the factors influencing domain selection pertain to the ozone model. Then the specifications for the MM5 meteorological modeling domain are discussed. There is a close relationship between the CAMx and MM5 grids to ensure that meteorological information is transferred accurately from MM5 to CAMx.

The MM5 uses a Lambert Conformal Projection (LCP) grid system. CAMx can use several different grid projection systems including the LCP as well as others (e.g., UTM, Lat/long, and Polar Stereographic). In order to minimize any interpolation of the meteorological variables from MM5 to CAMx that could disrupt mass consistency it is preferred that CAMx use the same coordinate system as MM5. Thus, an LCP coordinate system will be adopted for CAMx.

LAMBERT CONFORMAL PROJECTION (LCP) DEFINITION

Several parameters define a Lambert Conformal Projection (LCP) horizontal grid coordinate system, namely a latitude/longitude "center" (0 km, 0 km) point, two true latitude parallels (that are typically 30 and 60 degrees), and a grid origin offset from the "center" and the east-west and north-south extent of the modeling domain. The TCEQ has defined an LCP coordinate system for use in all current episode development in Texas (Houston/Galveston, Beaumont/Port-Arthur, Dallas/Fort-Worth, Northeast Texas and San Antonio/Austin) to promote consistency between modeling projects and emissions inventories. The Texas standard LCP coordinate system is defined with the central coordinate of the LCP grid at 100°W and 40°N with true latitude parallels at 30°N and 60°N. The Texas standard LCP grid definition was adopted for the Northeast Texas ozone modeling.

CAMx DOMAIN

The following factors were considered in defining the CAMx air quality modeling grid:

- Placing a high resolution (4 km) grid over the key monitors, sources and urban areas in Northeast Texas.
- The Northeast Texas 4 km grid must be large enough to include local and nearby major sources of emissions.
- The regional domain must extend far enough upwind to include all sources that might contribute substantially to elevated ozone levels in Northeast Texas.
- The CAMx grid must closely match the MM5 grid to minimize distortion of the meteorological variables in transferring data from MM5 to CAMx.

These issues are discussed further below and a CAMx grid is recommended.

Horizontal Extent and Grid Spacing

EPA's draft guidance on applying models for 8-hr ozone (EPA, 1999) includes the following recommendations:

1. Use nested grids. The fine grid provides higher resolution in the area of interest, and coarse grid provides computational efficiency over the larger modeling region;
2. The grid spacing over the receptor areas of interest should ideally be 4-5 km and should not be larger than 12 km;
3. Use a grid spacing of 36 km or less for the regional domain;
4. Make the regional domain large enough to include approximately 2 days of transport distance upwind of the area of interest.

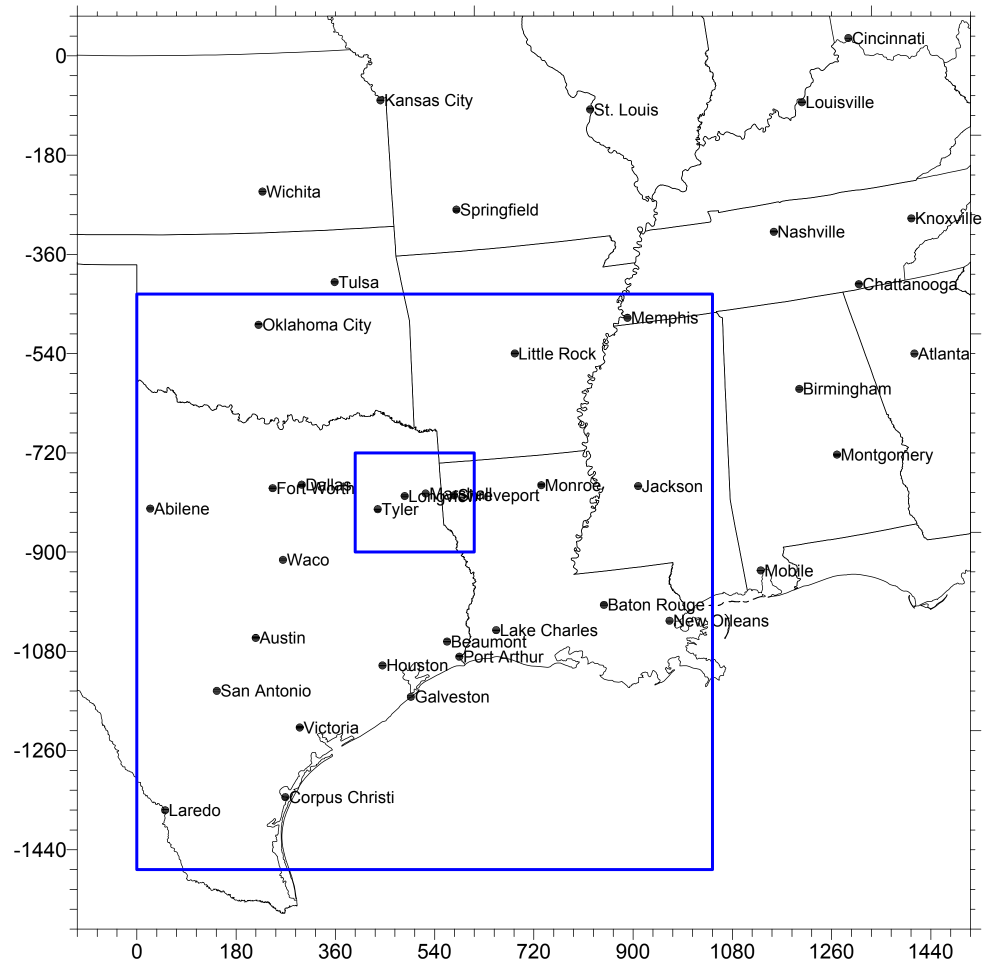
Additional requirements follow from the selection of MM5 as the driving meteorological model coupled with the desire to closely match the CAMx and MM5 grids:

5. Grid spacings for the nested grids must be multiples of three (e.g. 36/12/4 km).
6. Both grids must be defined in a Lambert Conformal Projection (LCP).

Based on these considerations, the CAMx grid for Northeast Texas will use 4 km and 12 km fine grids nested within a 36 km coarse grid. The coordinate system for the grids will be Lambert Conformal with the central coordinate of the LCP grid at 100°W and 40°N. The CAMx domain is shown in Figure 4-1.

The 36 km and 12 km grids shown in Figure 4-1 are the same as are being used for other ozone modeling studies in Texas. Having several modeling studies use a consistent grid system leads to efficient use of previous emissions inventory work and modeling experience. The 36 km coarse grid has been expanded further northeast relative to previous regional modeling studies in Northeast Texas. This expansion addresses concerns that during ozone episodes in Texas with winds from the northeast, there may be long-range transport of background ozone from as far as the lower midwest. Back trajectory analyses have suggested that under these conditions air mass transport times from the midwest to Texas may be 2-3 days, so this modeling domain is consistent with EPA's guidance that regional domains should account for potential transport distances of about 2 days upwind.

The 12 km grid includes all of the areas in eastern Texas that are conducting ozone modeling so that a consistent 12 km grid can be used in all studies. In addition, the 12 km grid includes a substantial area that would be upwind of Texas during an ozone episode with easterly or northeasterly winds. This is important to accurately represent any influence of ozone transport since ozone formation is modeled more accurately by a 12 km grid than a 36 km grid. The intention is to accurately model potential transport of ozone from areas at a distance upwind of about one State.



