

Appendix H
1999 Base Case Modeling and Performance Analysis

**Development of the September 13-20, 1999 Base Case Photochemical Model for
Austin's Early Action Compact**

Submitted to

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Executive Summary

Austin is currently preparing an Early Action Compact (EAC) for submission to the Texas Commission on Environmental Quality (TCEQ) and the United States Environmental Protection Agency (U.S. EPA). The purpose of this report is to document the background and methodology used to develop the Base Case photochemical model that will serve as the technical foundation for Austin's EAC and to demonstrate that the model achieves performance criteria established by the U.S. EPA.

The area has utilized resources from the State of Texas' Near Non-attainment Areas Program to develop a conceptual model of meteorological conditions during high ozone events in Central Texas. The conceptual model was used to select the September 13-20, 1999 multi-day high ozone episode for development with the Comprehensive Air Quality Model with Extensions (CAMx) photochemical grid model. The September 13-20, 1999 modeling episode fulfills both the requirements of the U.S. EPA's *Draft Guidance on the Use of Models and Other Analyses in Attainment Demonstrations for the 8-Hour Ozone NAAQS* (1999) and the U.S. EPA's *Protocol for Early Action Compacts* (2003) that require representation of meteorological regimes typical of ozone exceedances. The episode covers one synoptic cycle for ozone in Austin with two initialization days and six high ozone days. It includes two weekend days (September 18th and 19th), such that control strategies can be evaluated with different emission characteristics.

The model domain is a nested regional/urban scale 36-km/12-km/4-km grid. The area has conducted extensive refinements and analyses of the MM5 version 3.5 meteorological model configuration, emission inventories, boundary and initial conditions, and dry deposition algorithms, since initiating development of the photochemical model in 2001. Comprehensive discussions of the model development are provided in the forthcoming report.

In accordance with U.S. EPA guidance, a MOBILE6.2-based inventory for on-road mobile source emissions has been developed for the Austin metropolitan area. Emissions for non-road mobile sources were developed using the U.S. EPA's NONROAD2002a model. Emissions from non-road mobile sources, stationary sources, and area sources have been estimated for Austin and other urban areas in the 4-km domain, using local activity data when available.

Model performance has been evaluated using statistical and graphical metrics for both 1-hour and 8-hour averaged ozone concentrations. The September 13-20, 1999 CAMx photochemical model meets or exceeds established U.S. EPA performance criteria for attainment demonstrations.

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1. Background

Austin is one of five areas that have received funding from the Legislature of the State of Texas to address ozone air quality issues through the Near Non-attainment Areas Program. The Capitol Area Planning Council (CAPCO) coordinates air quality planning activities in Austin. The area is currently preparing an EAC. The purpose of this report is to document the background and methodology used to develop the Base Case photochemical model that will serve as the technical foundation for Austin's EAC and to demonstrate that the model achieves performance criteria established by the U.S. EPA.

1.1 Overview of Photochemical Modeling Activities in the Austin Area

Over the past six years, the Austin area has utilized its resources from the Texas Near Non-attainment Areas Program to develop photochemical models for air quality planning. Similar to the ozone non-attainment areas in Texas, the Austin area has struggled with achieving acceptable model performance. The area initially leveraged a regional photochemical model developed by the Texas Commission on Environmental Quality (TCEQ) for June 18-22, 1995 (The University of Texas at Austin, 2000). Several enhancements were made for photochemical modeling in the Austin area including modification of the modeling domain to a 32-km/16-km/4-km nested domain and incorporation of link data for Travis County on-road mobile source emissions, biogenic emission estimates from GLOBEIS2 and recent land cover surveys, and non-road mobile emissions estimates from the U.S. EPA's NONROAD Model. Evaluation of the model's performance indicated a strong under prediction tendency. Significant concern was expressed about the accuracy of modeled wind fields away from monitors and aloft, the inability of the Systems Application International Meteorological Model (SAIMM) to replicate small-scale land/sea breeze circulations along the Gulf Coast, and the sensitivity of model performance in Houston/Galveston to changes in the emissions inventory. Because of the model's relatively poor performance, the Austin area and the TCEQ decided not to use this modeling episode to evaluate regional and local emissions strategies.

Instead, in 2000, the area chose to modify the model-ready enhanced emissions inventory developed for the June 1995 episode and pursue modeling a July 7-12, 1995 episode. ENVIRON initially developed the July episode for the San Antonio area with the Urban Airshed Model-IV (UAM-IV) in 1997 (ENVIRON International Corporation, 1997). The Alamo Area Council of Governments (AACOG), which coordinates air quality planning activities in San Antonio, requested that ENVIRON model this episode using CAMx (ENVIRON International Corporation, 1998). The TCEQ suggested that the Austin area update their existing June 1995 modeling emission inventory and leverage AACOG's CAMx model for their air quality planning activities.

The University of Texas at Austin (UT), under contract to CAPCO, modified the emissions for the June 1995 episode to obtain day-specific biogenic emissions, on-road mobile emissions, and NO_x emissions from electric generating units for the July 7-12, 1995 episode (McDonald-Buller, 2000). The Regional Atmospheric Modeling System (RAMS, version 3a) simulations for OTAG were the basis of the meteorological data for July 7-12, 1995. The model's performance in the Central Texas grid during the July 7-

12, 1995 episode was considerably better than during the June 18-23, 1995 episode. The TCEQ considered the performance of the model during the July 7-12, 1995 episode to be sufficient for *initial* air quality planning studies in both Austin and San Antonio. Both areas developed 2007 projected inventories for use with this episode and examined the impacts of reductions in ozone precursor emissions from different emission source sectors.

1.2 Photochemical Modeling for Austin's Early Action Compact

Conceptual models of meteorological conditions that occurred during high ozone events were used to select another modeling episode in 2001. Austin collaborated with San Antonio, Victoria, Corpus Christi, and the TCEQ to develop a photochemical model for a September 13-20, 1999 ozone episode. The protocol for the model's development and evaluation was written by ENVIRON and is presented in Appendix A. The areas have jointly worked for two years to improve this photochemical model, which is now being used for the Early Action Compacts for Austin and San Antonio. The following report describes the selection, development, and performance evaluation of this model. The remainder of the report is subdivided into the following sections:

Section No.	Description
2.	Ozone conceptual model for the Austin area
3.	Episode selection
4.	Model domain
5.	Meteorological modeling for the September 13-20, 1999 episode
6.	Emission inventory development for the September 13-20, 1999 CAMx model
7.	Land use data
8.	Dry deposition algorithms
9.	Chemistry data
10.	Boundary and initial conditions
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2. Ozone Conceptual Model for the Austin Area

The development of a conceptual model, which describes local meteorological conditions and associated large-scale weather patterns experienced during periods of high ozone, is the first step in episode selection. This report summarizes the conceptual model for multi-day high ozone events in the Austin area. A detailed discussion of the conceptual model is presented in Appendix B.

2.1 Datasets

The development of the ozone conceptual model for the Austin Area was based primarily on ozone and meteorological data collected during the 1993 through 2002 period. These years were selected because:

1. The conceptual model should be based on data collected during periods with emissions similar to current inventories; and
2. These data are available from several sources, including the U.S. EPA's Aerometric Information Retrieval System (AIRS) Database.

Both local and national datasets were used to develop the ozone conceptual model. Ozone and meteorological data collected at three Austin Area Continuous Air Monitoring Stations (CAMS) were utilized for the historical trend and data analyses. In addition, data collected at the San Marcos and Fayette County monitoring locations were used to estimate regional levels of background ozone. Table 1 presents a summary of identification and geographic data for each monitoring location. Figure 1 is a map showing the locations of the CAMS monitoring stations. The CAMS 3 site, located at Murchison Middle School, collected continuous measurements during the 1993 through 2002 period. The CAMS 25 monitoring station, located at the intersection of Parmer Lane and Mopac, was active from 1993 until the site was dismantled in February 1997. The site was relocated to the Audubon monitoring station (CAMS 38), located about 18 miles northwest of downtown Austin, in March 1997. Both the Murchison and Audubon monitoring stations continue to collect ozone and meteorological data through the present period. Monitoring at the San Marcos and Fayette County stations began in 1998. Monitoring at the San Marcos monitoring station was discontinued in August 2002. Data collected at all CAMS locations are archived by TCEQ as hourly averages, and are available via the Internet through the AIRS Database (<http://www.epa.gov/airs>).

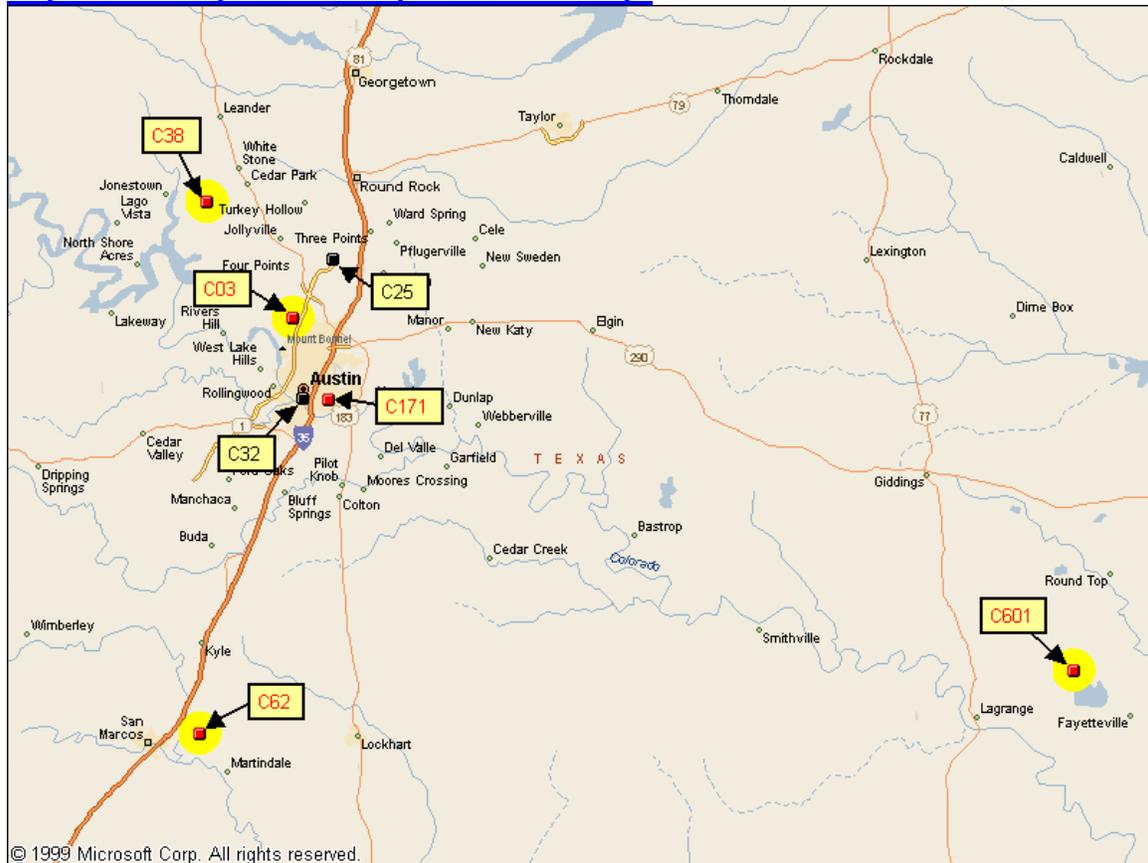
Analyses of the prevailing large-scale weather patterns were based on surface and upper-air weather maps provided by the National Weather Service. All weather maps analyzed were obtained from UNISYS (<http://weather.unisys.com>). The UNISYS archive of surface and upper air maps is currently available for the 1996 through present period.

Regional transport was investigated via the Lagrangian trajectory model HYSPLIT (Hybrid Single-Particle Lagrangian Integrated Trajectory) developed by a joint effort between the National Oceanic and Atmospheric Administration and Australia's Bureau of Meteorology (ARL) (<http://www.arl.noaa.gov/ready/hysplit4.html>). Most trajectories for

Table 1. Description and Location of Ozone Monitoring Stations in the Austin Area

Monitor Name	CAMS #	AIRS ID	Address	Active Years during 1993 – present
Audubon	38	48-453-0020	12200 Lime Creek Rd.	Mar. 1997 – present
Fayette County	601	48-149-0001	636 Roznov Rd.	Jul. 1998 - present
Murchison	3	48-453-0014	3724 North Hills Dr.	1993 – present
Parmer	25	48-453-0003	Parmer Lane at Mopac	1993 – Feb. 1997
San Marcos	62	48-055-0062	2041 Airport Dr.	Aug. 1998 – Aug. 2002

Figure 1. Location of Austin Area Monitors by CAMS # (Active monitors labeled in red. Ozone is not monitored at C171.) Courtesy of TCEQ Website <http://www.tceq.state.tx.us/updated/air/monops>



the 1993 through 1996 period were calculated based on the three-dimensional wind field provided by the Nested Grid Model (NGM) model forecast. The NGM dataset is archived by ARL with a 2-hour time resolution and a 180-km spatial resolution. Trajectories for the 1997 through 2002 period were primarily calculated from the three-dimensional wind field provided by the Eta Data Assimilation System (EDAS). The EDAS datasets are archived by ARL with a 3-hour time interval over an 80-km grid.

2.2 Ozone Trends

For purposes of this report, high ozone days were defined as those days exhibiting a peak 8-hour average ozone concentration greater than 75 ppb. The threshold value of 75 ppb was selected because:

1. The U.S. EPA guidance suggests 75 ppb as the lower threshold for an 8-hour averaging period for these analyses (U.S. EPA, 1999); and
2. A 75 ppb threshold provides a large enough dataset to allow robust statistics for the Austin Area.

During the 1993 through 2002 period, one or more Austin monitoring stations measured 75 ppb or greater on 173 dates. The annual number of high ozone days ranged from a minimum of 6 during 1996 to 34 during 1999. Annual 8-hour design values (i.e., annual fourth highest 8-hour averaged daily peak ozone concentrations) for Austin for the years 1988 through 2002 are presented in Figure 2.

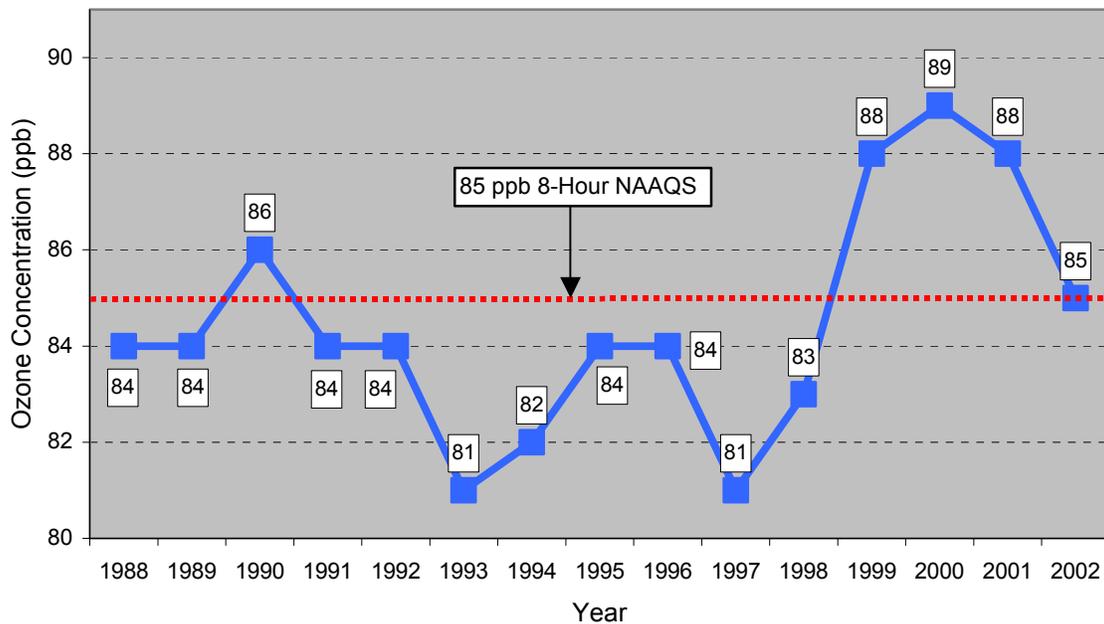


Figure 2. 8-Hour Ozone Design Values for Austin: 1988-2002

Higher ozone concentrations are typically measured at the Audubon location. Audubon, on average, measures an 8-hour peak concentration that is 7.5 percent greater than that measured at Murchison. Higher concentrations are equally likely to be measured at Murchison on days characterized by northeasterly, easterly, and southeasterly afternoon winds. During southeasterly flow, Audubon is likely better positioned to capture a portion of the downwind ozone plume. The consistent high bias at Audubon even during periods of easterly or northeasterly flow suggests there may be additional or alternate contributing factors to the observed bias between the two monitoring stations. Since the Murchison monitoring station is located relatively closer to the major transportation arteries in the region, NO from newly emitted mobile vehicle exhaust may react with some of the ozone to produce a localized decrease in ozone concentrations at the Murchison monitoring station. Interestingly, the bias decreases somewhat on days characterized by peak 8-hour ozone concentrations of 85 ppb or greater. Calm winds are often observed on these days, and the high ozone concentrations associated with the Austin plume are more likely to remain within the Austin urban area.