CAMx GRID DIMENSIONS
LCP Grid with reference origin at (40 N, 100 W)

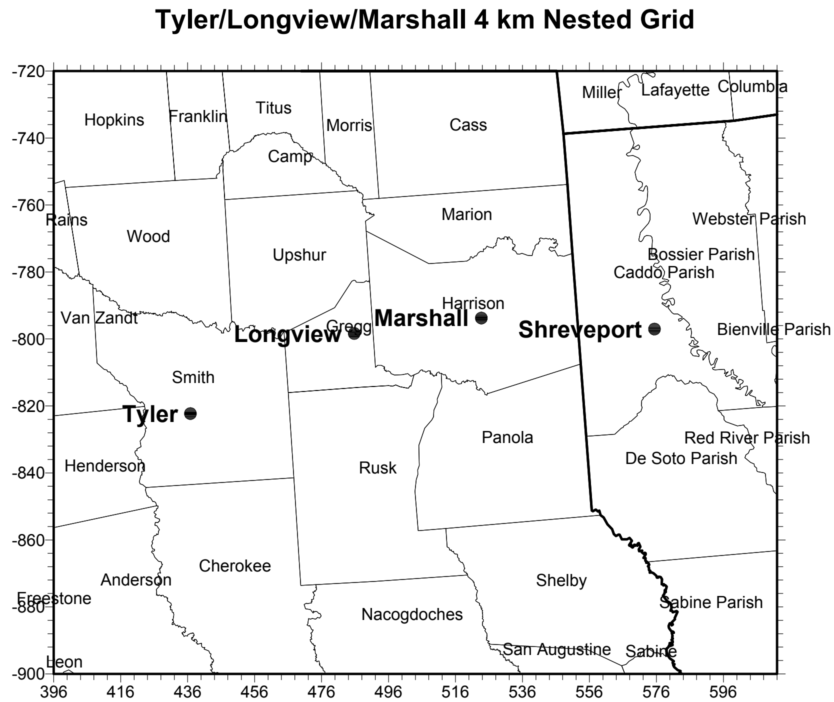
36 km Grid: 45 x 46 cells from (-108, -1584) to (1512, 72)
12 km Grid: 87 x 87 cells from (0, -1476) to (1044, -432)
4 km Grid: 54 x 45 cells from (396, -900) to (612, -720)

(nested grid dimensions do not include buffer cells)

Figure 4-1. CAMx grids for the Northeast Texas regional scale modeling of August 1999.

The 4 km grid covers the Tyler/Longview/Marshall area (Figure 4-2) and includes all of the emission sources in the immediate vicinity of the Tyler, Longview and Marshall ozone monitors. The 4 km grid includes all of the major sources in Northeast Texas that are part of the control strategies developed in previous modeling studies. The 4 km grid also includes the Shreveport urban area.

The 4 km grid is smaller than was used in previous ozone modeling of Northeast Texas (ENVIRON 1999a). The 4 km grid in the previous studies needed to be larger because the July 1997 episode was an urban scale model with no regional grid outside the 4 km grid, and therefore the 4 km grid needed to be large enough to contain any potential recirculation patterns.



CAMx GRID DIMENSIONS
LCP Grid with reference origin at (40 N, 100 W)

4 km Grid: 54 x 45 cells from (396, -900) to (612, -720)

(nested grid dimension does not include buffer cells)

Figure 4-2. Detail of the CAMx 4 km grid for the Northeast Texas regional scale modeling of August 1999.

Vertical Layers

EPA's current guidance on applying models for 8-hr ozone (EPA, 1999) includes the following recommendations on vertical layer structure:

1. Use 7-9 layers in the planetary boundary layer (PBL, the daily maximum mixing depth);
2. The surface layer should be no thicker than 50 m;
3. No layer within the Planetary Boundary Layer (PBL) should be thicker than 300 m; and
4. Add 1 or 2 layers above the PBL.

The CAMx and MM5 layer structures are shown in Figure 4-3. The CAMx layers exactly match the first 15 layers in MM5 up to approximately 4000 m above ground level (AGL). Under typical elevated ozone conditions in Northeast Texas the maximum depth of the PBL (i.e. mixing height) is about 1500-2000 m AGL. This means that MM5 and CAMx have about 10 layers within the typical maximum PBL and a 20 m surface layer. CAMx has about 5 layers above the PBL and below the model top. MM5 has more total layers than CAMx because the MM5 must be applied through at least the entire depth of the troposphere in order to capture weather systems. There is no advantage to extending the CAMx domain above about 4 km in order to model ozone within the PBL.

Layer	sigma	pressure	height	thickness	CAMx Layers
28	0.0000	50.00	18874.41	1706.76	
27	0.0250	73.75	17167.65	1362.47	
26	0.0500	97.50	15805.17	2133.42	
25	0.1000	145.00	13671.75	1664.35	
24	0.1500	192.50	12007.40	1376.75	
23	0.2000	240.00	10630.65	1180.35	
22	0.2500	287.50	9450.30	1036.79	
21	0.3000	335.00	8413.52	926.80	
20	0.3500	382.50	7486.72	839.57	
19	0.4000	430.00	6647.15	768.53	
18	0.4500	477.50	5878.62	709.45	
17	0.5000	525.00	5169.17	659.47	
16	0.5500	572.50	4509.70	616.58	
15	0.6000	620.00	**3893.12**	579.34	--15---
14	0.6500	667.50	**3313.78**	546.67	--14---
13	0.7000	715.00	**2767.11**	517.77	--13---
12	0.7500	762.50	**2249.35**	491.99	--12---
11	0.8000	810.00	**1757.36**	376.81	--11---
10	0.8400	848.00	**1380.55**	273.60	--10---
9	0.8700	876.50	**1106.95**	266.37	---9---
8	0.9000	905.00	**840.58**	259.54	---8---
7	0.9300	933.50	**581.04**	169.41	---7---
6	0.9500	952.50	**411.63**	166.65	---6---
5	0.9700	971.50	**244.98**	82.31	---5---
4	0.9800	981.00	**162.67**	65.38	---4---
3	0.9880	988.60	**97.29**	56.87	---3---
2	0.9950	995.25	**40.43**	20.23	---2---
1	0.9975	997.62	**20.19**	20.19	---1---
0	1.0000	1000.00	**0.00**	=============Surface======	

Figure 4-3. MM5 and CAMx vertical grid structures for regional scale modeling of August 1999. Layers are based on 28 sigma-p levels (including the surface) and heights (m) are above sea level according to a standard atmosphere; pressure is in millibars.

MM5 DOMAIN

The MM5 coarse and nested grids are shown in Figure 4-4 and are defined on the same LCP projection as CAMx. However, MM5 has an outer 108 km grid to capture the continental scale meteorology and to accommodate certain MM5 grid specification requirements. The MM5 36, 12 and 4 km grids are slightly larger than the corresponding CAMx grids to remove any artifacts (i.e., numerical noise) that can arise in MM5 adjacent to fine grid boundaries. The MM5 modeling uses the data-assimilation package (4DDA) to nudge the MM5 predictions toward 3-hourly, 40 km gridded meteorological analysis fields from the Eta Data Assimilation System (EDAS). Therefore, the MM5 108 km domain is sized to fit within the spatial limits of the EDAS fields. In this case, the southern edge of the MM5 domain is pushed to the southern limit of the EDAS fields. This is necessary in order to model the flow over the entire Gulf of Mexico, and to provide sufficient room for all the nested grid boundaries in southern Texas and northern Mexico. The MM5 vertical layers are shown in Figure 4-3, above.

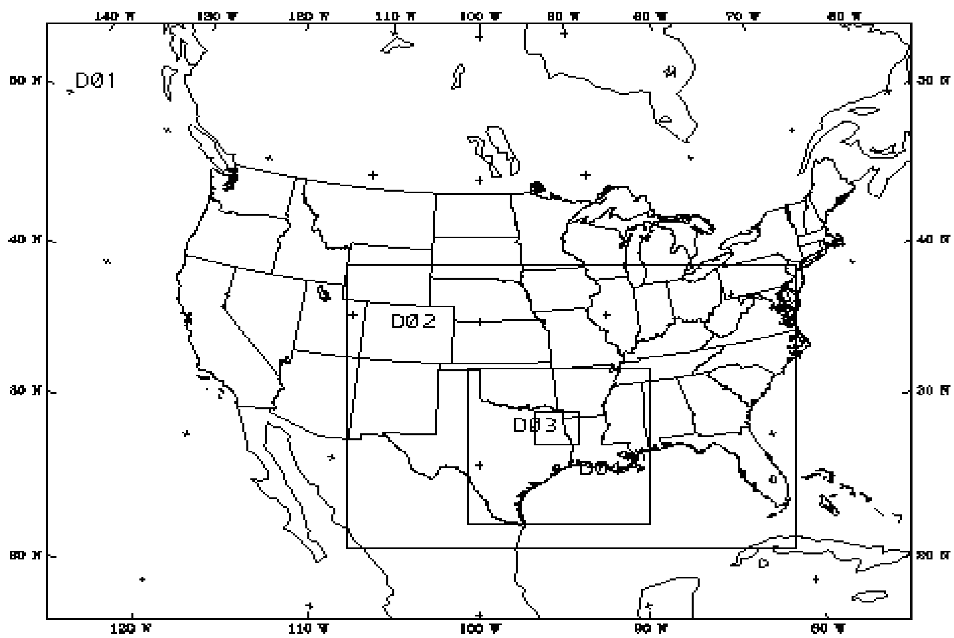


Figure 4-4. MM5 grid system (108/36/12/4 km) for Northeast Texas regional scale modeling of August 1999.

5. METEOROLOGICAL MODELING

The application of the MM5 meteorological model to prepare input fields for the ozone modeling is a complicated exercise that is governed by its own protocol. This section describes the general procedures that will be used in the meteorological modeling. It is understood that the application of a complex model like MM5 should not be undertaken using a prescriptive, pre-determined approach. Therefore, after the base case meteorology is established and performance evaluation testing is done, some model options and configurations may need to be refined during the project to improve model performance.

MM5 APPLICATION

We will operate the MM5 utilizing its Four Dimensional Data Assimilation (FDDA) capabilities. When used as a predictive (or forecasting) model, the MM5 is subject to a growing amount of error over the course of an extended simulation due to uncertainties in initial/boundary conditions, limits in spatial and temporal resolution, and simplifications in the governing equations. In simulations of historical episodes (as opposed to actual forecasting), FDDA is used to "nudge" model predictions toward observational analyses and/or discrete measurements to control model "drift" from conditions that actually occurred. This approach has consistently been shown to provide powerful advantages in running predictive mesoscale models for multi-day episodes, and has become a standard for photochemical applications.

For this project, we will supply the FDDA system with gridded meteorological analyses derived from the Eta Data Assimilation System (EDAS), which is archived at the National Center for Atmospheric Research (NCAR). Beginning in 1996, the EDAS provides 3-hourly gridded meteorological fields developed from the initialization cycle runs of the National Weather Service's Eta operational forecast model, which ingests observations from a combination of several systems (routine measurements from surface and upper air sites, radar networks, and satellite profilers). The EDAS domain covers most of the North American continent on a Lambert Conformal grid with 40 km grid spacing, and extends vertically from the surface to 50 mb (~20 km) with more than 20 pressure levels of data. We will augment this database with specialized data in the south-central U.S. to maximize performance in the areas of interest. These supplemental data include a wind profiler network (operated by the Forecast Systems Laboratory of NOAA), the EPA AIRS, observations from the Big Bend Regional Aerosol and Visibility Observation Study (BRAVO), which was operated in Texas between July and October 1999, and any local data available from Texas and Oklahoma.

Model Setup

The MM5 provides a wealth of options to configure the model for various parameterizations and physics packages. We will configure the model using the most appropriate options for each nested grid and for the meteorological conditions existing in the area of concern. A key MM5 option is which Planetary Boundary Layer (PBL) scheme to use.

We are currently evaluating several PBL schemes for applications in central Texas and will consider the following PBL schemes for the Northeast Texas MM5 modeling.

- MRF
- Blackadar
- Gayno-Seaman TKE
- ETA
- Pleim-Xiu

There has been a general realization among the MM5 user community that the MM5 Five-Layer Soil Model that has been used for MM5 modeling in the past may be too simple for land-surface processes, and that a more sophisticated Land-Surface Model (LSM) may be important for mesoscale meteorology modeling. Land-surface processes control the surface sensible and latent heat fluxes, which in turn strongly influence ground level air temperature, humidity and PBL development. As these parameters are especially critical for successful air pollution modeling, a more sophisticated LSM will be used in this application. Currently, two new LSM models are available in MM5, the Oregon State University LSM and Pleim-Xiu LSM models, are available in the MM5 version 3.5.

The Pleim-Xiu LSM, coupled with its own Planetary Boundary Layer (PBL) scheme, was employed in this work.

An initial MM5 run will be made that invokes the FDDA capabilities of the model, and that is configured with the physical treatments and options that, in our experience, have worked best in past photochemical modeling exercises. This configuration includes:

- FDDA analysis nudging on the 108/36/12 km grids:
    - 3D analysis nudging above the boundary layer -- MM5 is nudged toward 3-hourly EDAS analysis of wind, temperature, and humidity, which are improved by the surface and upper-air station observation data.
    - Surface analysis nudging within the boundary layer -- MM5 is nudged toward 3-hourly gridded surface analysis data generated by RAWINS program
- Simple-ice cloud microphysics will be employed for all grids.
- The Kain-Fritsch cumulus parameterization, which accounts for the effects of sub-grid scale convective activity, will be invoked for all grids except the 4 km nests. Sub-grid convection is not needed for the 4 km grid because MM5 can explicitly resolve convection at this grid scale.
- The Pleim-Xiu level-surface model. Coupled with its own PBL scheme will be employed in this work.
- The RRTM long wave scheme, which accounts for solar and terrestrial radiation impacts due to the presence of clouds, will be used for all grids.

Other MM5 configurations would be considered as needed, and we envision several additional MM5 sensitivity runs will be required to optimize performance. The types of additional simulations issues may include:

- Observational (or point) nudging of surface and profiler wind observations in the 4 km grid (as opposed to analysis nudging).
- Intensity and level of observational nudging (i.e., which data to assimilate at what strengths).
- The impact of the size of the 4 km nested grid on the MM5 simulation.
- The impact of alternative cumulus parameterizations and boundary layer treatments.
- The impact of altering soil characteristics and moisture content.

Performance Evaluation

Output from MM5 will be compared against meteorological observations from the various networks operating in Texas and throughout the south-central U.S. This will be carried out both graphically and statistically to evaluate model performance for winds, temperatures, boundary layer heights, and the placement, intensity, and evolution of key weather phenomena. The focus of this evaluation will center on performance in the 4 km grid. However, a regional analysis would also be carried out in different sections of the 12 km and 36 km MM5 domain.

The problem with statistics is that the more data pairings that are summarized in a given metric, the better the statistics generally look, and so calculating a single set of statistics for the entire 36 km domain would not yield significant insight into performance. Therefore, a series of three to four sub-regional analyses of MM5 performance would be conducted. Results from the local and sub-regional evaluations should give clues as to any necessary modifications to be made in the MM5 configuration.

GRID NESTING

Two-way nesting refers to the transfer of large-scale information down to nested grids, and the feedback of smaller scale influences up to larger grids. We will operate MM5 using two-way nesting for the 108/36/12 km grid simulation, and establish adequate model performance for the synoptic and larger-mesoscales before proceeding with the applications on the 4 km grid. However, we propose to operate MM5 using one-way nesting for the 4 km grid. In this approach, after the 108/36/12 km simulation is complete, 12 km grid results are extracted each hour to supply boundary information to the 4 km grid. Then MM5 is run separately for the 4 km grid, but the simulation results are not passed back to influence the 12 km results. This is a common practice among many mesoscale modelers because it allows the model to respond to the boundary conditions and fine grid parameters without a computational penalty. Our experience is that expansive 4 km MM5 simulations run quite slowly (even on our latest fast multi-processor machines), which limits our ability to run sensitivity tests if the complete 108/36/12/4 km grid system is run simultaneously. In our proposed approach, multiple MM5 runs for the 4 km nest can be made relatively quickly to optimize the model performance.