2.3 Meteorological Characteristics of Multi-Day High Ozone Events

High ozone concentrations occur preferentially during the August through early October period in the Austin area. Local meteorological measurements on high ozone days indicate an average daily maximum temperature of 92 °F and an average resultant mean wind speed of only 3.1 mph. Decoupling of the surface layer from the prevailing synoptic-scale circulation often results in rather variable morning wind directions. By late morning, mechanical mixing by convective thermals brings higher momentum air dominated by the large-scale flow to the surface, and afternoon winds typically blow from the northeast, east, or southeast.

A multi-day high ozone episode typically begins immediately after the passage of a weak frontal trough. These fronts provided little relief in terms of temperature, but represent a transition zone between drier continental air to the north and tropical maritime air from the Gulf of Mexico to the south. A ridge of surface high pressure advances southward into Texas behind the dissipating front. These high pressure systems are characterized by meteorological conditions highly favorable to the formation and accumulation of ground-level ozone, including light wind speeds, abundant sunshine, warm temperatures, and subsidence (sinking air) that inhibits vertical mixing and traps pollutants in a shallow layer near the surface.

The clockwise circulation around the surface ridge of high pressure, typically centered over the Central Plains or Ohio/Mississippi River Valleys, generates northeasterly or easterly flow that transports continental air and haze into eastern Texas. This continental airmass is often characterized by reduced visibility, and likely contains elevated concentrations of ozone and its precursor compounds associated with both biogenic and anthropogenic emissions. High ozone levels are often monitored throughout eastern Texas during these periods. Peak 8-hour ozone concentrations at the San Marcos and Fayette County monitoring stations under these conditions average 80-85% of the observed Austin maximum, suggesting significant regional transport of background ozone into Central Texas. With background levels ranging from 65 ppb to 85 ppb on

most high ozone days, even small contributions of ozone formed from local source emissions in the Austin area can result in a violation of the 8-hour NAAQS of 0.08 ppm.

3. Episode Selection

Since weather maps are readily available only for the 1996 through the current period, weather maps were only reviewed for multi-day high ozone episodes during the 1996 through 2002 period. For purposes of this review, a multi-day high ozone episode was defined as at least two consecutive days with daily peak 8-hour ozone concentrations greater than 75 ppb, with at least one day reaching 85 ppb. The dates of all reviewed events for the 1999 through 2002 period are listed in Table 2.

Given the historical preference for events to occur in August and September, emphasis was placed on high ozone episodes that occurred during these months. Though admittedly subjective, case studies were chosen to demonstrate the prevailing large-scale weather patterns that typically dominate during periods characterized by high ozone. A consistent large-scale weather pattern associated with multi-day high ozone episodes includes the migration of surface and/or upper level high-pressure systems across eastern Texas. These high-pressure systems are associated with meteorological conditions that favor the formation and accumulation of ground-level ozone. In addition, the large-scale clockwise flow around the high-pressure systems results in substantial regional transport of continental air, which contains elevated levels of background ozone and its precursor compounds, into eastern Texas.

Table 2. High Ozone Episodes during the 1999 through 2002 Period

Dates (mm/dd/yy)	Duration (Number of Days)	Daily Peak 8-Hour Ozone Concentrations (ppb)
8/03/99 – 8/07/99	5	82, 84, 103 , 98, 90
8/15/99 – 8/17/99	3	84, 96 , 80
8/20/99 – 8/21/99	2	93, 98
8/30/99 – 9/02/99	4	94 , 94 , 93, 89
9/15/99 – 9/20/99	6	79, 86, 100, 99, 101 , 88
9/23/99 – 9/24/99	2	79, 89
10/13/99 – 10/14/99	2	87, 87
8/01/00 – 8/02/00	2	85, 86
8/12/00 – 8/13/00	2	76, 88
8/31/00 – 9/07/00	8	80, 88, 89, 87, 79, 97 , 77, 79
9/15/00 – 9/18/00	4	83, 81, 77, 100
5/23/01 – 5/24/01	2	85 , 77
6/23/02 – 6/25/02	3	92, 100 , 75
9/11/02 – 9/14/02	4	76, 87, 96 , 91

Appendix B presents detailed discussions of the case studies examined for the Austin area. The Austin, San Antonio, Corpus Christi, and Victoria areas eventually selected September 15-20, 1999 as the joint near non-attainment area photochemical modeling episode, with September 13-14 included as model initialization days. The discussion below summarizes the atmospheric conditions during this episode.

Table 3 presents the maximum 8-hour ozone concentrations for selected metropolitan areas. High ozone concentrations were monitored across eastern Texas. Maximum ozone concentrations of 85 ppb or greater were measured in Austin on five consecutive days. Peak ozone levels reached 99 ppb, 99 ppb, and 101 ppb on the 17th, 18th, and 19th, respectively.

Table 3. Daily Peak 8-Hour Ozone Concentrations in Eastern Texas during September 15, 1999 through September 20, 1999

Date	Austin	Beaumont/ Pt. Arthur	Corpus Christi/ Victoria	Dallas/ Ft. Worth	Houston/ Galveston/ Brazoria	San Antonio	Tyler/ Longview/ Marshall
9/15/99	78	70	82	80	97	82	85
9/16/99	85	89	81	78	104	85	82
9/17/99	99	69	86	99	111	76	86
9/18/99	99	101	89	99	98	96	91
9/19/99	101	100	88	96	120	91	97
9/20/99	87	79	99	92	124	86	110

Mid-September was characterized by warm temperatures and low humidities associated with a continental airmass. During September 12th through 14th, a vigorous low-pressure system associated with a southward-moving cold front moved east and northeast through the U.S. northern plains and Great Lakes regions. The surface front passed through the Austin area on September 13th, transporting cooler and drier air into Texas. Surface winds in Austin were northeasterly during this period, and daily maximum temperatures reached the low 90s. Daily peak 8-hour ozone concentrations ranged from 55 ppb to 65 ppb. By September 15th, the upper-level low-pressure system lifted into eastern Canada, and zonal flow dominated most of the southern United States. Figure 3 shows 32-hour back trajectories for September 15, 1999 through September 20, 1999. A second surge of cold air entered Central Texas as Hurricane Floyd moved north along the Eastern Coast. Overnight lows dropped into the mid-50s and 60s in Central Texas.

The subtropical jet settled east-west across northern Texas throughout the remainder of the period, and shower activity in Dallas through the 17th was likely associated with a weak wave of low pressure propagating along the subtropical jet. A few isolated showers due to convergence along the dissipating surface trough occurred in Central and South

Texas during this period as well; however, conditions in Austin remained clear and rain-free. Maximum 8-hour ozone concentrations at Fayette County and San Marcos ranged between 65 ppb to 70 ppb on the 15th and 16th, suggesting high regional levels. The rather stagnant atmospheric conditions, coupled with transport of continental haze into Central Texas, contributed to a daily maximum 8-hour ozone concentration of 86 ppb on the 16th.

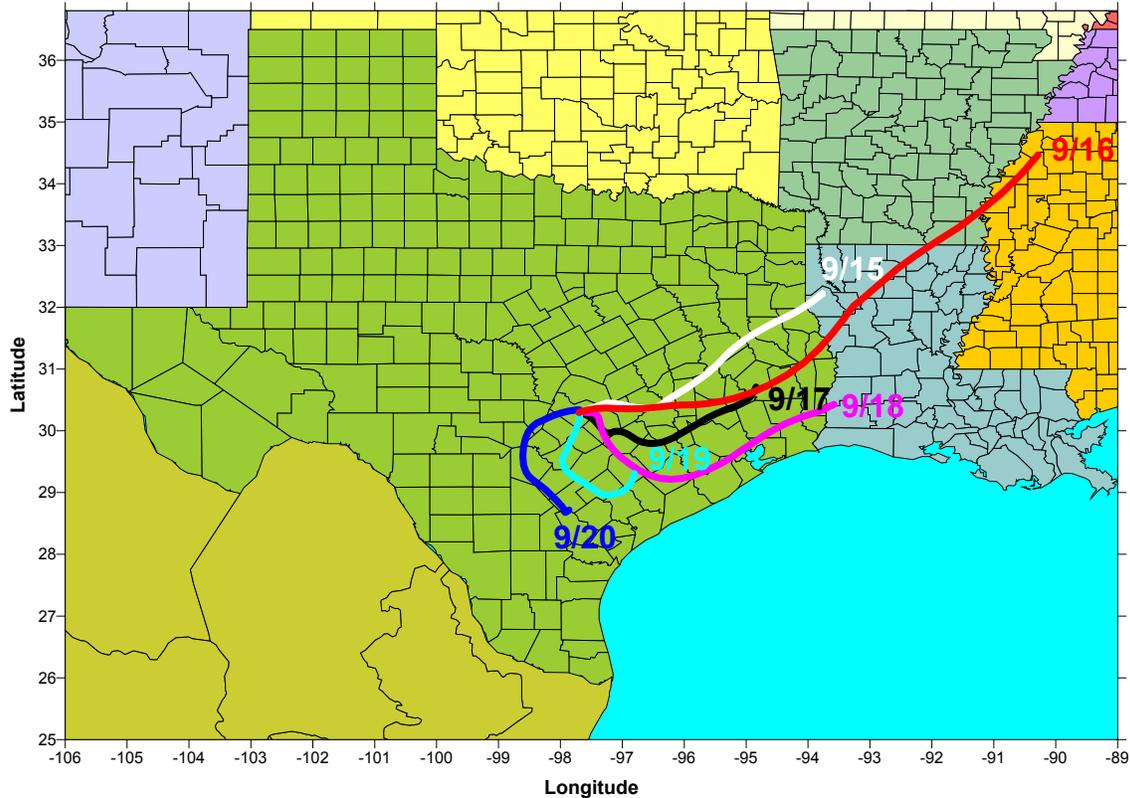
By the 18th, the strong surface ridge of high pressure centered over the Central Plains on the 15th had moved eastward to near Virginia. Clockwise flow around this ridge resulted in more southeasterly flow after the 16th. During the 17th through 19th, maximum 8-hour ozone concentrations at Fayette County and San Marcos ranged from 75 ppb to 85 ppb. Clear skies dominated Central Texas. As surface wind speeds decreased from approximately 5 mph to less than 3 mph, peak ozone concentrations reached 99 ppb in the Austin Area on the 17th and 18th. Fog and/or haze were reported on some days, likely associated with transport of continental haze, and indicated an extremely stagnant lower atmosphere. Daily maximum temperatures increased to the mid-90s by the 19th, and the highest ozone concentration of 101 ppb was measured in Austin. Tropical Storm Harvey formed in the central Gulf of Mexico and began to move northeasterly. This tropical circulation may have enhanced subsidence in Texas, though the impact of the system appears minimal. By September 19th, southerly flow had returned to Central Texas as the surface ridge of high pressure, now located over the northeastern U.S., was rapidly weakening and moving to the northeast ahead of a second cold front. Winds in Austin became southwesterly on the 20th, immediately ahead of a second frontal passage late on September 20th. This front brought strong northerly winds and much colder and drier air to Texas.

The U.S. EPA's *Draft Guidance on the Use of Models and Other Analyses in Attainment Demonstrations for the 8-Hour Ozone NAAQS* (1999) is the principal guidance document for areas submitting EACs. The guidance specifies four primary criteria for selecting meteorological episodes to model:

1. "Choose a mix of episodes which represent a variety of meteorological conditions which frequently correspond with 8-hour daily maxima > 84 ppb at different monitoring sites.
2. Model periods in which observed 8-hour daily maximum concentrations are close to the average 4th high 8-hour daily maximum concentrations.
3. Model periods for which extensive air quality and meteorological databases exist.
4. Model a sufficient number of days so that the modeled attainment test applied at each monitor violating the NAAQS is based on several days."

The guidance also indicates that tradeoffs among the four primary criteria may be necessary. In addition, the U.S. EPA's *Protocol for Early Action Compacts* (2003) specifies that "a 1999 or later episode reflective of a typical ozone season exceedance that meets the U.S. EPA's episode selection guidance to ensure that representative meteorological regimes are considered" must be included.

Figure 3. 32-Hour Back-Trajectories for September 15, 1999 through September 20, 1999



The September 13-20, 1999 modeling episode fulfills both the requirements of the U.S. EPA draft guidance and the protocol for representation of meteorological regimes typical of ozone exceedances. Although on some days of the episode, maximum daily 8-hour ozone concentrations exceeded the annual design values shown in Figure 2, the episode is an ideal example of the high ozone episodes described in the conceptual model for the Austin area. Extensive air quality and meteorological databases specifically for Central Texas are not available. The episode covers one synoptic cycle for ozone in both Austin and San Antonio with two initialization days and six high ozone days, which achieves the objectives of the fourth criteria specified by the U.S. EPA. In addition, the episode includes two weekend days (September 18th and 19th), such that control strategies can be evaluated with different emission characteristics. An important consideration in selecting this episode was that high ozone concentrations were observed throughout Central Texas, which had not necessarily been the case for previous modeling episodes. Thus, the areas of Austin, San Antonio, Corpus Christi, and Victoria, along with the TCEQ, could combine their resources for development of a new episode that focused specifically on conditions associated with high ozone in Central Texas and that was not leveraged from other areas, such as Houston and Dallas.

The forthcoming sections document the specification of the modeling grid, the development of the meteorological input, emission inventories, boundary and initial

conditions for the episode, and the results of the model performance evaluation. The initial development of the model was performed by ENVIRON International Corporation (ENVIRON) with assistance in the meteorological model development from the University of Texas (UT), and emission inventory development from CAPCO, AACOG, the City of Victoria, the City of Corpus Christi and their contractors. The TCEQ provided oversight and technical assistance throughout the process.

4. Model Domain

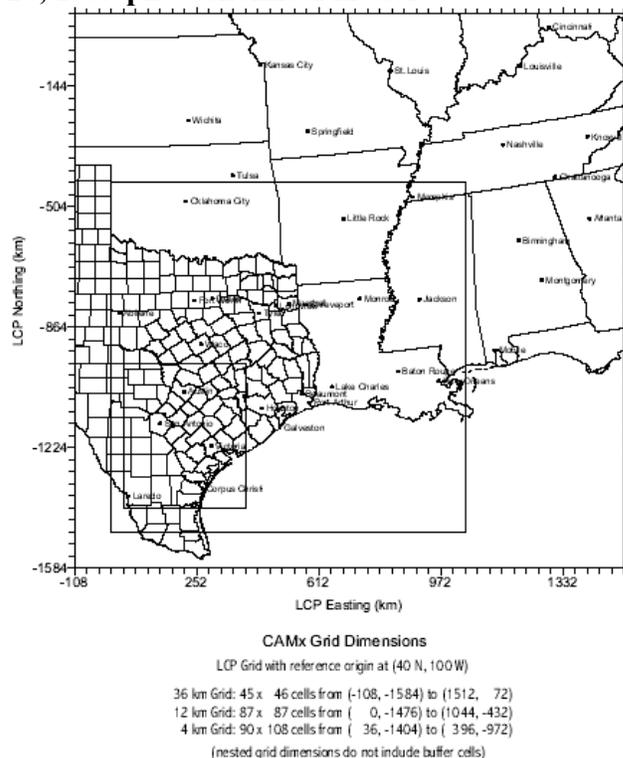
Detailed discussion of the modeling domain can be found in Emery *et al.* (2002). Portions of that discussion are replicated below for the sake of clarity.

The nested regional/urban scale 36-km/12-km/4-km grid developed by ENVIRON is shown in Figure 4. The grid formulation was selected to achieve several objectives:

1. Grid spacings must be in multiples of three for the MM5 meteorological model.
2. The 4-km domain must incorporate Austin, San Antonio, Victoria, and Corpus Christi and surrounding rural areas with large sources of nitrogen oxides (NO_x).
3. The regional domain should be large enough to account for upwind sources that may contribute to elevated ozone levels in Central Texas.