6. CAMx INPUT DATA PREPARATION

VERSION OF CAMx

The current publicly available version of CAMx is Version 4.02 released on July 9, 2003. CAMx version 4.02 will be used for the Northeast Texas ozone modeling.

EMISSIONS

CAMx requires two types of emission input files:

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

(2) Elevated emissions from major point sources are injected into CAMx at the coordinates of each source. The plume rise for each source is calculated by CAMx from stack parameters so that the emissions are injected into the appropriate vertical layer. Emissions from selected major NOx emitters may be treated with the CAMx Plume-in-Grid (PiG) module.

The emission files will be prepared using version 2x of the Emissions Processing System (EPS2x). The emissions model must perform several tasks:

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

Chemical speciation: Emission estimates for total VOC must be converted to the more detailed chemical speciation used by the Carbon Bond 4 (CB4) chemical mechanism in CAMx. Total unspeciated NOx emissions must be allocated to NO and NO_2 components.

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

Growth and Controls: Emissions estimated for one year may need to be adjusted for use in different year. In this project, the base year inventory may be for the same year as the modeling episode (1999) and so no adjustments will be needed. The 8-hour ozone modeling will rely upon modeling changes in emissions and air quality from 2002 to 2007. The 2002 emission inventory will use actual 2002 data wherever possible (e.g., CEM data for major NOx point sources) and otherwise will use projections from 1999(or a more recent year) to 2002. The 2007 future case inventories will be adjusted for growth and controls anticipated in the attainment year.

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

The outputs from the emissions model are called the "model-ready" emissions, and they are day-specific, gridded, speciated and temporally (hourly) allocated. EPS2x performs all of the processing steps for the anthropogenic emissions. The biogenic emissions are prepared using a different model (GloBEIS) because they are based on different input data and have specialized processing requirements (e.g., dependence on temperature, solar radiation and drought conditions).

Emissions Processing System (EPS2x)

The anthropogenic emission inventories will be processed using ENVIRON's enhanced version 2 of the Emissions Processing System (EPS2x). The original EPS2 was developed for EPA in the early 1990's. Design constraints imposed by the limited computer systems available at the time severely compromised performance for current regional modeling applications. However, EPS2 has all of the capabilities required for this study, and particular strengths of EPS2 include excellent reporting and QA capabilities and good documentation. ENVIRON has implemented several code revisions that greatly improve the speed of EPS2. With these modifications, the ENVIRON version of EPS2 has sufficient speed to perform the emissions modeling required for this project.

Anthropogenic Emissions Data Sources

The primary sources of emissions for the Northeast Texas ozone modeling study will be the NCTCOG (North Central Texas Council of Governments), TCEQ and the EPA. In the Northeast Texas CMSA and 4 km grid area, local data from the North Central Texas Council of Governments (NCTCOG) will be used. NCTCOG will conduct traffic demand modeling and develop day/hour specific link based emissions using the EPA MOBILE6 model. NCTCOG will also develop an offroad emissions inventory based on economic information, survey data, and the latest version of the EPA NONROAD model.

TCEQ data will be the preferred data source for point sources and all other areas in Texas. The most recent version of EPA's 1999 National Emissions Inventory (NEI) database will be used for most other states in the regional domain. Some data from the Louisiana Department of Environmental Quality (LA DEQ) will be used. The latest EPA emissions models will be used to estimate mobile source emissions, MOBILE6 for onroad mobile sources and NONROAD for offroad mobile sources.

Table 6-1 summarizes the source for emissions data that will be used in the Northeast Texas modeling.

Table 6-1. Summary of emissions data sources.

Category	Area	Data Source
Mobile	Northeast Texas	TTI link-based, MOBILE6.2
	Other Texas	TTI county level, MOBILE6.2
	Outside Texas	EPA NET99, MOBILE6.2
Offroad	Northeast Texas	NETAC data, NONROADv2002 model
	Other Texas	TCEQ data, NONROADv2002 model
	Outside Texas	EPA NET99 data, NONROADv2002 model
Area	Northeast Texas	NETAC data
	Other Texas	TCEQ data
	Outside Texas	EPA NET99 (area and offroad are combined)
Point	Northeast Texas	EPA acid rain data and NETAC data
	TX and LA EGU	EPA acid rain data processed by TCEQ
	Texas other	1999 TCEQ PSDB
	Louisiana other	LA DEQ provided to TCEQ
	Other	EPA NET99
Offshore	Texas	TCEQ offshore and shipping emissions
Biogenic	Texas	GloBEIS3.1 with TCEQ LULC data and drought adjustment
	Outside Texas	GloBEIS3.1 with BELD3 LULC data and drought adjustment

Note: EGU means electricity generating unit, i.e., utility boilers.

Biogenic Emissions

Biogenic emission inventories will be based on the most modern and scientifically advanced tool currently available, which is GloBEIS version 3.1. The State of Texas sponsored the development of GloBEIS through several projects performed by ENVIRON, the University of Texas at Austin, and the National Center for Atmospheric Research (NCAR). The GloBEIS model is publicly available at http://www.globeis.com along with a User's Guide and the report describing the model development. The key advantages of GloBEIS are: updated (BEIS3) emission factors; flexibility to incorporate detailed landuse data; ability to use solar radiation data from GOES satellite imagery; and built in QA and reporting functions. GloBEIS3 has several other advanced features including modeling the effects of drought or prolonged periods of high temperature. Biogenic emissions with/without drought conditions will be estimated using GloBEIS3.1.

QUALITY ASSURANCE

Thorough quality assurance of the emissions processing is essential for this study to provide meaningful results. We will address this by setting up independent QA/QC procedures for each stage in the emissions processing. The primary QA/QC strategies will be as follows:

1. Review EPS2x log files from each processing step for error messages.
2. Track emissions totals through processing to ensure that data integrity is maintained.
3. Prepare emissions summary tables by source category.

4. Review emission density and tile plots prepared with PAVE and compare to LU/LC and vegetation data.
5. Evaluate day-to-day variation in emissions for consistency with expected changes due to temperature, day-of-week, etc.

METEOROLOGY

CAMx requires meteorological input data for the parameters described in Table 6-2.

Table 6-2. CAMx meteorological input data requirements.

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

All of these input data will be derived from the MM5 results. MM5 output fields will be translated to CAMx-ready inputs using ENVIRON's MM5CAMx translation software. This program performs several functions:

1. Extracts data from MM5 grids and adjusts as appropriate to the corresponding CAMx grid.
2. Performs mass-weighted vertical aggregation of data for CAMx layers that span multiple MM5 layers.
3. Diagnoses key variables that are not directly output by MM5 (e.g., vertical diffusion coefficients and cloud information).

The MM5CAMx program has been written to carefully preserve the consistency of the predicted wind, temperature and pressure fields output by MM5. This is the key to preparing mass-consistent inputs for CAMx, and therefore for obtaining high quality performance from CAMx.

The data prepared by MM5CAMx will be directly input to CAMx with the exception of the vertical diffusivity coefficients (Kv). Vertical diffusivities are an important input to the CAMx simulation since they determine the rate and depth of mixing in the planetary boundary layer (PBL) and above. In general, our experience has been that diffusivities from meteorological models require careful examination before they are used in air quality modeling. This may be because the photochemical model results are much more sensitive to diffusivities than the meteorological model results. We will evaluate the CAMx diffusion inputs by comparing several calculation approaches, and by analyzing available sounding data from profilers and rawinsondes. Based on prior experience, we will likely apply minimum diffusivity values to the between layers 1 and 2 to ensure that nocturnal stability near the surface is not over-stated. The minimum value used will depend upon landuse (e.g., urban, forest, agricultural, water, etc.) to represent different impacts of mechanical mixing and surface heat input (e.g., urban heat island effect).