The 32-hour back trajectories during this episode extended from southeastern Missouri. Thus, ENVIRON set the northern boundary for the 36-km domain to include the lower Ohio River Valley and the eastern boundary to include Atlanta and large NO_x sources in the Tennessee Valley. The 12-km domain incorporated all of eastern Texas, including the ozone non-attainment areas of Dallas/Fort Worth, Houston/Galveston, and Beaumont/Port Arthur. The grid formulation meets the requirements of the U.S. EPA (1999), which recommends horizontal grid cell sizes in regional domains to be less than or equal to 36 km, and in urban scale domains to be 4-5 km. The spatial extent of the domain is sufficient to evaluate the impacts of both local and regional emission controls.

Figure 4. Nested 36-km/12-km/4-km modeling domain used for the September 13-20, 1999 photochemical model.



5. Meteorological Modeling for the September 13-20, 1999 Episode

This section summarizes the development of the meteorological modeling using the Fifth Generation Pennsylvania State University/National Center for Atmospheric Research (PSU/NCAR) Mesoscale Model (MM5). The final MM5 application for the September 13-20, 1999 modeling episode was developed through a number of individual simulations and sensitivity studies performed during the 2001 through 2003 period. An overview of these studies is provided in this section. Full documentation can be found in Emery and Tai (2001), Emery *et al.* (2002), and Emery *et al.* (2003).

5.1 Original MM5 Modeling

The original meteorological modeling for the September 13-20, 1999 ozone episode was based on MM5 version 3.4 and was completed and documented by Emery and Tai (2001). Telescoping nested grids (108/36/12/4-km) were used to resolve the flow and thermodynamic fields over the south-central U.S and within southern Texas. The finest grid was defined with a 4-km grid point spacing that included all of the major urban centers within southern Texas and the Texas Gulf Coast. Given the time and resource limitations for the MM5 modeling component of this original study, only four different MM5 configurations were evaluated.

Certain performance problems were identified from statistical summaries, MM5 output fields, and subsequently from the air quality modeling results (Emery *et al.*, 2002). The best performing run was referred to as Run 4c, and provided generally acceptable performance when appropriate modifications to soil moisture parameters were applied to represent drought conditions throughout much of Texas. Notable issues that remained included:

- A consistent over prediction of wind speed at night, and under predictions during the daytime, on both the 4-km and 12-km grids. These results could have been caused by any number of problems, including an overly excited low-level jet stream, consistent over prediction of surface pressure over Texas, and inadequate treatments in the boundary layer parameterization.
- A common over prediction tendency in early-morning temperatures that was likely related to a lack of near-surface nocturnal stabilization at night or deficiencies in the radiation algorithm.
- Marginal performance for humidity and for the overall pressure pattern covering the south-central U.S, which affected wind speed/direction.

Subsequently, close examination of the vertical mixing predictions in East Texas modeling work (Emery *et al.*, 2003) showed inexplicable geographic variations in mixing that appeared to be a result of the Gayno-Seaman boundary layer scheme used in all four original MM5 simulations. Similar problems were discussed by several presenters at a July 2002 U.S. EPA workshop on meteorological modeling for air quality applications; it was also learned that a recently discovered deficiency in the Gayno-Seaman boundary layer scheme could be a leading contributor to the diurnal wind performance problems,

and ultimately the morning temperature issues. Based on information gained in attending this workshop, a new MM5 configuration was recommended that simply replaced the Gayno-Seaman approach with an alternative methodology.

A comparison of modeled and observed pressure and wind data also showed that MM5 consistently developed a high-pressure ridge system over Texas during the September episode. The simulated high was more intense and extended farther into Texas than was actually measured. This caused the simulated winds over south-central Texas to exhibit more northerly and easterly directions rather than developing the observed southerly trends later in the period. ENVIRON and UT hypothesized that this problem was a result of inaccuracies in the observational analyses used in the MM5 data-nudging scheme.

5.2 Additional MM5 Modeling

Given that several known deficiencies remained in the original MM5 simulations, and that certain CAMx performance problems were likely linked to these deficiencies, Austin, San Antonio, Victoria, Corpus Christi, and the TCEQ requested additional simulations and analyses with MM5 in an attempt to minimize errors associated with the meteorological characterization. UT and ENVIRON investigated causes of the MM5 performance issues in a cooperative effort documented by Emery *et al.* (2003).

5.2.1 Meteorological Sensitivity Tests

It was assumed that MM5 performance was subject to a combination of errors associated with model inputs and the choice of internal algorithms. Based upon new analyses and various sensitivity runs, ENVIRON and UT attempted to improve overall MM5 performance through the use of new databases and model configurations that followed from earlier recommendations and that had since been shown to work better in other applications throughout the country. The following modifications to the MM5 configuration were recommended:

- Change to an alternative boundary layer scheme (Blackadar or Medium Range Forecast (MRF)) to investigate sensitivity to boundary layer mixing;
- Change to an alternative radiation scheme (Rapid Radiative Transfer Model (RRTM)) that is known to perform better in the humid Texas climate and may reduce the morning over-predicted surface temperatures;
- Utilize interactive multi-layer soil moisture schemes now available with the latest release of MM5 (v3.5) that would provide a more realistic feedback between soil and atmosphere; and
- Test the effects of alternative observational analyses and four-dimensional data assimilation (FDDA) techniques that may better characterize conditions in the south-central U.S.

A series of relatively simple meteorological sensitivity tests were performed in an effort to improve the model performance. The tests are listed in Table 4 in order of incremental change:

Table 4. Summary of Meteorological Sensitivity Tests

Run ID	Configuration-
Run 5c	Identical to Run 4c (the best performing of the original runs reported by Emery and Tai, 2002), except that the Blackadar planetary boundary layer (PBL) scheme was replaced by the Gayno-Seaman PBL scheme.
Run 5	Identical to Run 5c except that the Dudhia Cloud radiation scheme was replaced by the RRTM radiation scheme.
Run 5b	Identical to Run 5 except that data from the Texas Coastal Ocean Observation Network (TCOON) and National Oceanic and Atmospheric Administration (NOAA) National Buoy Center were added to the original observational FDDA input dataset.
Run 5d	Identical to Run 5b, except that the MRF PBL scheme replaced the Blackadar PBL scheme.
Run 5e	Identical to Run 5d, except that the standard 5-layer soil model was augmented by the bucket soil moisture option, and Run 5e used the standard climatological default soil moisture to define the initial soil conditions by land use category (up to this point, soil moisture was reduced 25% from standard values as in the original Run 4c).
Run 5f	Identical to Run 5e, except that the reduced soil moisture was used similarly to Runs 4c and 5-5d.
Run 5i	Identical to Run 5d except that the number of vertical layers was increased from 28 to 41, resulting in about twice the vertical resolution between approximately 250 and 4600 meters above the surface.
Run 5h	Identical to Run 5e (bucket soil moisture with standard default initial soil moisture values) except that the number of vertical layers was increased from 28 to 41.

Sensitivity runs using the Dudhia Cloud scheme were unable to replicate the amplitude of the diurnal temperature cycle. It appeared that the Dudhia scheme over estimated the amount of radiation absorbed and re-radiated by the atmosphere, primarily resulting in nighttime minimum temperatures that are too warm. Use of the RRTM radiation scheme in place of the Dudhia Cloud approach greatly improved the simulation of the

observed diurnal temperature range, although maximum temperatures remained too cool.

Runs with the Blackadar PBL scheme overestimated both daytime and nighttime wind speeds. This suggested that the Blackadar approach is overly aggressive in the vertical transfer of momentum, and higher winds near the top of the boundary layer may be mixed to the surface too rapidly. The associated under prediction of maximum temperatures could be related to the deeper mixing of surface heat. The MRF PBL scheme improved the prediction of both daytime and nighttime wind speeds, although nighttime wind speeds remained biased too high. Daytime maximum temperatures warmed by 1-2 K but remained below the observations on most days.

The introduction of the bucket soil moisture option produced a consistent increase in wind speed compared to the standard 5-layer soil model. The prediction of maximum temperatures improved slightly during the final days of the episode.

MM5 was configured to run with 41 layers instead of 28 in order to investigate the effects of increased vertical resolution. Based on recent discussions within the MM5 community, higher resolution (more than 30 layers) in the vertical direction is recommended and widely adopted. Interestingly, the 41 layer runs did not indicate any obvious improvement in performance at the surface or within the boundary layer in this case.

A qualitative review revealed that surface pressure patterns predicted by both the Blackadar and MRF runs were similar and compared well with observations. Cloud type and coverage across the 4-km domain were also similar throughout the episode, although the Blackadar runs produced slightly greater amounts of low-level cloudiness over South Texas and the adjacent Gulf on some days. In agreement with observations, rainfall was not predicted on the 4-km domain by either set of sensitivity runs after the 14th. The MRF PBL scheme systematically produced a deeper mixed layer than the Blackadar runs. On average, the afternoon MRF heights were greater by 25-35%.

Overall, Run 5d produced the best results of the eight sensitivity runs. Daytime wind speeds were slightly over-predicted during the first half of the episode and slightly under predicted thereafter. Nighttime wind speeds were over-predicted through the 18th. Predictions of wind direction exhibited a northerly bias, which was a consistent result across all sensitivity runs. Temperature performance was acceptable, although maximum temperatures were underestimated by 1-2 K. The surface humidity bias was negative on most days compared to Run 4c, likely because of the more rapid and deeper mixing associated with the MRF boundary layer approach relative to the Gayno-Seaman option. The humidity performance is not particularly good, and may be cause for concern. Errors in humidity may not significantly impact the performance of the photochemical model; however, substantial errors suggest that the PBL schemes may not be accurately simulating the spatial and temporal evolution of the boundary layer,

particularly along the coast. It should be mentioned that determining performance along the coast is challenging. Slight errors in wind speed and direction and inaccuracies in the details of the coastline can produce errors in the thermodynamic structure even if the PBL is well simulated overall.

5.2.2 Revised MM5 Applications

Based upon results of the MM5 sensitivity tests described above and new information regarding MM5 performance from a July 2002 U.S. EPA workshop, a new MM5 application was designed in an attempt to improve known deficiencies and to access additional modeling capabilities in the newly released MM5 version 3.5. The modified configuration included:

1. The same four-domain nested mesh with 108/36/12/4-km resolution, but with an expanded 36-km grid in order to move possible 108/36 boundary artifacts away from the area of interest and to better simulate the dominant regional-scale meteorology over the entire central U.S. that dictated flow and pressure patterns in Texas during the episode.
2. The coupled Pleim-Xiu Land Surface Model and boundary layer model, which required additional datasets such as soil type, vegetation categories, deep soil temperature, and vegetation fraction archived at the National Center for Atmospheric Research (NCAR).
3. Three-hourly observational “analysis” fields from the Eta Data Assimilation System, (EDAS) as opposed to EDAS “initialization” data used in previous modeling to establish initial/boundary conditions and inputs to the MM5 FDDA package.
4. Incorporation of routine surface and upper-air observation data obtained from NCAR archives into the EDAS fields processed for each MM5 modeling grid. This modification was made to ensure that the mesoscale and local meteorological features in the south-central U.S. were faithfully characterized in the EDAS analysis dataset. This preprocessing step was skipped in the original application because it was believed that the relatively high spatial and temporal resolution of the EDAS fields was sufficient to capture these details.
5. Use of the RRTM radiation scheme for all grids, based on the favorable results from the sensitivity tests.
6. Use of two-way interactive nesting for all grids. The 4-km grid was run as an independent one-way nest in the original application.
7. Modifications to the FDDA nudging technique to include two-dimensional surface analysis nudging, altered nudging strengths, and recommendations of Dr.

Nelson Seaman at the Pennsylvania State University. The TCOON and NOAA buoy data were also added to the observation FDDA nudging inputs.

Cloud options remained consistent with the original Run 4c and Run 5 series summarized above. Namely, resolved cloud microphysics were treated with the “simple ice” mechanism, and sub-grid scale clouds on the 108/36/12-km grids were modeled with the “Kain-Fritsch” approach.

It was realized that the relatively simple “five-layer” soil model used previously did not adequately handle complex surface-atmosphere interactions, and that more sophisticated Land Surface Models (LSMs) could provide important advantages for mesoscale modeling. Surface-atmosphere processes control the direction and magnitude of sensible and latent heat transfer, which in turn define surface temperature, humidity and boundary layer development. Because these parameters are especially critical for successful air pollution modeling, a more sophisticated LSM was adopted for the revised MM5 application. The Pleim-Xiu approach was selected based on outstanding results achieved and reported by air quality planning organizations in the midwestern United States and on modeling conducted by ENVIRON in other parts of the country.

Revised MM5 applications are referred to as the “Run 6” series. Four different MM5 runs were undertaken, as listed below:

Table 5. Summary of Revised MM5 Applications

Run ID	Configuration
Run 6c	As described above, including two-dimensional (2-D) surface nudging toward wind, temperature, and humidity analyses, and soil moisture nudging toward surface humidity, applied to all but the 4 km domain.
Run 6d	Identical to Run 6c, except soil moisture nudging was turned off.
Run 6e	Identical to Run 6c, except 2-D analysis and soil moisture nudging was applied to the 4 km domain.
Run 6f	Identical to Run 6e, except with additional surface observations from TCOON and NOAA National Buoy Center sites in the observation nudging database.

Diurnal trends of wind speed in Run 6c were much better simulated than in Run 4c, with stronger speeds in the afternoon and lighter speeds at night. Although daytime wind speeds tended to be over predicted during the first four days of the simulation, they corresponded well to the observations from September 17th through September 20th. However, the diurnal temperature range was suppressed, with cooler afternoon maxima and warmer morning minima. Diurnal trends of moisture were marginally better than in Run 4c.

The diurnal temperature range improved significantly when the soil moisture nudging was turned off, but remained worse than in Run 4c. Afternoon wind speeds were even stronger than in Run 6c, and moisture performance exhibited a larger gross error on all days. With the addition of 2-D analysis and soil moisture nudging on the 4-km domain (Run 6e), wind speed gross error was reduced on all days. Run 4c had a smaller gross error during the model initialization period, but Run 6e was superior with respect to wind speed and direction from September 17th through September 20th. The diurnal temperature range was much improved over the previous Runs 6c and 6d, and comparable to Run 4c, although temperatures were slightly under predicted. Humidity was generally higher compared to the other runs but agreed well with observed values.

5.3 Final MM5 Configuration for the September 13-20, 1999 Photochemical Model

Based upon the results summarized above, the UT /ENVIRON team suggested that the areas use the MM5 Run 5d set of meteorological fields for their photochemical model. However, the team also recommended that a final hybrid simulation be conducted that incorporated many of the important FDDA and input database changes adopted in MM5 Run 6f, but that maintained the simpler MRF PBL scheme and five-layer soil model of Run 5d. This additional simulation was performed by UT in May 2003 and is referred to as Run 5g. The model physics and options of Run 5g are summarized below:

- 28 sigma levels
- Expanded 36-km domain used in Run 6f
- Two-way interactive 108/36/12/4-km grids
- FDDA analysis nudging on the 108/36/12-km grids:
 - Three-dimensional (3-D) analysis nudging: MM5 was lightly nudged toward 3-hourly gridded EDAS analysis of winds (in the boundary layer and aloft) and temperature and humidity (only above the boundary layer), which were improved by the blending of routine surface and upper-air observational data
 - 2-D surface analysis nudging: MM5 was lightly nudged toward 3-hourly gridded surface analyses of winds, temperature, and humidity.
- Observation nudging on the 12/4-km grids: MM5 was strongly nudged toward discrete hourly wind observations from routine and special measurement networks operating in Texas during the episode.
- MRF PBL
- Simple ice cloud microphysics
- Kain-Fritsch cumulus parameterization except on 4-km grid
- Five-layer soil model
- RRTM radiation scheme
- Reduced soil moisture and thermal inertia to account for drier conditions

Run 5g exhibited improved simulation of surface temperature and pressure gradients over Texas compared to Run 5d. Temperature and humidity performance at surface observations stations for Run 5g also improved relative to Run 5d. Run 5g wind speed and direction predictions for Central Texas during the first half of the episode were

slightly degraded compared to Run 5d; however, along the coast, Run 5g showed enhanced onshore afternoon flow that was in better agreement with observations. Few differences were noted for other predicted fields. In particular, mixing depths simulated by Run 5d and Run 5g were virtually identical. Overall, the performance of the Run 5d and Run 5g models were quite similar. However, given that the EDAS analysis fields used for the large-scale grid nudging for Run 5g showed better agreement with observations compared to the EDAS initialization fields used for Run 5d, the Run 5g configuration was accepted as the final MM5 simulation by Austin, San Antonio, Victoria, Corpus Christi, and the TCEQ. The Run5g configuration is the basis for the meteorological fields for the September 13-20, 1999 photochemical model that is being used by Austin and San Antonio for their Early Action Compacts.

5.4 Statistical Evaluation of MM5 Run 5g Performance

A quantitative assessment of MM5 performance was undertaken to evaluate winds, temperature, and humidity at all available surface observation stations across the 4-km domain. This statistical assessment was performed on all MM5 simulations using the METSTAT program developed by ENVIRON (2001). The METSTAT program generates pairings of observations and predictions and calculates statistical measures for wind speed, wind direction, temperature, and humidity. The following statistical metrics were examined:

- Bias error – mean difference between pairings of predicted and observed data over a region.
- Gross error – mean absolute value of difference between pairings of predicted and observed data over a region.
- Root Mean Square Error (RMSE) – the square root of the mean of the squared difference between pairings of predicted and observed data over a region.
- Index of agreement (IOA) – at each monitoring site, calculate the sum of the absolute value of the difference between the prediction and the mean of the observations and the absolute value of the difference between the observation and the mean of the observations. These sums are added over all monitoring sites and divided into the square of the RMSE. This value is then subtracted from one.

Performance goals for the above parameters were established from a comparison of statistical summaries of the results of nearly thirty regional meteorological model simulations used to drive photochemical models throughout the country. Performance goals were chosen to establish a level of performance that most past modeling has achieved and to filter out those applications that exhibit particularly poor performance. It should be stressed that these goals are guided by the results of meteorological models that have been accepted and used in support of historical regulatory photochemical air quality modeling efforts. The performance goals will require refinement as the state of the science of meteorological modeling improves.

Mean daily statistics from Run 5g for the San Antonio/Austin, Corpus Christi/Victoria, and Houston/Galveston sub-domains are compared with statistical benchmarks in Table

6. The importance of the various meteorological input fields on CAMx air quality modeling can be ranked as follows (in descending order):

1. Surface and vertical profiles of wind speed/direction;
2. Boundary layer mixing depth and intensity;
3. Temperature (primarily the extent to which it influences boundary layer characterization, but secondarily, the extent to which it affects chemical reaction rates);
4. Humidity and clouds (assuming cloud cover was insignificant, which was the case during this episode).

Table 6 reveals that excellent performance for wind speed and direction and good performance for temperature and humidity was achieved by the Run 5g simulation on the 4-km domain. The reader is cautioned that these results are based on comparisons to observations obtained from ground-level monitoring stations. Upper air observations in the 4-km domain were limited to two locations. Vertical profiles of observed wind, temperature, and humidity were available from the Corpus Christi National Weather Service rawinsonde station. Vertical profiles of boundary layer winds were available from a special air quality study (Big Bend Regional Aerosol and Visibility Observational) profiler located in Llano, Texas. As summarized in Emery *et al.* (2003), Run 5g and Run5d achieved the best performance at these two monitoring stations.

Table 6. Comparison of mean daily statistics against statistical benchmarks for the 4-km subdomains. Values in red denote statistics outside the benchmarks.

Parameter	Benchmark	Episode Mean		
		Austin/ San Antonio	Corpus Christi/ Victoria	Houston/ Galveston/ Beaumont/ Port Arthur
Wind Speed RMSE	2.0	1.2	1.3	1.3
Wind Speed Bias	± 0.5	0.0	0.5	0.4
Wind Speed IOA	0.60	0.68	0.81	0.63
Wind Direction Gross Error	30	36	23	30
Wind Direction Bias	± 10	-6	-5	2
Temperature Gross Error	2.0	2.1	1.3	1.5
Temperature Bias	± 0.5	-1.3	0.4	-0.6
Temperature IOA	0.80	0.92	0.92	0.95
Humidity Gross Error	2.0	1.4	2.4	1.1
Humidity Bias	± 1.0	-0.3	-1.6	-0.3
Humidity IOA	0.60	0.47	0.53	0.61

5.5 Processing of MM5 Meteorological Fields for CAMx

Meteorological data from the Run 4c, Run 5d, Run 5g, and Run6f simulations were used to generate the required three-dimensional gridded meteorological fields shown in Table 7 for the September 13-20, 1999 CAMx model. The MM5 output fields were translated to CAMx-ready inputs using ENVIRON's MM5CAMx translation software. This program performs several functions:

- Extracts wind, temperature, pressure, humidity, cloud, and rain fields from each MM5 grid that matches the corresponding CAMx grid;
- Performs mass-weighted vertical aggregation of data for CAMx layers that span multiple MM5 layers;
- Diagnoses fields of vertical diffusion coefficient (K_v), which are not directly output by MM5 (K_v was diagnosed using the O'Brien 1970 method);
- Outputs the meteorological data into CAMx-ready input files.

Table 7. Meteorological data requirements for CAMx.

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	3-D gridded cloud cover for each hour
Rainfall Rate (in/hr)	2-D gridded rainfall rate for each hour

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

Most data prepared by MM5CAMx were directly input to CAMx. A single 40-meter deep CAMx surface layer was extracted from the aggregation of the lowest two 20-meter MM5 layers. The vertical layer structures for MM5 and CAMx are shown in Figure 5. The CAMx vertical layer structure is consistent with recommendations in the U.S. EPA's 8-hour modeling guidance (1999) which specifies that the surface layer should be no more than 50 meters deep, no layer beneath the mixing height should be greater than about 300 meters thick, 7-9 vertical layers with the planetary boundary layer and 1-2 layers above it (Emery *et al.*, 2002).

The horizontal extent of the MM5 4-km domain was defined to be much larger than the CAMx 4-km domain (the MM5 domain reached to the Texas-Louisiana border). The

differences in spatial extents of the domains could lead to inconsistencies in the flow and hydrodynamic fields just inside and along the eastern boundary of the CAMx 4-km grid and 12-km grids, if meteorological fields for the 12-km CAMx grid were derived only from the 12-km MM5 output. To ensure consistency for this portion of the CAMx grids, an alternative approach was designed. The 4-km meteorological output fields were extracted for the entire MM5 4-km grid coverage using MM5CAMx, averaged to 12-km resolution, then used to replace the meteorological fields on that portion of the CAMx 12-km grid.

Figure 5. Vertical layer structure for MM5 and CAMx for the September 13-20, 1999 episode modeling.

k	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	--12---
14	0.6500	667.50	3313.78	546.67	
13	0.7000	715.00	2767.11	517.77	--11---
12	0.7500	762.50	2249.35	491.99	
11	0.8000	810.00	1757.36	376.81	--10---
10	0.8400	848.00	1380.55	273.60	---9---
9	0.8700	876.50	1106.95	266.37	---8---
8	0.9000	905.00	840.58	259.54	---7---
7	0.9300	933.50	581.04	169.41	---6---
6	0.9500	952.50	411.63	166.65	---5---
5	0.9700	971.50	244.98	82.31	---4---
4	0.9800	981.00	162.67	65.38	---3---
3	0.9880	988.60	97.29	56.87	---2---
2	0.9950	995.25	40.43	20.23	---1---
1	0.9975	997.62	20.19	20.19	
0	1.0000	1000.00	0.00	=====Surface=====	

An alternative set of vertical diffusivity input fields were developed for CAMx. Vertical diffusivities (K_v) are an important input to the CAMx simulation because they determine the rate and depth of mixing in the PBL and above. Original diffusivity fields derived by MM5CAMx were passed through an additional algorithm that sets minimum K_v values between layers 1 and 2 to ensure that nocturnal stability near the surface is not overstated. The minimum value is dependent upon land use (e.g., urban, forest, agricultural, water, etc.) to represent different impacts of mechanical mixing and surface heat input (e.g., urban heat island effect).

6. Emission Inventory Development for the September 13-20, 1999 CAMx Model

Emission inventories for the Austin, San Antonio, and Victoria areas have undergone extensive refinement and scrutiny since the September 13-20, 1999 episode was selected for photochemical modeling. Documentation of this work has been included in a number of reports: Murphy *et al.* (2003), Jimenez *et al.* (2002), Pavlovic (2002), Emery *et al.* (2002), and AACOG (2001). Austin's 1999 emission inventory, which is the basis for the emission inputs to the September 13-20, 1999 photochemical model, is documented in a separate report (CAPCO, 2003) in accordance with EAC reporting requirements. The purpose of the discussion below is to summarize sources of emission inventory data used in the photochemical model, to note specific emission processing steps, and to present the spatial distribution of NO_x and volatile organic compound (VOC) emissions in the five-county Austin area.

Tables 8 and 9 present a summary of total daily anthropogenic NO_x and VOC emissions, respectively, for the five counties in the Austin Metropolitan Statistical Area. Anthropogenic emissions are greatest in Travis County, which includes the City of Austin. Onroad mobile sources contribute nearly 60% of the total anthropogenic NO_x emissions in the five-county area, followed by area and nonroad mobile sources, which contribute just over 20%. Anthropogenic VOC emissions in the five-county area are dominated by emissions from area and nonroad mobile sources, which account for almost 70% of the total anthropogenic inventory. Emissions from onroad mobile sources account for the majority of the remaining anthropogenic VOC inventory.

Spatial distributions of NO_x emissions from area and nonroad mobile sources, low-level point sources, elevated point sources, and on-road mobile sources at 0800 on September 17 (weekday) are shown in Figures 6, 7, 8, and 9, respectively. Similar maps for VOC emissions are shown in Figures 10, 11, 12, and 13, respectively. It is important that the reader note variations in scales on maps for different source categories. This was done intentionally because substantial differences in the magnitude of emissions existed between source categories. Map scales were adjusted for each source category in order to show the spatial distributions of emissions.

Emissions from area and non-road sources in Central Texas are concentrated within central Travis County, central and eastern Williamson County, and central Bexar County. Isolated point sources are located within the Austin and San Antonio areas, but emissions from stationary source categories are significantly denser in southeastern Texas and along the Gulf Coast. Emissions from on-road mobile sources in Central Texas are concentrated along the I-35 corridor within and between the Austin and San Antonio Metropolitan Statistical Areas.

Biogenic emissions are a strong function of land cover, ambient temperature, and solar radiation. Biogenic emissions for the 4-km Central Texas domain were estimated from version 2.2 of the Global Biosphere Emissions and Interaction System (GloBEIS) using land use/land cover data developed by the TCEQ, interpolated temperatures from National Weather Service observations, and solar radiation data from GOES satellite data analyzed by the University of Maryland (Jimenez *et al.*, 2002). Spatial distributions of

isoprene emissions in the 4-km domain on September 19, 1999, the day with the greatest total biogenic VOC emissions in the 4-km domain, and September 13, 1999, the day with the smallest total biogenic VOC emissions, are shown in Figure 14 and Figure 15, respectively. Biogenic emissions for the regional 12-km and 36-km grids were prepared in the same manner as the 4-km grid. However, land use/land cover data for states other than Texas were obtained from the U.S. EPA's BELD 3.1 database (Jimenez *et al.*, 2002).

Data sources and applicable processing notes/assumptions for Central Texas (4-km domain) anthropogenic emission inventories used in the September 13-20, 1999 photochemical modeling episode are summarized in Table 10.

Emission inventories for the Houston/Galveston and Beaumont/Port Arthur areas were supplied by the TCEQ. Emissions from electric generating units in the Houston/Galveston and Beaumont/Port Arthur areas were based on the TCEQ's Point Source Database for September 1999 supplemented with additional data from the U.S. EPA's 1999 Acid Rain Database. Emissions from other industrial point sources in the Houston/Galveston and Beaumont/Port Arthur areas were generated by the TCEQ for the August 22-September 1, 2000 CAMx modeling episode currently being used for the Houston/Galveston area Mid-Course Review (MCR). The TCEQ specified that Austin and San Antonio should use this inventory without any adjustment to 1999 because these estimates are expected to be relatively stable (Powell and Breitenbach, 2004).

Emission inventories for electric generating units in the remainder of Texas (i.e., outside of the Austin, San Antonio, Victoria, Corpus Christi, Houston/Galveston, and Beaumont/Port Arthur areas) were obtained from the TCEQ and supplemented with additional data from the U.S. EPA's Acid Rain Database. Emissions from other industrial point sources in the remainder of Texas were supplied by the TCEQ and were based on the TCEQ's Point Source Database for September 1999. Temporal and chemical speciation profiles for all Texas point sources were provided by TCEQ. With the exception of point sources in Louisiana, for which emissions data was obtained by the TCEQ directly from the Louisiana Department of Environmental Quality (LDEQ), all point source emission inventories for the regional domains (12-km and 36-km) outside of Texas were based on the 1999 National Emissions Inventory (NEI) Version 2 for Criteria Pollutants.

Emissions from area and non-road mobile sources in the Houston/Galveston area were generated by the TCEQ for the August 22-September 1, 2000 CAMx modeling episode for the MCR. Emissions from area sources were adjusted for 1999 using EGAS v. 4 factors, while emissions from nonroad mobile sources were adjusted using the ratio between the 1999/2000 emissions generated by the NONROAD2002a model. The August 22-September 1, 2000 TCEQ emission inventories for area and nonroad sources for Texas counties outside of the Austin, San Antonio, Victoria, Corpus Christi, and Houston/Galveston areas were used instead of the U.S. EPA's 1999 NEI Version 2 because they include emission estimates by the TCEQ for oil and gas production in Texas based on survey data. The TCEQ supplied temporal and chemical speciation profiles for

these emissions. All area and non-road mobile source emission inventories for the regional domains (12-km and 36-km) outside of Texas were based on the 1999 NEI Version 2 for Criteria Pollutants.

The TCEQ provided MOBILE6 based emission files for 2000 for the Houston/Galveston Area. Emissions for an average weekday (Aug. 30th), Friday (Aug. 25th), Saturday (Aug. 26th), and Sunday (Aug. 27th) were adjusted to obtain estimates for 1999 and incorporated into the emission inventory for the September 13-20th, 1999, modeling episode. Emissions from on-road mobile sources for Texas counties outside of the Austin, San Antonio, Victoria, Corpus Christi, and Houston/Galveston areas were based on MOBILE5 estimates. All on-road mobile source emission inventories for the regional domains (12-km and 36-km) outside of Texas were based on the 1999 NEI Version 2 for Criteria Pollutants.

Table 8. Daily NO_x emissions from anthropogenic sources in the five-county Austin area in 1999

	Date (mm/yy)	NO_x Emissions (tpd) in 1999
Area and Nonroad Mobile Source Emissions	09/13	37.02
	09/14	37.02
	09/15	37.02
	09/16	37.02
	09/17	37.02
	09/18	26.65
	09/19	25.97
	09/20	37.02
On-Road Mobile Source Emissions	09/13	94.50
	09/14	96.53
	09/15	98.80
	09/16	100.04
	09/17	90.51
	09/18	60.35
	09/19	46.22
	09/20	97.79
Point Source Emissions	09/13	30.46
	09/14	29.36
	09/15	30.04
	09/16	29.51
	09/17	28.90
	09/18	28.47
	09/19	29.34
	09/20	33.49
Total Anthropogenic Emissions	09/13	161.98
	09/14	162.91
	09/15	165.86
	09/16	166.57
	09/17	156.43
	09/18	115.47
	09/19	101.53
	09/20	168.30

Table 9. Daily VOC emissions from anthropogenic sources in the five-county Austin area in 1999.

	Date (mm/yy)	VOC Emissions (tpd) in 1999
Area and Nonroad Mobile Source Emissions	09/13	115.96
	09/14	115.96
	09/15	115.96
	09/16	115.96
	09/17	115.96
	09/18	101.92
	09/19	71.28
	09/20	115.96
On-Road Mobile Source Emissions	09/13	44.34
	09/14	45.57
	09/15	46.35
	09/16	46.58
	09/17	53.74
	09/18	39.10
	09/19	34.23
	09/20	50.09
Point Source Emissions	09/13	3.28
	09/14	3.19
	09/15	3.17
	09/16	3.20
	09/17	3.21
	09/18	3.21
	09/19	3.19
	09/20	3.24
Total Anthropogenic Emissions	09/13	163.58
	09/14	164.72
	09/15	165.48
	09/16	165.74
	09/17	172.91
	09/18	144.23
	09/19	108.70
	09/20	169.29

Figure 6. Area and nonroad mobile source NOx emissions within the 4-km domain at 0800 on September 17, 1999.