OTHER INPUT DATA

Initial and Boundary Conditions

Boundary and Initial Conditions

The initial conditions (ICs) are the pollutant concentrations specified throughout the modeling domain at the start of the simulation. Boundary conditions (BCs) are the pollutant concentrations specified at the perimeter of the modeling domain throughout the simulation. The boundary conditions are shown in Table 6-3 and varied by boundary segment as shown in Figure 6-1. The ozone BC was set to 40 ppb, which is the value commonly considered to be the continental background and used for ozone modeling studies. The NOx BC was set to 1.1 ppb, which is low but not exceptionally clean. The VOC BCs varied by boundary segment over a range from 9 to 50 ppbC according to broad differences in land cover. The higher VOC BCs in the Northeast/East boundary segment are for areas with higher biogenic emissions (Goldan et al., 1995; Watkins et al., 1995). The lower VOC BCs along the West boundary segment are for dryer areas with lower biogenic emissions. The lowest VOC BCs are over the Gulf of Mexico and these low values were also used for all boundaries above an altitude of 1700 m. The initial conditions were set to the lowest (Gulf of Mexico) BC values.

Table 6-3. Boundary concentrations for different boundary segments shown in Figure 5-4.

Species	East/Northeastern Boundary	Western Boundary	Southern Boundary
O3 (ppb)	40.0	40.0	40.0
NOx (ppb)	1.1	1.1	1.1
VOC (ppbC)	50.5	22.3	9.3

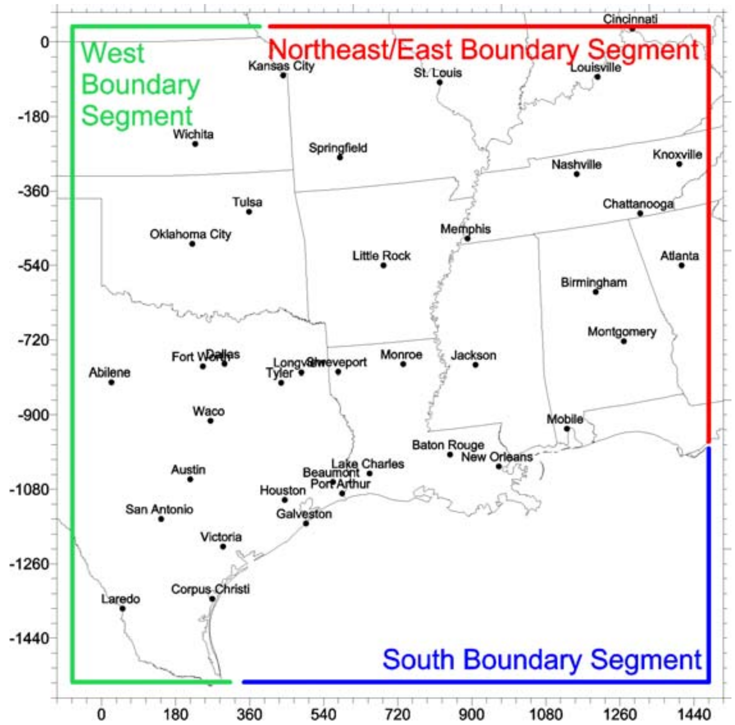


Figure 6-1. CAMx 36 km regional modeling domain showing boundary segments that are assigned different boundary conditions (BCs).

Surface Characteristics (Land Use)

CAMx requires gridded land use data to characterize surface boundary conditions, such as surface roughness, deposition parameters, vegetative distribution, and water/land boundaries. CAMx land use files provide the fractional contribution (0 to 1) of eleven land use categories (Table 6-4) to the surface area of grid cell. Gridded geographic data will be developed from USGS 200 m resolution landuse/landcover and topographic databases.

Table 6-4. CAMx land use categories and the default surface roughness values (m) and UV albedo assigned to each category.

Category Number	Land Cover Category	Surface Roughness (meters)	UV Albedo
1	Urban	3.00	0.08
2	Agricultural	0.25	0.05
3	Rangeland	0.05	0.05
4	Deciduous forest	1.00	0.05
5	Coniferous forest including wetland	1.00	0.05
6	Mixed forest	1.00	0.05
7	Water	0.0001	0.04
8	Barren land	0.002	0.08

Category Number	Land Cover Category	Surface Roughness (meters)	UV Albedo
9	Non-forested wetlands	0.15	0.05
10	Mixed agricultural and range	0.10	0.05
11	Rocky (with low shrubs)	0.10	0.05

Chemistry Data

Chemistry Parameters File

The CAMx "chemistry parameters" file determines which photochemical mechanism is used to model ozone formation. CAMx will be run with an updated version of the Carbon Bond 4 mechanism (CB4), referred to as mechanism 3 in CAMx, which is described in the CAMx User's Guide (ENVIRON, 2003a). Mechanism 3 is the CB4 mechanism with updated radical-radical termination reactions and updated isoprene mechanism as used for the OTAG modeling and other previous TCEQ modeling studies.

Photolysis Rate File

The CB4 mechanism also includes several "photolysis" reactions that depend upon the presence of sunlight. The photolysis rates input file determines the rates for chemical reactions in the mechanism that are driven by sunlight. Photolysis rates will be calculated using the Tropospheric visible Ultra-Violet (TUV) model developed by the National Center for Atmospheric Research (Madronich, 1993 and 2002). TUV is a state-of-the-science solar radiation model that is designed for photolysis rate calculations. TUV accounts for environmental parameters that influence photolysis rates including solar zenith angle, altitude above the ground, surface UV albedo, absorption by aerosols (haze), and stratospheric ozone column.

Albedo, Haze and Stratospheric Ozone Column

The albedo/haze/ozone input file is used in conjunction with the photolysis rates input file to specify several of the environmental factors that influence photolysis rates. The photolysis rates and albedo/haze/ozone files must be coordinated to function together correctly. The surface UV albedo will be calculated based on gridded land use data using the land use specific UV albedo values given in Table 6-4. The albedo varies spatially according to the land cover distribution, but does not vary with time. The total ozone column will be based on satellite data from the Total Ozone Mapping Spectrometer (TOMS), which are available from a web site maintained by the NASA Goddard Space Flight Center (http://jwocky.gsfc.nasa.gov). Daily ozone column are available at 1.25° longitude by 1° latitude resolution and were mapped to the CAMx grid. The haze optical depth will be set to a clean regional value of 0.1.

CAMx MODEL OPTIONS

CAMx has several user-selectable options that are specified for each simulation through the CAMx control file. Most of these options follow naturally from other choices about model inputs. There are three main optional inputs that must be decided for this project: the advection scheme, the plume-in-grid scheme, and the chemistry solver. The recommended choices for these options are discussed below. See the CAMx User's Guide (ENVIRON, 2003a) for more details on these options. The selection for each option will be decided at the stage of the base case model performance evaluation and then held fixed for the remainder of the project.

Advection scheme: CAMx has three optional methods for calculating horizontal advection (the movement of pollutants due to horizontal winds) called Smolarkiewicz, Bott and Piecewise Parabolic Method (PPM). The Smolarkiewicz scheme has been used for many years, and was used in many previous studies in Texas with CAMx and the Urban Airshed Model (UAM). The Smolarkiewicz scheme has been criticized for causing too much artificial diffusion of pollutants, tending to "smear out" features and artificially overstate transport. The Bott and PPM schemes are newer and have less artificial diffusion than the Smolarkiewicz scheme. The Piecewise Parabolic Method will be used for this study since it has provided optimum results in previous work. Sensitivity to other advection options may be evaluated in the base case depending upon model results.

Plume-in-Grid: CAMx includes an optional sub-grid scale plume model that can be used to represent the dispersion and chemistry of major NOx point source plumes close to the source. We will use the Plume-in-Grid (PIG) sub-model for major NOx sources (i.e., point sources with episode average NOx emissions greater than 10 tons per day). Sensitivity to PIG treatment may be examined in diagnostic tests for the base case.