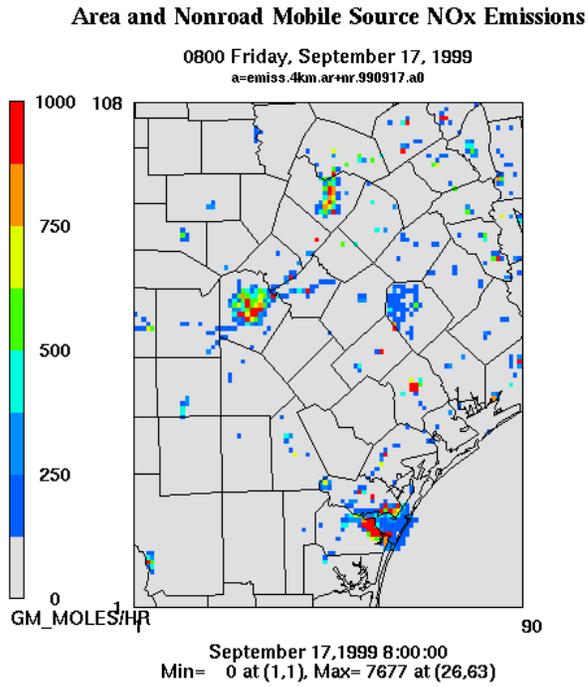


Figure 7. Low-level point source NOx emissions within the 4-km domain at 0800 on September 17, 1999.

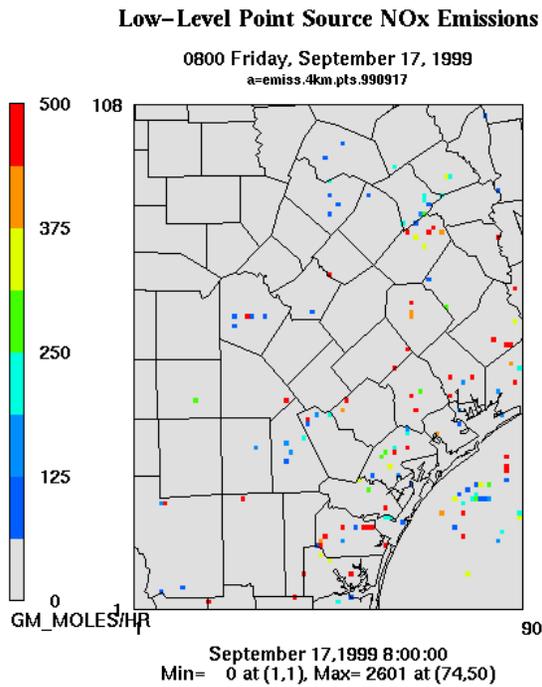


Figure 8. Elevated point source NOx emissions within the 4km domain at 0800 on September 17, 1999.

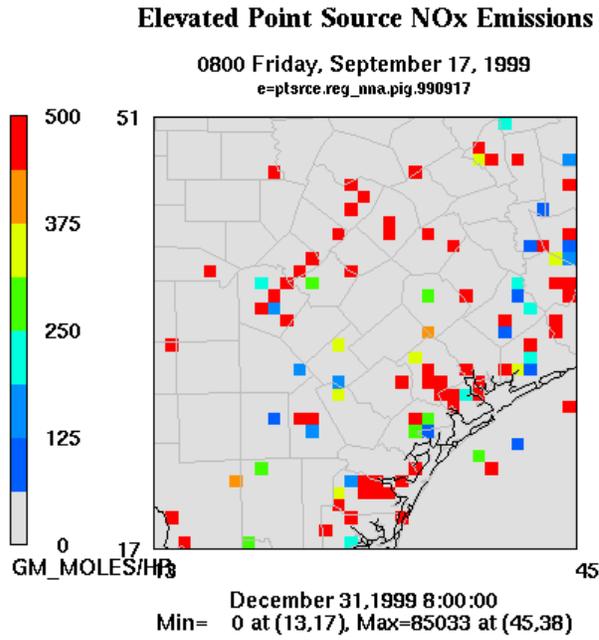


Figure 9. On-road mobile source NOx emissions within the 4-km domain at 0800 on September 17, 1999.

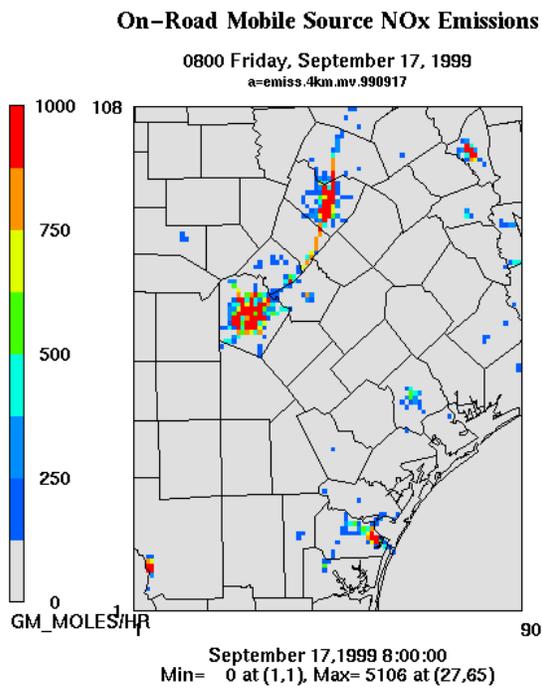


Figure 10. Area and nonroad mobile source VOC emissions within the 4-km domain at 0800 on September 17, 1999.

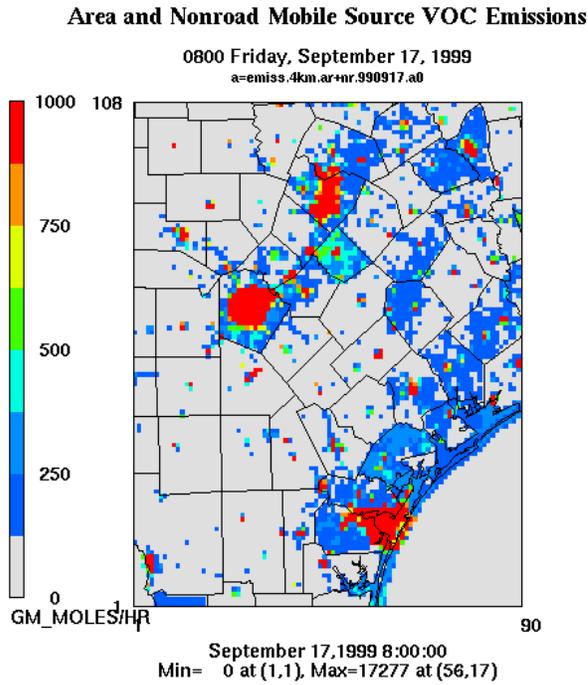


Figure 11. Low-level point source VOC emissions within the 4-km domain at 0800 on September 17, 1999.

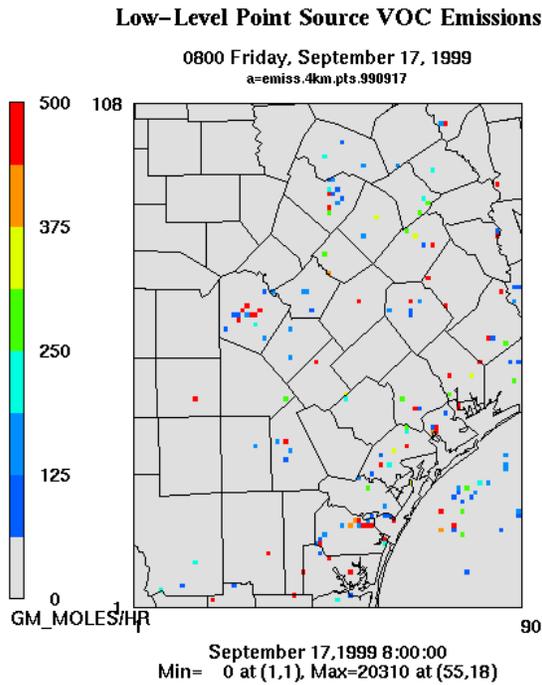


Figure 12. Elevated point source VOC emissions within the 4km domain at 0800 on September 17, 1999.

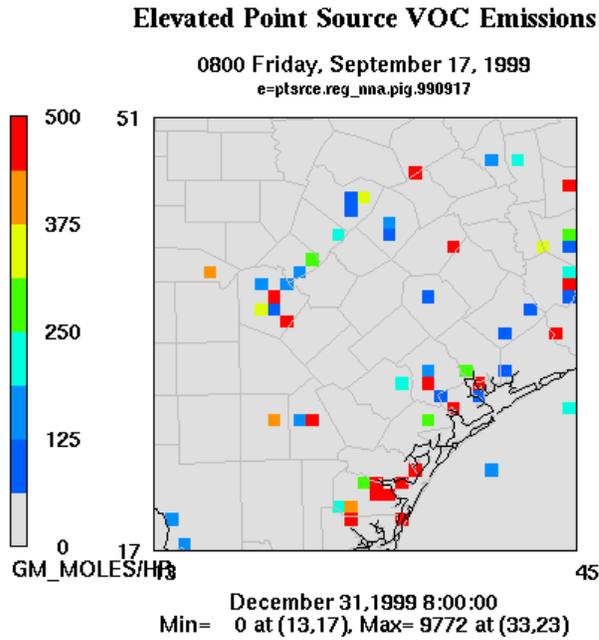


Figure 13. On-road mobile source VOC emissions within the 4-km domain at 0800 on September 17, 1999.

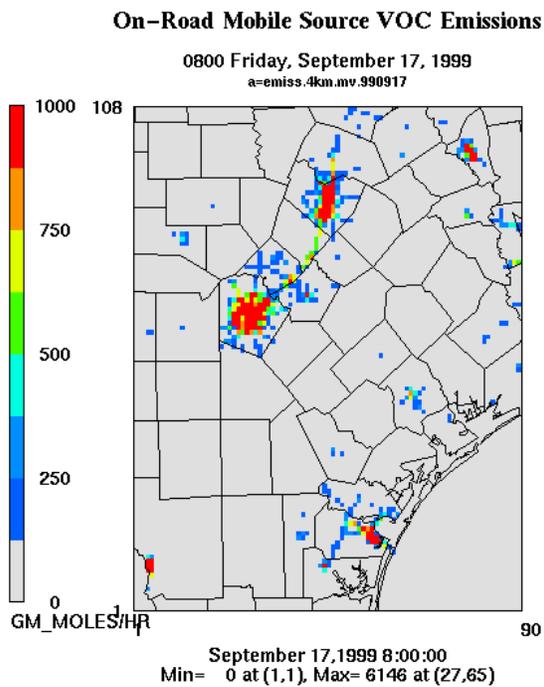


Figure 14. Isoprene emissions within the 4-km domain at 1400 on September 13, 1999.

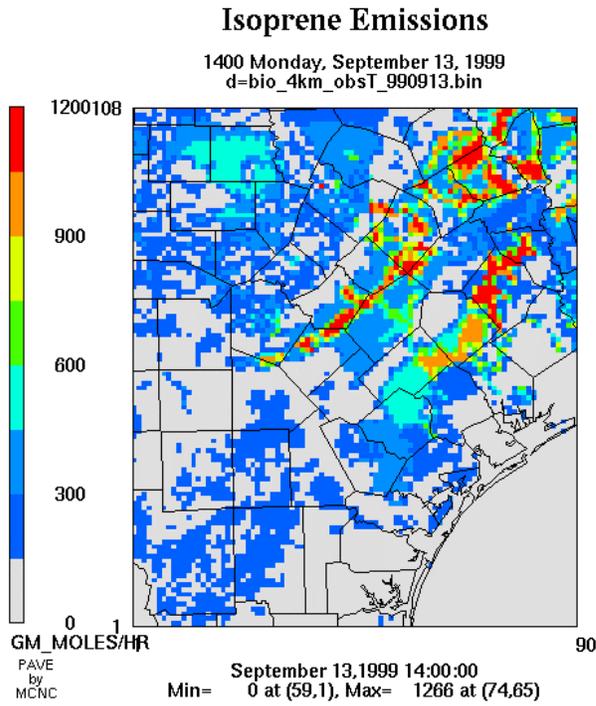


Figure 15. Isoprene emissions within the 4-km domain at 1400 on September 19, 1999.

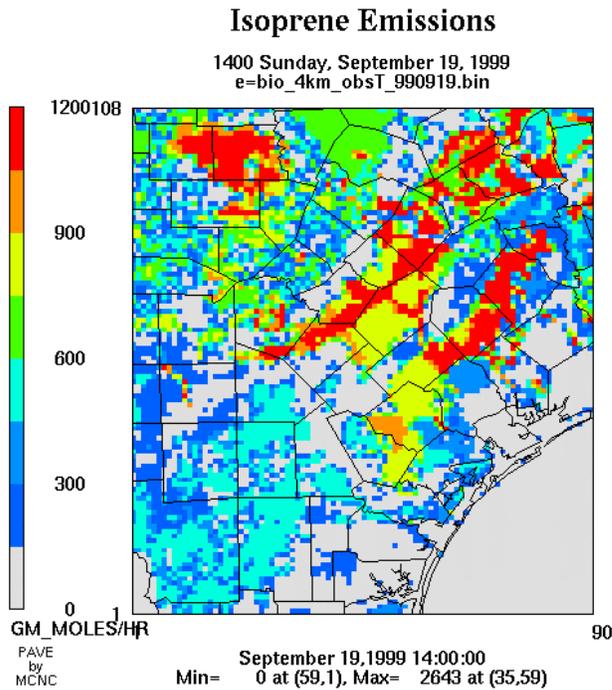


Table 10. Anthropogenic emission data sources for the 4-km domain.

Region/Source Category	Data Source	Assumptions/Processing Notes (if applicable)
Austin		
On-road Mobile	Emission factors obtained from the U.S. EPA's MOBILE6.2 model in combination with a travel demand model run by the Texas Transportation Institute (TTI). Link-based emissions developed for Hays, Travis, and Williamson Counties. Non-link based emissions developed for Bastrop and Caldwell Counties by applying factors to adjust from 1999 county-wide MOBILE5 totals to 1999 county-wide MOBILE6.2 totals provided by TTI.	For the link-based counties in the Austin and San Antonio areas, average weekday (Sep. 20 th), Friday (Sep. 17 th), Saturday (Sep. 18 th), and Sunday (Sep. 19 th) data were obtained from the TCEQ. Day-specific temperature and humidity adjustments were made to average weekday emissions (Sep. 20 th) to obtain day-specific emissions for the remaining weekdays in the episode (Sep. 13 th -16 th).
Area	Local survey data prepared by CAPCO.	Chemical speciation and chemical/temporal cross-references and profiles based on original ENVIRON data supplemented by local surveys or EPA defaults.
Non-road Mobile	NONROAD2002a with local survey data prepared by CAPCO.	Fuel parameters for NONROAD model based on data collected by the TCEQ (Brown, 2003). Chemical speciation and chemical/temporal cross-references and profiles based on original ENVIRON data supplemented by local surveys or EPA defaults.
Point	TCEQ Point Source Database with local data from Austin Energy.	Chemical speciation and chemical/temporal cross-references and profiles as used for the TexAQS2000 EI and provided by Ron Thomas of TCEQ.
San Antonio		
On-road Mobile	Emission factors obtained from the U.S. EPA's MOBILE6.2 model in combination with a travel demand model run by the Texas Transportation Institute (TTI). Link-based emissions developed for Bexar County. Non-link based emissions developed for Comal, Guadalupe, and	For the link-based counties in the Austin and San Antonio areas, average weekday (Sep. 20 th), Friday (Sep. 17 th), Saturday (Sep. 18 th), and Sunday (Sep. 19 th) data were obtained from the TCEQ. Day-specific temperature and humidity adjustments were made