Chemistry Solver: There are two options for the numerical solution scheme for the gas phase chemistry. Changing the chemistry solver option does not alter the chemical mechanism. The first option is the CMC fast solver that has been used in every prior version of CAMx. The second option is an IEH solver. The CMC solver is fast and more accurate than most chemistry solvers used in current ozone models. The IEH solver is even more accurate than the CMC solver but significantly slower. Because of its speed, the CMC solver will be used for this study. Sensitivity to using the IEH solver may be examined in diagnostic tests for the base case if appropriate.

Drought Stress

Analyses conducted by the Department of Agriculture (Figure 6-2) show that much of the Northeast Texas CAMx modeling domain was experiencing drought conditions during the August 1999 episode period. Drought stress affects vegetation and can influence ozone by changing the biogenic emissions and dry deposition rates. The effects of drought on biogenic emissions are considered in GloBEIS3 (Guenther et al., 2002; Yarwood et al., 2002) in relation to the Palmer drought index (SPI) calculated by the Dept. of Agriculture. Figure 6-2 shows an archived *forecast* of the expected drought conditions for August 1999, but the National Weather Service Climate Prediction Center also analyses actual drought conditions based on recorded meteorological data. The actual drought condition data will be used in the ozone modeling as described below.

Drought affects dry deposition by changing how ozone diffuses into the leaf cuticles through the stomata and is destroyed by contact with the leaf tissue (Weseley, 1989). One response of plants to moderate drought is to partially close leaf stomata in an attempt to reduce water loss. Figure 6-3 shows the GloBEIS relationship between drought stress on stomatal conductance.

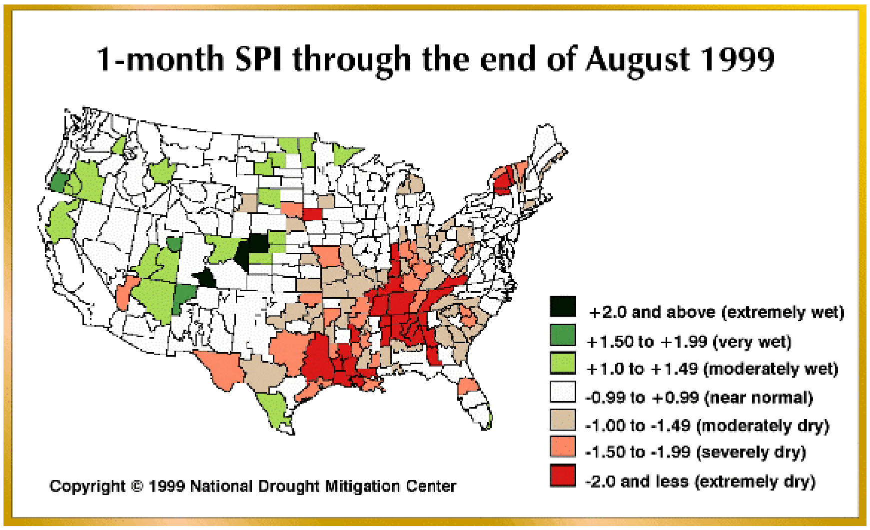


Figure 6-2. 1-month Standardized Precipitation Index ending in August 1999, indicating levels of drought relative to climatological norms in each climate zone.

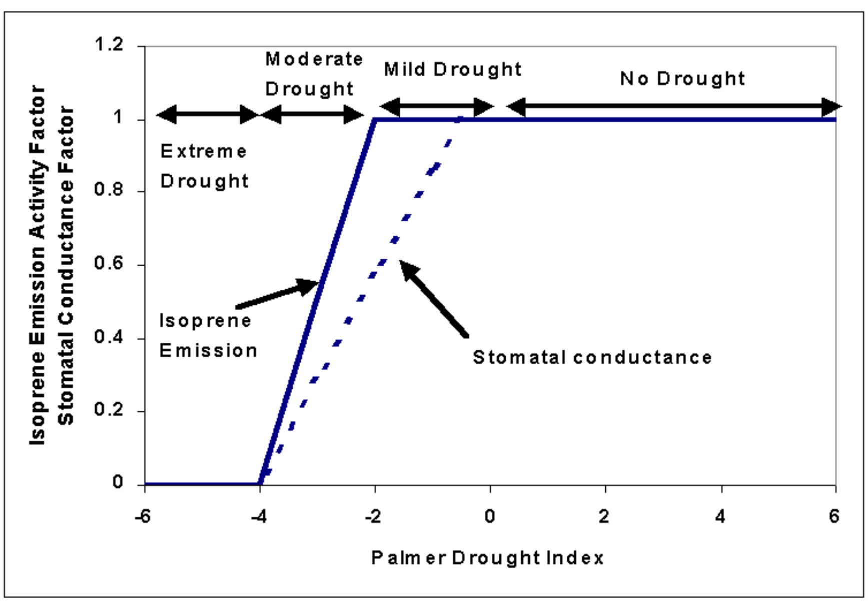


Figure 6-3. The GloBEIS3 relationship between leaf stomatal conductance and drought stress.

ENVIRON has modified CAMx version 4.02 to read an input file that specifies the Palmer Drought Index (PDI) value for each grid cell. This PDI value is used in the dry deposition algorithm to change the stomatal conductance. For moderate drought conditions (PDI of −1 to −3) the stomatal conductance is multiplied by 50%. For severe drought conditions (PDI less than −3) the stomatal conductance is reduced to near zero. This update to the CAMx code will be included in the next public release of CAMx and will be used to model the effect of drought stress on ozone levels.

The drought index input files will be generated from Palmer Drought Index (PDI) data obtained from the National Weather Service Climate Prediction Center. Drought severity is reported weekly for each climate division as defined by the Climate Prediction Center. These data are available from the FTP site (ftp://ftp.ncep.noaa.gov/pub/cpc/htdocs/temp2/) for the time period of interest.

7. BASE YEAR MODEL PERFORMANCE EVALUATION

For the base year modeling, CAMx will be run for the August 13-22, 1999 episode and the performance of the model will be evaluated against available air quality data. The purpose of the evaluation is to build confidence in the model's reliability as an ozone prediction tool. The proposed evaluation plan will follow the procedures recommended in the EPA guidance documents for 1-hour ozone (EPA, 1991) and 8-hour ozone (EPA, 1999).

APPROACH TO MODEL PERFORMANCE EVALUATION

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

- **The Model Should be Viewed as a System.** When we refer to evaluating a "model" we include not only the CAMx photochemical model, but its various companion preprocessor models (e.g., meteorological and emissions models) the supporting aerometric and emissions database, and all other related analytical and numerical procedures used to produce modeling results.

- **Model Acceptance is a Continuing Process of Non-Rejection.** Over-reliance on explicit or implied model "acceptance" criteria should be avoided, including EPA's performance goals (EPA, 1991). Models should be accepted gradually as a consequence of successive non-rejections, and confidence builds as the model undergoes a number of different applications (hopefully involving stressful performance testing) without encountering major or fatal flaws that cause the model to be rejected.

- **Criteria for Judging Model Performance Must Remain Flexible.** This approach recognizes that the model can give the right answers for various combinations of wrong inputs. Statistical tests are a first step in the performance evaluation, but not in themselves final or definitive. The model output must also be compared to time series and geographical plots as well as precursor data when it is available. Performance may even be degraded as new information and procedures are inserted into the model, because new elements may illustrate the presence of compensating errors that were previously unknown.

- **Previous Experience is Used as a Guide for Judging Model Acceptability.** Interpretation of the CAMx modeling results for the episode, considered against the backdrop of the quality of the meteorological and emissions inputs and previous modeling experience will aid in identifying potential performance problems and suggest whether the model should be modified, tested further, or rejected.