	Wilson Counties by applying factors to adjust from 1999 county-wide MOBILE5 totals to 1999 county-wide MOBILE6.2 totals provided by TTI.	to average weekday emissions (Sep. 20 th) to obtain day-specific emissions for the remaining weekdays in the episode (Sep. 13 th -16 th).
Area	Local survey data prepared by AACOG.	Chemical speciation and chemical/temporal cross-references and profiles based on original ENVIRON data supplemented by local surveys or EPA defaults.
Non-road Mobile	NONROAD2002a with local survey data prepared by AACOG.	Chemical speciation and chemical/temporal cross-references and profiles based on original ENVIRON data supplemented by local surveys or EPA defaults.
Point	TCEQ Point Source Database with local survey data.	Chemical speciation and chemical/temporal cross-references and profiles as used for the TexAQS2000 EI and provided by Ron Thomas of TCEQ.
Victoria		
On-road Mobile	Link-based MOBILE6 emission files for Victoria County obtained from the TCEQ.	For Victoria County, average weekday (Sep. 13 th), Friday (Sep. 17 th), Saturday (Sep. 18 th), and Sunday (Sep. 19 th) data were obtained from the TCEQ. Day-specific temperature and humidity adjustments were made to average weekday emissions (Sep. 13 th) to obtain day-specific emissions for the remaining weekdays in the episode (Sep. 14 th -16 th , 20 th).
Area	Special fire inventory study conducted by UT. ENVIRON statewide trends inventory for other sources, except oil and gas, which was estimated from local survey data collected by Pollutions Solutions (1996).	Chemical speciation and chemical/temporal cross-references and profiles based on original ENVIRON data supplemented by local surveys or EPA defaults.
Non-road Mobile	NONROAD2002a. Locomotive data from ENVIRON statewide trends inventory. Local survey data for aircraft and airport ground support equipment. NEI v.1 data for air taxis.	Fuel parameters for NONROAD model based on data collected by the TCEQ (Brown, 2003). Day-specific meteorological data for NONROAD2002a model from

		National Weather Service Observations. Chemical speciation and chemical/temporal cross-references and profiles based on original ENVIRON data supplemented by local surveys or EPA defaults.
Point	TCEQ Point Source Database with day-specific data from British Petroleum, Dow, DuPont, Formosa Plastics, American Electric Power, and GulfSouth Pipeline Company.	Day-specific upset/maintenance emissions provided by Formosa, DuPont, and Dow. UT generated CB4 speciation for units at Dow and DuPont using Carter's emitdb. Chemical speciation and chemical/temporal cross-references and profiles as used for the TexAQS2000 EI and provided by Ron Thomas of TCEQ.
Corpus Christi		
On-road Mobile	Link-based MOBILE6 emission files for Nueces and San Patricio Counties obtained from the TCEQ.	
Area	Local data	Chemical speciation and chemical/temporal cross-references and profiles based on original ENVIRON data supplemented by local surveys or EPA defaults.
Non-road Mobile	Local data	Chemical speciation and chemical/temporal cross-references and profiles based on original ENVIRON data supplemented by local surveys or EPA defaults.
Point	Local data	Chemical speciation and chemical/temporal cross-references and profiles as used for the TexAQS2000 EI and provided by Ron Thomas of TCEQ.
Other Counties Not in Near Nonattainment Areas, but within 4-km Domain		
On-road Mobile	Emissions for non-link counties based on MOBILE5 estimates.	
Area	TexAQS2000 EI provided by Jim MacKay of TCEQ (data filename:	Chemical speciation and chemical/temporal cross-

	ams.TX_00.area_base2). Control factors to project emissions to 1999 (using EGAS Model, 2000) provided by Steven Smeltzer of AACOG.	references and profiles as used for the TexAQS2000 EI and provided by Jim MacKay of TCEQ. Additional EPA default cross-references and profiles added by UT-Austin for missing SCCs.
Nonroad Mobile	TexAQS2000 EI provided by Jim MacKay of TCEQ (data filename: ams.TX_00.NR_base2). Control factors to project emissions to 1999 (using Nonroad Model, 2000) provided by Steven Smeltzer of AACOG.	Chemical speciation and chemical/temporal cross-references and profiles as used for the TexAQS2000 EI and provided by Jim MacKay of TCEQ. Additional EPA default cross-references and profiles added by UT-Austin for missing SCCs.
Point	TCEQ Point Source Database	Chemical speciation and chemical/temporal cross-references and profiles as used for the TexAQS2000 EI and provided by Ron Thomas of TCEQ.

7. Land Use Data

Gridded land use data to characterize surface boundary conditions for the episode was developed by ENVIRON (Jimenez *et al.*, 2002). These data were generated from the same data used to generate spatial emission surrogates. ENVIRON developed software to process the raw spatial surrogate data into eleven landuse categories used by CAMx, to grid the data to the 36, 12, and 4-km CAMx grids, and to write the results in an appropriate format for input to CAMx.

8. Dry Deposition Algorithms

Dry deposition algorithms in CAMx are based on the regional-scale deposition model developed by Wesely et al. (1989). These algorithms have been widely used in both field applications and air quality models.

ENVIRON and UT reviewed the Palmer drought severity index, shown in Figure 16, for eastern Texas and found a moderate level of drought stress during the episode. Although the MM5 models accounted for reduced soil moisture, the original dry deposition algorithm in the September 13-20, 1999 CAMx model did not account for vegetation moisture stress. Because of the potential influence of drought stress on the uptake of pollutants through plant stomata and the importance of dry deposition as a physical removal process for ozone and other secondary pollutants, ENVIRON initiated changes to the CAMx deposition algorithms for the September 13-20, 1999 episode.

The current formulation of Wesely's dry deposition model in CAMx can be manipulated to account for drought stress through the use of vegetation moisture stress codes. Wesely supplies minimum bulk stomatal resistances by season and land use type. High resistances (9999) represent no deposition through the stomata. Vegetation moisture stress codes (istress of 0=unstressed; istress of 1=stressed, istress of 2=extremely stressed) essentially define factors by which minimum bulk stomatal resistances are increased/decreased to reflect drought conditions: if istress =1 then the stomatal resistance is increased by a factor of two; if istress = 2, then the stomatal resistance is increased by a factor of 10. ENVIRON increased drought stress codes over land use categories by one to reflect summer drought conditions for those land use categories that did not already have very high minimum bulk stomatal resistances. With the approval of the TCEQ and the U.S. EPA, Austin adopted these modifications for the September 13-20, 1999 photochemical model.

**Figure 16. Long-term Palmer drought severity index for September 18, 1999
(NOAA Climate Prediction Center, 2003).**

9. Chemistry Data

Chemistry data, developed by ENVIRON (Emery *et al.*, 2002), are summarized in Table 11.

Table 11. Summary of chemistry data for the September 13-20, 1999 CAMx model.

Input Data/Specification	Description
Chemistry Parameters	CB4 with current radical termination reactions and isoprene mechanism
Photolysis rates	TUV version 4
Albedo/Haze/Ozone File	<ul style="list-style-type: none">• Surface UV albedo from gridded land use data• Total ozone column data from satellite data from the Total Ozone Mapping Spectrometer (TOMS)• Haze optical depth field assumed spatially and temporally constant at 0.1.

10. Boundary and Initial Conditions

A number of sensitivity studies focusing on boundary and initial conditions were conducted following the initial CAMx model performance evaluation of the September 13-20, 1999 episode. The results of the model performance evaluation and CAMx simulations conducted by ENVIRON suggested that the September 1999 episode was promising, but required additional refinement to improve performance. Daily peak and daily mean 1-hour ozone concentrations were under predicted by 10-20% and 10-30%, respectively, at each ambient monitoring site. Although the unpaired peak accuracy and normalized gross error met U.S. EPA criteria for 1-hour averaged ozone concentrations on most days, the relative bias failed to meet U.S. EPA criteria in all near non-attainment areas on at least one episode day.

U.S. EPA default boundary and initial conditions, which were used in the original modeling, are shown in Table 12. The AACOG initiated sensitivity studies that focused on increasing ozone concentration from 40 ppb to 60 ppb along all boundaries of the 36-km domain and in the initial conditions supplied to CAMx. Model performance improved significantly and indeed, U.S. EPA performance criteria for unpaired peak accuracy, normalized bias, and gross error, were met on most days in Central Texas. The AACOG and UT, on behalf of CAPCO, then undertook a number of sensitivity studies to further elucidate the influence of boundary and initial conditions on model performance:

- Increase ozone concentrations along the northern and eastern boundaries from 40 ppb to 60 ppb.
- Increase ozone concentrations along the northern boundary from 40 ppb to 60 ppb.
- Increase ozone concentrations along the eastern boundary from 40 ppb to 60 ppb.
- Increase initial ozone concentrations from 40 ppb to 60 ppb.

In conjunction with the sensitivity studies, UT also examined whether the increase in ozone concentrations upwind and along the boundaries could be supported by ambient monitoring data during the episode. UT developed time series from relevant U.S. EPA AIRS monitors as well as from the IMPROVE network. In total, data from sixteen states (Oklahoma, Kansas, Nebraska, Missouri, Iowa, Indiana, Illinois, Arkansas, West Virginia, Ohio, Kentucky, Tennessee, North Carolina, Georgia, South Carolina, Alabama) were examined. Although the sensitivity studies led to variable degrees of improvement in model performance, the ambient data did not support increasing ozone concentrations above 40 ppb along most boundaries throughout the episode. The exception was the area of domain that encompassed Tennessee and North Carolina, which experienced ozone concentrations in excess of 60 ppb on most episode days.

The TCEQ suggested that UT examine the effects of boundary and initial conditions used for the September 1993 photochemical model for Houston's State Implementation Plan on model performance. These boundary and initial conditions are currently being used for the August 13-22, 1999 episode for the Dallas/Fort Worth area, for the Longview/Tyler/Marshall area, and for Oklahoma (Yarwood, 2003).

All of the model applications described above suffered from a tendency to underpredict regional ozone levels, which prompted a review of the boundary conditions. In particular, total VOC level of only 4.4 ppbC may be too low in areas of the regional modeling domain that are over land. Boundary condition values shown in Columns 1-3 of Table 12 were originally developed for the TCEQ's regional modeling of the September 1993 episode (Yocke *et al.*, 1996). These values varied by boundary segment, as shown in Figure 17, and were based on several data sources.

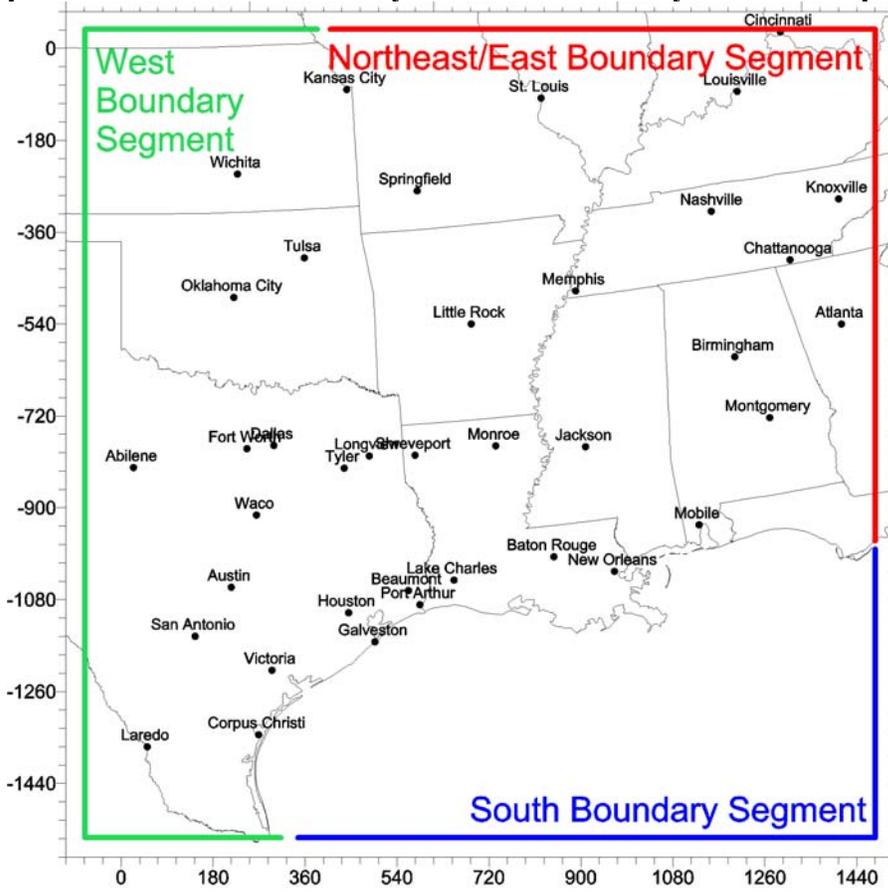
Concentrations along the East/Northeastern Boundary were based on U.S. EPA's guidance for UAM modeling (U.S. EPA, 1991) with carbon monoxide (CO) reduced from 350 ppb to 200 ppb and higher biogenic VOCs (isoprene, methanol, and ethanol) based on measurements at Kinterbish, Alabama for the Rural Oxidants in the Southern Environment Study (Goldan *et al.*, 1995). Western boundary concentrations were based on U.S. EPA's UAM modeling guidance (U.S. EPA, 1991) with CO reduced from 350 ppb to 200 ppb and were consistent with data from Niwot Ridge, CO (Watkins *et al.*, 1995). Southern boundary concentrations were based on the Gulf of Mexico Air Quality Study sponsored by the Minerals Management Service (MMS, 1995). Initial conditions were identical to those in Column 3.

UT conducted a sensitivity study using the September 1993 Houston/Galveston boundary and initial conditions and found improved model performance for the September 13-20, 1999 episode in Central Texas. The negative bias predicted by the original model was considerably reduced, and this metric, now fell within the range of U.S. EPA 1-hour averaged ozone concentration performance criteria. Model performance statistics will be described in detail below, but improved ozone predictions were observed throughout the regional domain, including in the Houston/Galveston area. Because of the significantly improved model performance and the robust technical basis of these data, Austin and San Antonio, in collaboration with the TCEQ, decided to use these boundary and initial conditions for the photochemical modeling for their Early Action Compacts.

Table 12. Boundary and initial conditions used by ENVIRON in the original model and by Austin in the final model for the Early Action Compact. Initial conditions were identical to concentrations along the western boundary. The EAC boundary and initial conditions are identical to those used in the September 1993 Houston/Galveston model for the State Implementation Plan.

Species	NE Boundary below 1700m (ppb) (EAC)	West Boundary below 1700 m (ppb) (EAC)	SE Boundary and Above 1700m (ppb) (EAC)	Default Initial and Boundary Conditions used in original modeling.
O3	40	40	40	40
CO	200	200	100	100
NO	0.1	0.1	0.1	0.000049
NO ₂	1	1	1	0.08555
HNO ₃	3	3	1	1.525
HNO ₂	0.001	0.001	0.001	0.000728
ALD2	0.555	0.555	0.05	0.1051
ETH	0.51	0.51	0.15	0.005315
HCHO	2.1	2.1	0.05	1.068
OLE	0.3	0.3	0.05	
PAR	14.9	14.9	7.6	3.078
TOL	0.18	0.18	0.0786	0.006043
XYL	0.0975	0.0975	0.0688	
ISOP	3.6	0.1	0.001	
PAN	0.1	0.1	0.1	0.03834
H ₂ O ₂	3	3	1	2.263
MEOH	8.5	0.001	0.001	
ETOH	1.1	0.001	0.001	

Figure 17. Map showing the delineation of boundary segments for the photochemical model used by Austin for the Early Action Compact.



11. CAMx Model Options

CAMx model options, established by ENVIRON (Emery *et al.*, 2002), are summarized in Table 13.

Table 13. Summary of options for the September 13-20, 1999 CAMx model.

Input Data/Specification	Description
Advection Scheme	Piece Parabolic Method (PPM)
Plume-in-Grid Model	Selected for major NO _x sources (≥ 10 tons/day) in 4 km grid
Chemical Mechanism	CMC fast solver

12. September 13-20, 1999 CAMx Model Performance

Model performance was evaluated using statistical and graphical metrics in accordance with U.S. EPA guidance (1999) for both 1-hour and 8-hour attainment demonstrations. Performance for both 1-hour and 8-hour predicted ozone concentrations was evaluated based on the seven monitors in the San Antonio, Austin, San Marcos, and Fayette County networks in Central Texas.

12.1 Model Performance: 1-Hour Averaged Ozone Concentrations

Statistical metrics and associated U.S. EPA performance criteria, if defined, for 1-hour averaged ozone concentrations include:

- Unpaired peak accuracy (U.S. EPA performance criteria: $\pm 20\%$)
- Average paired peak accuracy (U.S. EPA performance criteria not defined)
- Bias in peak timing (U.S. EPA performance criteria not defined)
- Normalized bias (U.S. EPA performance criteria: $\pm 15\%$)
- Normalized error (U.S. EPA performance criteria: $\pm 35\%$)

Time series plots of observed versus predicted 1-hour averaged ozone concentrations were also evaluated for the Central Texas monitors, other monitors within the 4-km domain, and monitors within the Houston/Galveston area.

Statistical metrics for 1-hour averaged ozone concentrations in Central Texas are summarized in Figure 18. Statistical metrics for 1-hour averaged ozone concentrations in Corpus Christi, Victoria, and Houston/Galveston are presented in Appendix C.