Incorporating these principals into an operational philosophy for judging model performance, we suggest the following approach for assessing the reliability of the CAMx model for control strategy development. The modeled ozone levels should be consistent with the goals and objectives proposed in Table 16-1 of EPA's draft modeling guidance for 8-hour ozone (EPA, 1999):

- The bias between the predicted and observed daily maximum 8-hour ozone at each monitor should be within about 20% for most monitors.
- The fractional bias between the predicted and observed daily maximum 8-hour ozone at each monitor should be within about 20% for most monitors.
- The correlation coefficient between the predicted and observed daily maximum 8-hour ozone should show moderate to large positive correlations.
- The normalized bias between the predicted and observed ozone (daily maximum 8-hour and 1-hour > 60 ppb) over all monitors should be better than ±5-15%.
- The normalized gross error between the predicted and observed ozone (daily maximum 8-hour and 1-hour > 60 ppb) over all monitors should be better than 30-35%.
- Scatterplots and quantile-quantile (Q-Q) plots of 8-hour and 1-hour ozone metrics should be reviewed.

These statistical evaluation methods provide goals, rather than criteria, for accepting model performance. If the model performance were better than all of these goals, the base case would not be rejected unless evidence from any supplemental diagnostic or sensitivity simulations suggests unusual or aberrant behavior.

If the base case fails one of the above general ranges, it would become necessary to explain why the performance is poorer than commonly achieved in similar applications and whether the problems will compromise the evaluation of emission control strategies. Without an explanation or working hypothesis, it is impossible to develop appropriate diagnostic and sensitivity tests, and the particular base case in question should be declared inadequate. After an assessment, there are several potential courses of action: (a) diagnose the causes of poor performance and rectify the problems, or (b) eliminate the poor-performing episode from use in strategy development and/or (c) identify an alternative episode for substitution in the study.

GRAPHICAL AND STATISTICAL EVALUATION

The evaluation of performance for the Northeast Texas 1-hour and 8-hour ozone modeling episode would be carried out in two sequential phases, beginning with the simplest comparisons of modeled and observed ground-level 1-hour and 8-hour ozone concentrations, and progressing to potentially more illuminating analyses if necessary (e.g., examination of precursor and product species, comparisons of pollutant ratios and groupings). The procedures outlined in the recent draft 8-hour modeling guidance illustrates the evolution in the EPA's previous 1-hour assessment procedures and provides a means by which to establish acceptable model performance:

1. Inspection of computer generated graphics, images and animations.
2. Calculation of ozone statistical metrics for bias, gross error and unpaired peak ozone.
3. Comparison of observed and predicted precursor emissions or species concentrations.
4. Comparison of observed and predicted ratios of indicator species.
5. Comparison of predicted source category contribution factors with estimates obtained using observational models.

6. Retrospective analyses in which air quality differences predicted by the model are compared with observed trends.

Sufficient fulfillment of these six points requires the availability of comprehensive measurement data on ozone and precursors from an extensive monitoring network. This may not be feasible in all cases, particularly in regards to precursor measurements. It is also quite possible that the list given above will change with the release of final guidance by EPA. Therefore, our proposed approach will consist of a blend of those points above and the three basic model performance steps outlined below. To the extent possible, each of the performance procedures described by EPA's 8-hour guidance will be addressed, and at a minimum, an explanation of why certain components cannot be fulfilled will be provided (e.g., insufficient observational data).

Initial screening of the CAMx base case ozone predictions will be performed for the modeling episodes in an attempt to identify obviously flawed model simulations and to implement improvements to the model input files in a logical, defensible manner. If the screening phase suggests that no obvious flaws or compensating errors exist in the simulation(s), then the work will progress to the operational evaluation. The screening evaluation will employ ozone performance statistics and plots. Graphical displays will be generated using a combination of several common software packages that the ENVIRON team possess in-house, most of which are readily accessible to the project sponsors. These software packages include the Microsoft Excel, Surfer, and publicly-available PAVE. Examples of the types of graphical displays to be considered for each base case include:

- Ozone time series plots of predicted and observed hourly and 8-hour ozone;
- Ground-level 1-hour and 8-hour ozone isopleths compared to real world data;
- Ozone observed/predicted concentration scatterplots;
- Bias and error statistics stratified by for day of episode and sub-region.

Experience in photochemical modeling is the best basis upon which to identify obviously flawed simulation results. Efforts to improve photochemical model performance, where necessary and warranted (i.e., to reduce the discrepancies between model estimates and observations), should be based on sound scientific principles. A "curve-fitting" or "tuning" activity is to be avoided. The following principles should govern the model performance improvement process (to the fullest extent possible given the project schedule):

- Any significant changes to the model or its inputs must be documented;
- Any significant changes to the model or its inputs must be supported by scientific evidence; analysis of new data, or by re-analysis of the existing data where errors or misjudgments may have occurred; and
- The TCEQ staff should review all significant changes to the model or its inputs and advise the Northeast Texas Photochemical Modeling Technical Committee.

If the initial examination of the CAMx ozone output does not reveal obvious flaws, the formal operational evaluation follows. This activity consists of evaluation of ozone precursors and sensitivity/diagnostic simulations. Graphical displays utilized in the screening evaluation for ozone will be generated for NOx and VOC data where available.

DIAGNOSTIC AND SENSITIVITY SIMULATIONS

Objectives

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

- Reveal model responses that are inconsistent with expectations or other model responses.
- Identify what parameters (or inputs) dominate (or do not dominate) model results.
- Examine the relationship between uncertainties in model inputs and model outputs (error propagation through the model).
- Identify alternate base cases that offer similar model performance and therefore identify potential compensating errors.
- Provide guidance for model refinement and data collection programs.

The exact number and nature of the sensitivity simulations that will be needed can only be assessed after the initial model performance evaluation is complete.

Tests That Are Not Recommended

With the advent of more sophisticated nested regional ozone models (such as CAMx) a number of sensitivity runs that were historically required by EPA guidance for the UAM-IV model are no longer needed or appropriate. These tests are zero-emission, zero initial condition, zero boundary condition runs and modified wind field tests such as halving the wind speeds. Physically unrealistic tests such as these can produce misleading results that are difficult to interpret. For the zero emission and zero IC/BC sensitivity tests, more can be learned from looking at sensitivity to alternate (but physically possible) inputs.

Ad-hoc, post processing modifications to wind fields outside of the meteorological models like MM5 are not recommended because they destroy consistency among the meteorological inputs (e.g., winds that are physically unrelated to pressures and temperatures). Other types of meteorological experiments such as alternate vertical eddy diffusivities or alternate vertical grid structures are potentially less destructive and may be more useful.

Recommended Tests

Sensitivity experiments will be considered as part of the performance evaluation analysis as appropriate. The potential need for and nature of these simulations will be discussed with the NETAC Technical Committee as required.

Potential diagnostic evaluation runs include changes to:

- Boundary conditions, sensitivity of local background concentrations to more or less polluted boundary and initial conditions.
- Biogenic emissions, to evaluate sensitivity to uncertainties in biogenic emissions due to canopy temperatures and drought during the episode.
- PiG treatment, to check ozone sensitivity to the implementation of this submodel for sources in the lignite belt.
- Advection solver, to evaluate impact of this model option on performance.
- Meteorology, specific diagnostic tests identified during the preparation of the meteorological modeling such as: alternate vertical diffusion coefficients to adjust daytime and night time mixing heights toward observed data; impacts of clouds on photolysis rates; and impact of wet deposition.

Potential sensitivity runs include:

- Sensitivity to reductions/increases in total anthropogenic VOC and/or NOx emissions.
- Sensitivity to reductions/increases in anthropogenic VOC and/or NOx emissions from specific source categories such as point, area, and mobile.
- Sensitivity to reductions/increases in anthropogenic VOC and/or NOx emissions from specific urban areas and source regions (e.g., distant or local).

USE OF CAMX PROBING TOOLS FOR DIAGNOSTIC EVALUATION

CAMx provides several "extensions" to the basic chemical/dispersion model, referred to as "probing tools", that provide information concerning source apportionment and the relative importance of various physical and chemical processes. These tools include the Ozone Source Apportionment Technology (OSAT and derivatives), the Integrated Process Rate Analysis Method (IPRAM), and the Decoupled Direct Method of tracking sensitivity coefficients to model inputs (DDM). All of these are described in the CAMx User's Guide for version 4.0 (ENVIRON, 2003).