With the exception of the normalized bias on the model initialization day of September 13, model performance in Central Texas met U.S. EPA performance criteria on every day of the episode. A persistent negative bias was observed during the episode throughout the 4-km domain and in the Houston/Galveston area. Although the improvements to the emission inventories, meteorological inputs, boundary and initial conditions, and dry deposition algorithms described above led to significant reductions in the negative bias relative to the original formulation of the model, the consistently low regional background ozone levels are continuing to be investigated through the use of process analysis.

One-hour time series at the seven Central Texas monitors are presented in Figures 19-25. Figures 26 and 27 present the 8-hour times series at the Murchison and Audubon monitoring stations, respectively. Although the model under predicts peak ozone concentrations in Austin, notably on September 20th, the model shows excellent replication of diurnal trends. Peak predicted ozone concentrations also tend to be under predicted in San Antonio, Fayette County, and San Marcos relative to peak observed concentrations. Diurnal trends are generally well replicated, although on some episode days, the model does not capture ozone titration at night in these areas.

12.2 Model Performance: 8-Hour Averaged Ozone Concentrations

The U.S. EPA has issued draft guidance on model performance metrics for 8-hour attainment demonstrations, but the metrics have not been widely applied to date. The U.S. EPA recommends the following metrics be used to assess the model's ability to predict mean 8-hour daily peak ozone concentrations:

- Bias between spatially paired means of observations and predictions of 8-hour daily maximum ozone concentrations, with predicted values based on grid cells 'near' a monitor.
- Correlation coefficient and scatter plot for average observed and predicted 8-hour daily maximum ozone concentrations.
- Temporal correlation coefficient of observed and nearby predicted 8-hour daily maximum ozone concentrations, which are spatially averaged. If the monitoring network is sufficiently large, concentrations should be grouped into upwind, downwind, and center city locations.
- Quantile-quantile plots
- Fractional bias

ENVIRON has developed a FORTRAN program and Microsoft Excel Macro to calculate normalized bias, normalized error, fractional bias, fractional error, and correlation coefficients and to prepare scatter plots of observed versus predicted 8-hour ozone concentrations and quantile-quantile plots. Recognizing that the evaluation of model performance for 8-hour averaged ozone attainment demonstrations is currently being applied for the first time in many areas throughout the United States and, consequently, could be subject to modifications in the future, ENVIRON used three different methodologies to select predicted ozone concentrations to compare to observed values:

1. The predicted daily maximum ozone concentration within grid cells 'near' a monitor, as defined by U.S. EPA guidance (1999);
2. The predicted daily maximum ozone concentration within grid cells 'near' a monitor that is closest in magnitude to the observed daily maximum at the monitor;
3. A bilinear interpolation of predicted daily maximum ozone concentration around the monitor location.

UT evaluated the software and applied it to assess the model's ability to replicate maximum observed 8-hour ozone concentrations in Central Texas. Because the monitoring network in Central Texas is not dense, Austin and San Antonio, in conjunction with the TCEQ and the U.S. EPA Region 6, decided not to group monitors, but rather to evaluate performance based on data from all stations. In accordance with U.S. EPA guidance, grid cells 'near' a monitor were defined as a 7x7 array of cells (U.S. EPA, 1999).

Statistical metrics for each methodology are presented in Tables 14, 15, and 16, respectively. Graphical metrics for each methodology are presented in Figures 28, 29, and 30, respectively. The U.S. EPA (1999) has recommended that the normalized bias and fractional bias be less than 20% of mean observed 8-hour daily maximum

concentrations. Regardless of the approach used to select the predicted maximum concentration, both metrics for Austin and San Antonio's September 13-20, 1999 CAMx model fall well within these criteria.

Figure 18. Statistical metrics of CAMx model performance for 1-hour averaged ozone concentrations in Central Texas.

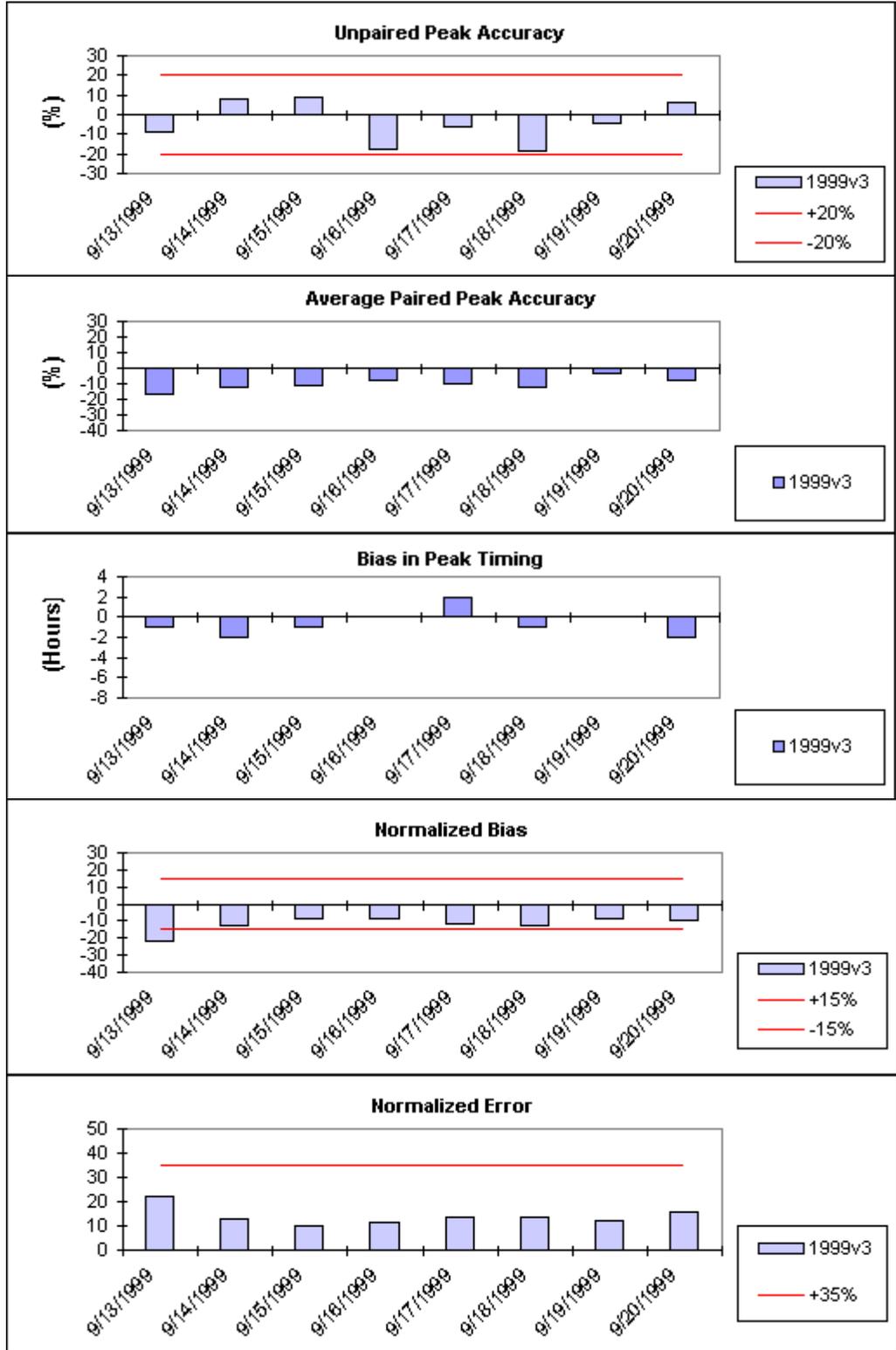


Figure 19. Time series of predicted versus observed 1-hour ozone concentrations during September 13-20, 1999 at Austin's Murchison monitor (CAM3:AIRS ID 484530014).

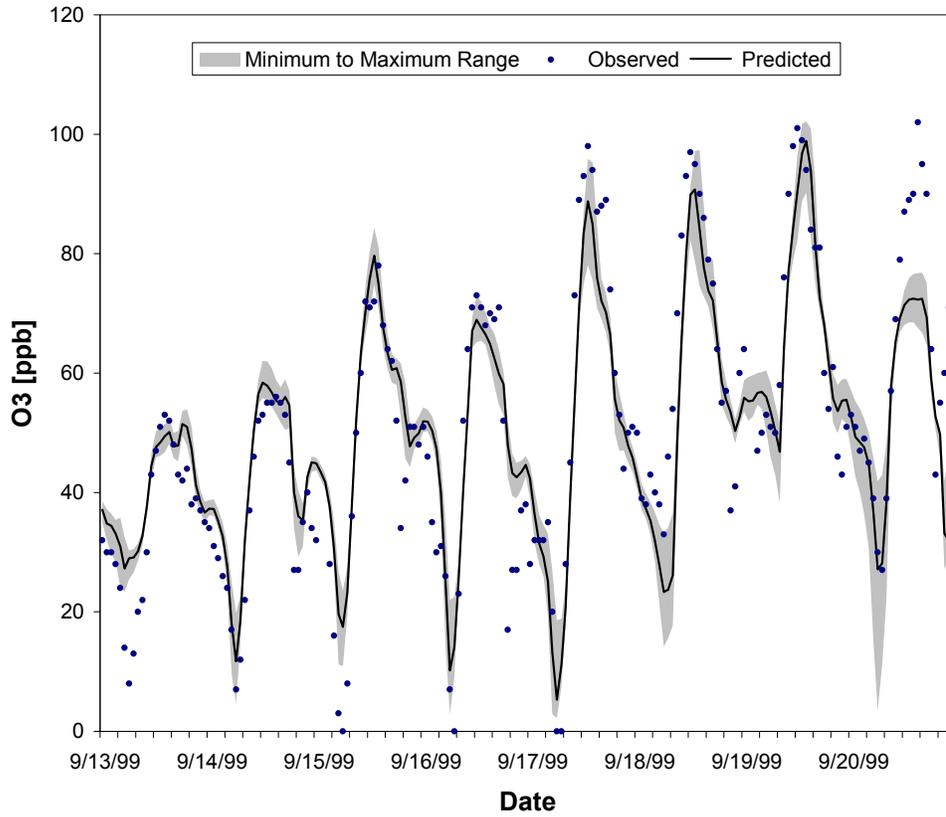


Figure 20. Time series of predicted versus observed 1-hour ozone concentrations during September 13-20, 1999 at Austin's Audubon monitor (CAMS 38:AIRS ID 484530020).

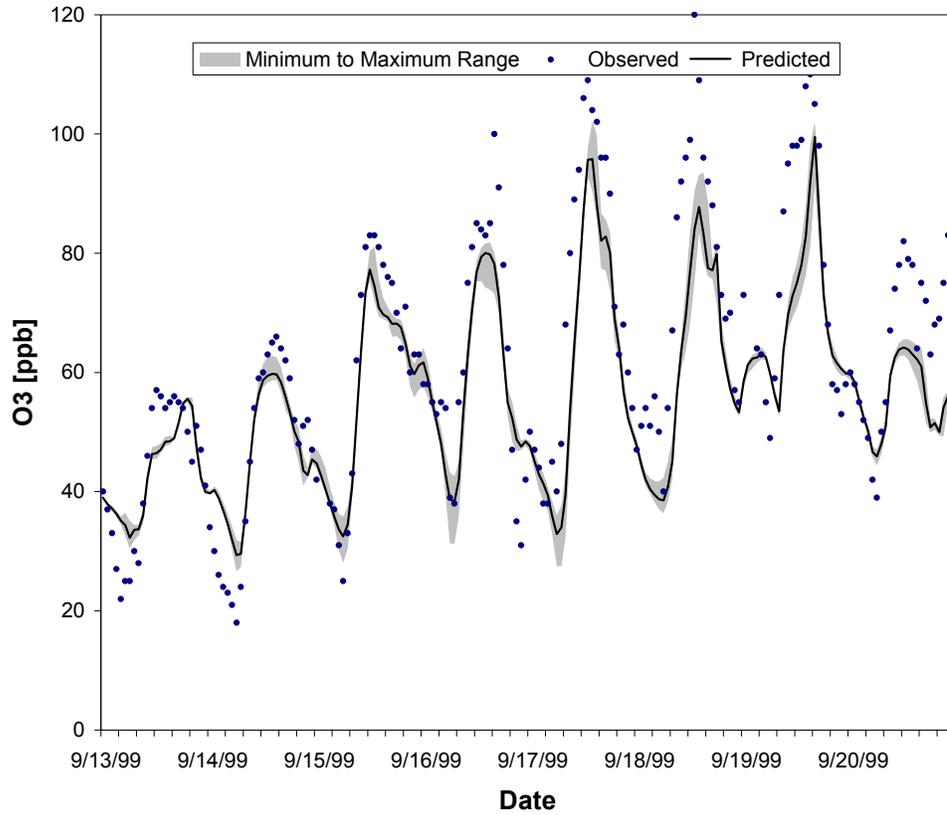


Figure 21. Time series of predicted versus observed 1-hour ozone concentrations during September 13-20, 1999 in San Antonio (AIRS ID 480290023).

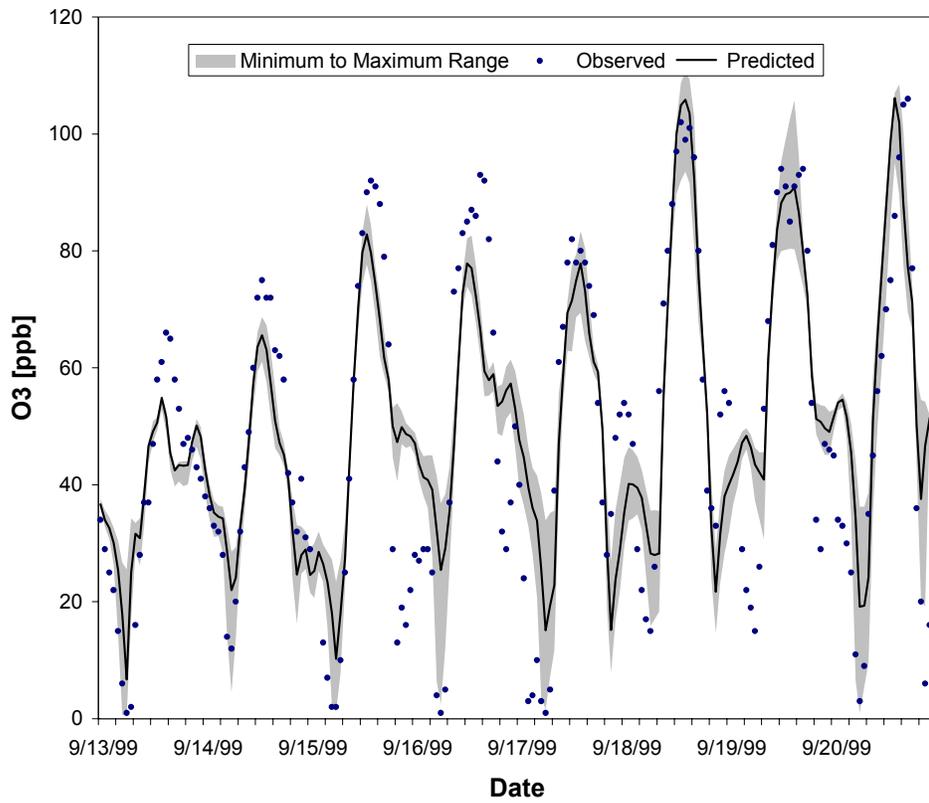


Figure 22. Time series of predicted versus observed 1-hour ozone concentrations during September 13-20, 1999 in San Antonio (AIRS ID 480290052).