For diagnostic purposes, the most useful tool is IPRAM, as this provides a wealth of information concerning the rates of change in ozone relative to transport and chemical processes. Reviewing this information can lead to insights into model performance and NOx/VOC-limited chemical kinetics in user-specified portions of the domain. Depending on project resources and schedule, use of IPRAM would be considered the primary tool for the diagnostic evaluation of the Northeast Texas CAMx Base Case simulations.

While OSAT and DDM would typically be used for assessing source apportionment for purposes of designing control strategy scenarios, both can be used in a diagnostic manner to assess the relative importance of various sources. In this way, the modeling team may be able to discover if a particular source area/category is having a stronger or weaker influence on ozone in key receptor areas than conceptually expected, and then undertake an investigation to determine if that response is appropriate or not. For understanding ozone contributions and identifying potential control strategy options, OSAT could be applied to generate source-receptor relationships. OSAT may be particularly useful for determining the level of ozone due to interstate and intrastate transport versus local sources in Northeast Texas.

8. ATTAINMENT DEMONSTRATION AND WEIGHT OF EVIDENCE ANALYSIS

INTRODUCTION

The ultimate use of the photochemical modeling database for Northeast Texas is the evaluation of alternative ozone emission control strategies and the demonstration that the selected ozone control plan will attain the 8-hour ozone standard by 2007. In this section we describe the procedures to be used to demonstrate attainment of the 8-hour ozone standard using the modeling results and additional data analyses to be undertaken to corroborate the modeled attainment demonstration test. The 8-hour ozone attainment demonstration test will follow EPA's draft 8-hour ozone guidance that uses the modeling results in a relative sense to scale current year observed 8-hour ozone Design Values to project the future-year 8-hour ozone Design Values (EPA, 1999). Data from the Longview, Tyler, Karnack and Waskom monitors will be used in the attainment test. The basic features of the 8-hour ozone modeled attainment test are described below with details contained in EPA's draft 8-hour ozone guidance (EPA, 1999).

EPA's draft guidance notes that there may be cases in which the modeled ozone attainment test does not project 8-hour Design Values of 84 ppb or lower (i.e., attainment), but there are reasons to believe that the selected control plan will achieve attainment. In this case, EPA's draft guidance has provisions for performing a Weight of Evidence (WOE) analysis that analyzes emissions and air quality data and the modeling results in more detail to provide a WOE attainment demonstration. A WOE attainment demonstration may be needed if the projected 8-hour ozone Design Value is above 84 ppb (although EPA notes that if it is above about 90 ppb a WOE test is not likely valid), or if there are insufficient modeled days with high ozone at an ozone monitor to perform the modeled attainment test. However, we believe that performing the additional data analyses activities identified in EPA's WOE analysis should be performed even if the modeled attainment test is passed and the WOE attainment test is not needed in order to provide corroborative evidence and more confidence that the selected 8-hour ozone control plan is a viable attainment plan. Thus, as part of the Northeast Texas 8-hour ozone study, the data analyses and other activities identified under EPA's WOE procedures will be carried out.

MODELED ATTAINMENT TEST

The modeled attainment test in the draft EPA 8-hour ozone guidance (EPA, 1999) will be used to demonstrate that the selected emissions control plan will achieve attainment in the future-year. This approach uses the modeling results in a relative fashion to perform Design Value scaling. The observed ozone 8-hour ozone Design Value at each monitoring site based on 2001-2003 data will be the starting point for the ozone Design Value scaling. The future-year for demonstrating attainment for the 8-hour ozone Early Action Compact (EAC) commitments is 2007. Once the model performance evaluation has shown that the model is replicating the observed ozone conditions for 1999, the model will be then applied using a 2002 emissions inventory to estimate conditions in 2002. There are several reasons why the NETAC

Technical committee, with approval from EPA and TCEQ, selected 2002 as the base year for the attainment demonstration:

- Significant emissions reductions were implemented for local major NOx point sources since 1999.
- Ozone levels have decreased since 1999 coincident with local emissions reductions.
- 2002 is the center of the 3-year period 2001-2003 that EPA will use for 8-hour ozone attainment designations.
- Projecting 2007 ozone levels from the more recent data (2002) will result in less overall uncertainty than projecting 2007 ozone levels from older (1999) data.

The emissions inventory will be projected to 2007 and the model would be run for 2007 to obtain 2007 8-hour ozone estimates. For each ozone monitor i and each episode day j modeled, a Relative Reduction Factor (RRF_{ij}) would be calculated that is the ratio of the 2007 to 2002 model estimated maximum 8-hour ozone concentrations "near" the ozone monitor on that day. With the 4-km grid spacing used in Northeast Texas in this study, "near" means the maximum ozone concentration on a 7 x 7 array of 4-km grid cells centered on the 4-km grid cell containing the ozone monitor in question (EPA, 1999).

Once day-specific RRFs have been estimated for each ozone monitor, an average monitor-specific RRF would be calculated using all episode days in which the 2002 estimated 8-hour ozone concentration was "close" to the observed 8-hour ozone Design Value for that day. EPA's draft guidance suggests defining close as within ±10 ppb but leaves the issue open to account for additional factors that can only be determined at the time of application.

The steps for performing the modeled attainment demonstration test are as follows (EPA, 1999):

1. Compute the site-specific observed 8-hour ozone Design Value based on 2001-2003 monitoring data;
2. Use the 2002 and 2007 modeling results to calculate a site-specific average RRF for each monitor;
3. Multiply the site-specific RRF obtained in Step 2 with the site-specific observed 2001-2003 8-hour ozone Design Value to obtain the projected 2007 8-hour ozone Design Value for that monitor. If the 2007 projected 8-hour ozone Design Value is 84 ppb or less at this site, then the 8-hour ozone attainment test is passed for this site.
4. Repeat Steps 1-3 for each monitoring sites with 2001-2003 8-hour ozone Design Values of 75 ppb or higher. If the test is passed at each monitoring site, the modeled attainment test is passed.

EPA's draft 8-hour guidance also has provisions for performing the attainment test at grid cells where the model consistently estimates high ozone concentrations but where no monitor is located. The attainment test for these "screened" grid cells will also be conducted following EPA's recommended procedures (EPA, 1999). ENVIRON has developed software to perform this analysis that has been tested in previous modeling studies for Northeast Texas (ENVIRON; 1999a, 2003b).

ADDITIONAL CORROBORATIVE ANALYSIS

Additional analysis of the modeling results and analysis of air quality and emissions data will be undertaken to corroborate the modeled attainment test and, if necessary, for use in a Weight of Evidence (WOE) attainment demonstration. These additional analyses will include, but not be limited to, the following.

Air Quality Data Analysis

The trend in 8-hour ozone concentrations and Design Values are analyzed at each monitor. The conceptual model for ozone in Northeast Texas will include trends in 1-hour and 8-hour ozone Design Values. Trends will also be calculated making adjustments to account for year-to-year variations in meteorological. The EPA draft guidance suggests using the Cox/Chu approach to factor out year-to-year meteorological variability when calculating ozone Design Value trends (Cox et al., 1993; 1996). Other approaches, with varying levels of sophistication, are also available. One component of the meteorological adjusted ozone trends that will be specific to Northeast Texas is factoring in the level of ozone transport days from the south that are highly correlated with 8-hour ozone exceedances in Northeast Texas.

Emissions Trends

The trends in ozone precursor emissions in the vicinity and upwind of the key ozone monitors will be documented. Trend in VOC and NOx emissions in the vicinity of Longview and Tyler will be examined along with trends in emissions in all of Northeast Texas as well as upwind areas (e.g., Louisiana and Texas).

In addition to an analysis of historical emission trends and their relationship with the trends in ozone concentrations discussed above, projected trends in emissions will also be made. Key future-years to be analyzed will be the EAC three-year attainment year period of 2005-2007 as well as 2012.

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