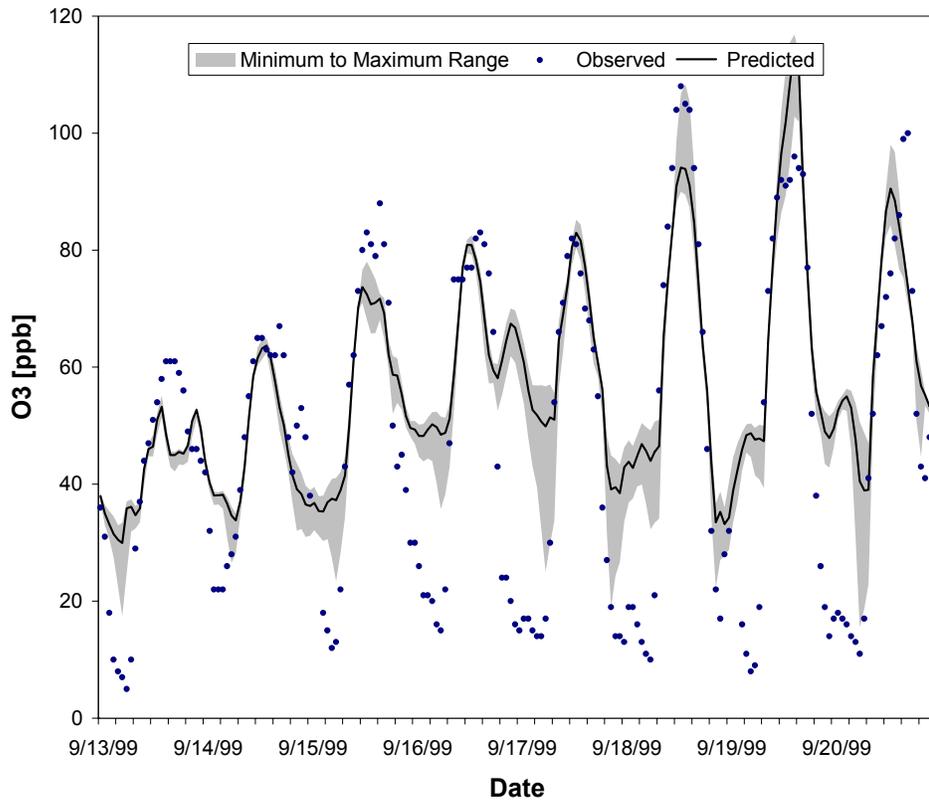


Figure 23. Time series of predicted versus observed 1-hour ozone concentrations during September 13-20, 1999 in San Antonio (AIRS ID 480290059).

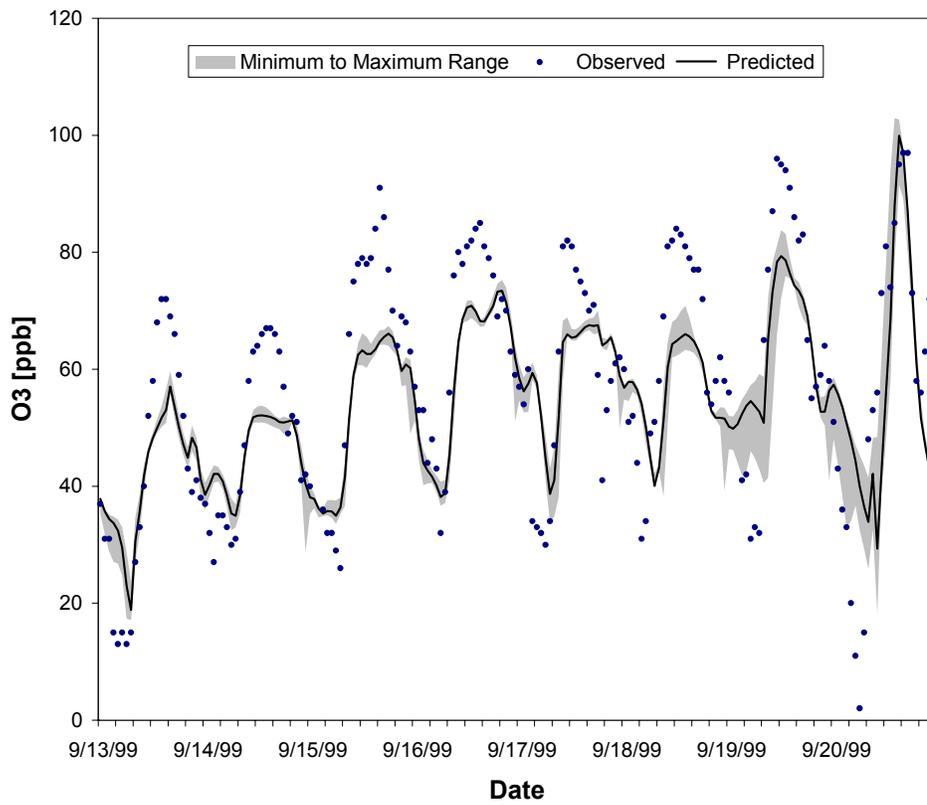


Figure 24. Time series of predicted versus observed 1-hour ozone concentrations during September 13-20, 1999 in Fayette (AIRS ID 481490001).

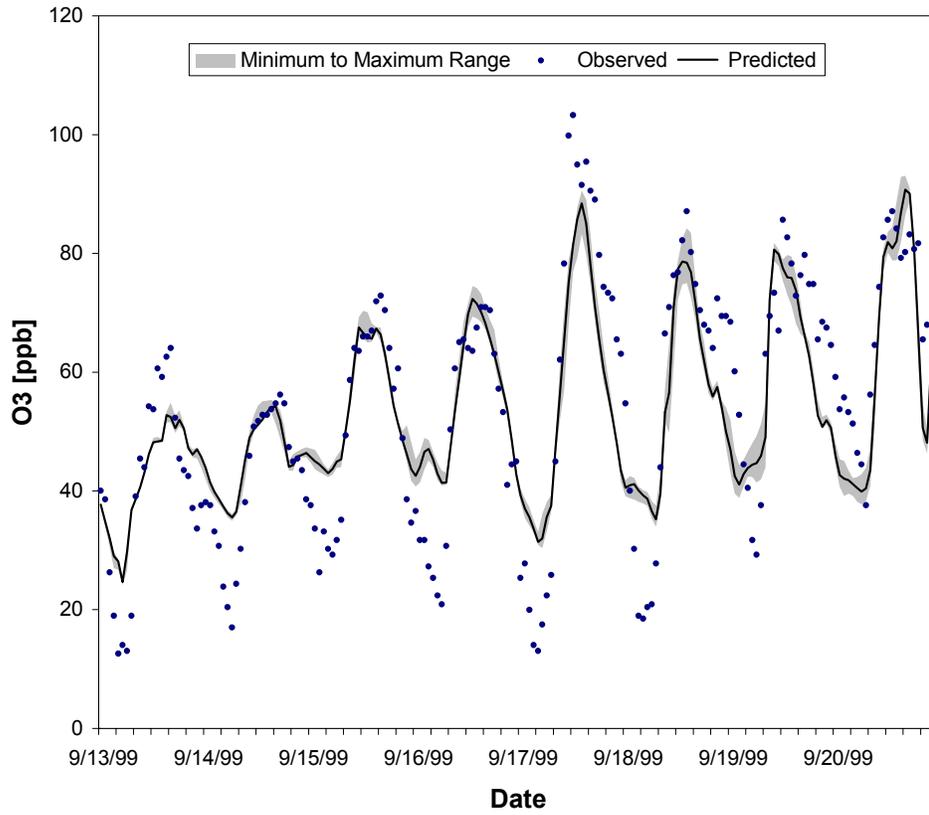


Figure 25. Time series of predicted versus observed 1-hour ozone concentrations during September 13-20, 1999 in San Marcos (AIRS ID 480550062).

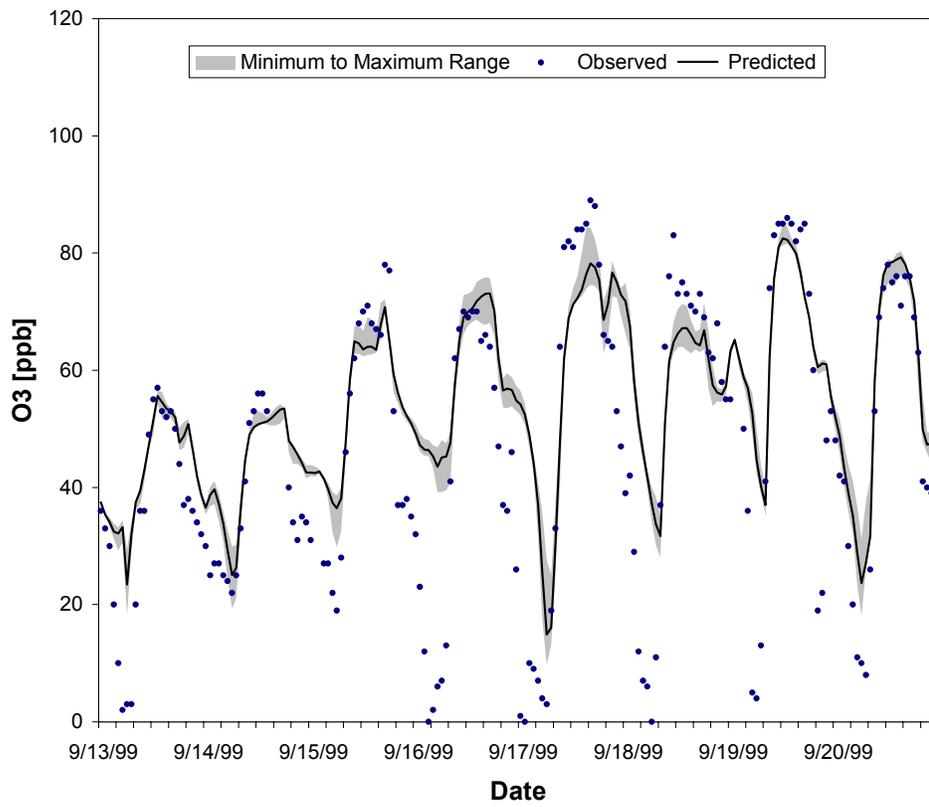


Figure 26. Time series of predicted versus observed 8-hour ozone concentrations during September 13-20, 1999 at Austin's Murchison monitor (CAM3:AIRS ID 484530014).

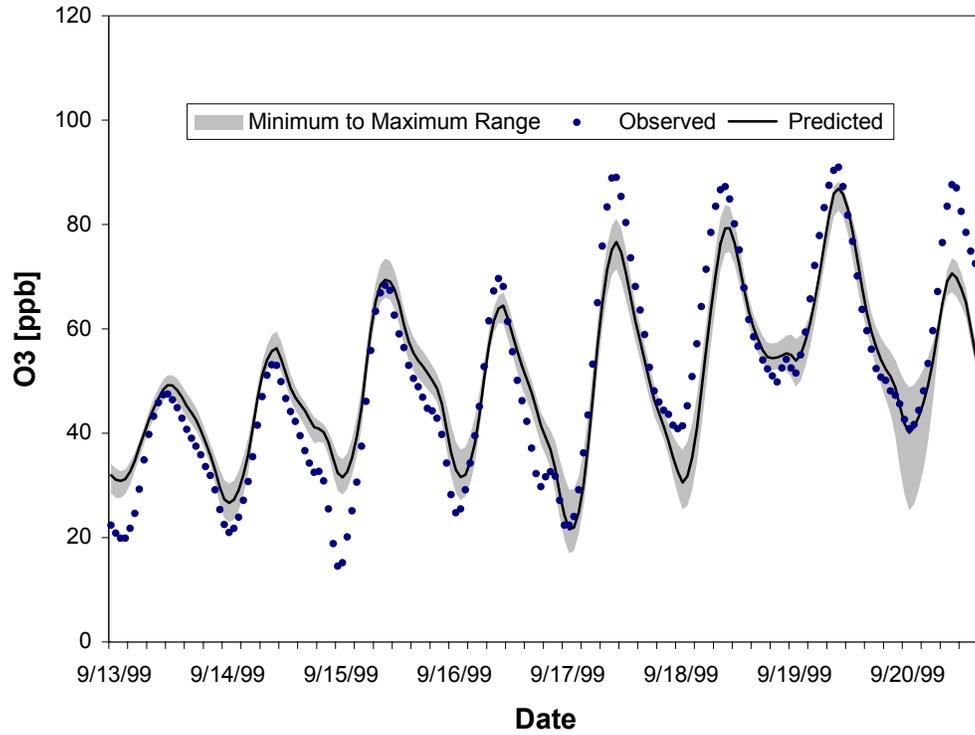


Figure 27. Time series of predicted versus observed 8-hour ozone concentrations during September 13-20, 1999 at Austin's Audubon monitor (CAMS 38:AIRS ID 484530020).

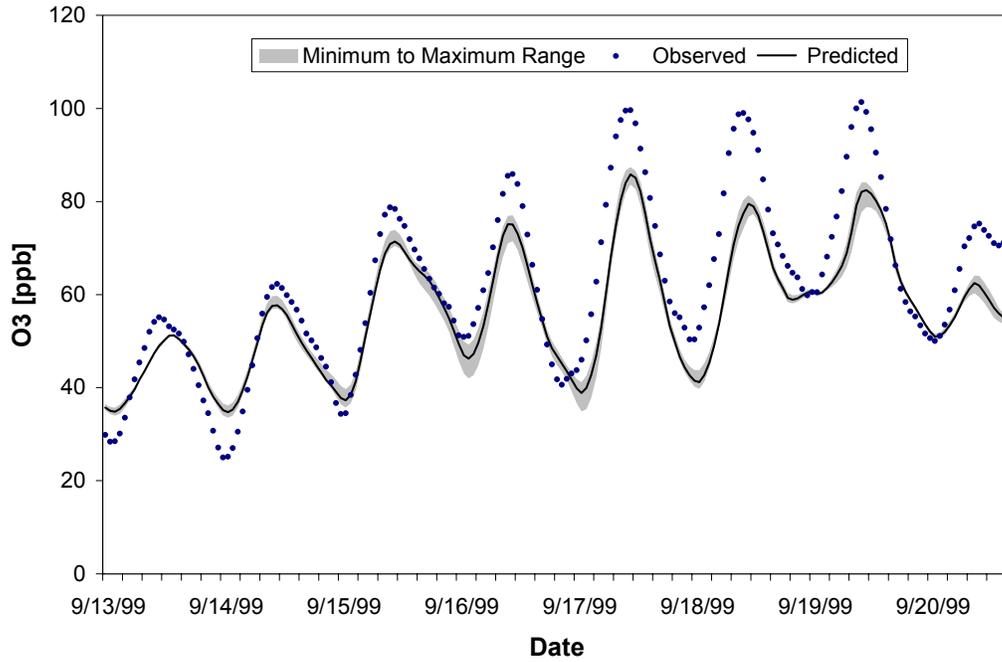


Table 14. Statistical metrics for 8-hour averaged ozone concentrations used to assess performance of the September 13-20, 1999 photochemical model in Central Texas. The metrics are based on the predicted daily maximum ozone concentration within a 7x7 array of grid cells ‘near’ each Central Texas monitor.

Date	Maximum Observed 8-Hour Ozone Concentration (ppb)	Maximum Predicted 8-Hour Ozone Concentration in Grid Cells Near Monitor (ppb)	Normalized Bias	Fractional Bias	Normalized Error	Fractional Error
9/13/99	55.70	52.53	-5.00	-5.54	9.68	10.03
9/14/99	60.54	60.28	0.36	-0.30	8.28	8.13
9/15/99	75.59	74.66	-0.68	-1.10	7.05	7.16
9/16/99	76.50	75.63	-0.32	-0.70	8.02	8.05
9/17/99	84.58	82.37	-1.93	-2.31	7.64	7.77
9/18/99	86.86	84.18	-3.03	-3.33	6.14	6.36
9/19/99	89.31	89.73	0.71	0.34	7.39	7.34
9/20/99	81.58	86.11	5.37	5.07	7.32	7.09

Table 15. Statistical metrics for 8-hour averaged ozone concentrations used to assess performance of the September 13-20, 1999 photochemical model in Central Texas. The metrics are based on the predicted daily maximum ozone concentration within a 7x7 array of grid cells ‘near’ each Central Texas monitor that is closest in magnitude to the observed daily maximum.

Date	Maximum Observed 8-Hour Ozone Concentration (ppb)	Maximum Predicted 8-Hour Ozone Concentration in Grid Cells Near Monitor that is Closest in Magnitude to the Observed Daily Maximum Ozone Concentration (ppb)	Normalized Bias	Fractional Bias	Normalized Error	Fractional Error
9/13/99	55.70	51.45	-7.18	-7.63	7.51	7.96
9/14/99	60.54	57.98	-3.97	-4.23	3.97	4.23
9/15/99	75.59	72.45	-3.89	-4.16	3.94	4.20
9/16/99	76.50	73.02	-4.15	-4.36	4.20	4.40
9/17/99	84.58	80.22	-4.78	-5.03	4.93	5.18
9/18/99	86.86	82.85	-4.52	-4.78	4.65	4.91
9/19/99	89.31	86.27	-3.20	-3.36	3.50	3.66
9/20/99	81.58	80.85	-0.97	-1.01	1.16	1.19

Table 16. Statistical metrics for 8-hour averaged ozone concentrations used to assess performance of the September 13-20, 1999 photochemical model in Central Texas. The metrics are based on a bilinear interpolation of predicted daily maximum ozone concentration around each Central Texas monitor.

Date	Maximum Observed 8-Hour Ozone Concentration (ppb)	Bilinear Interpolation of Maximum Predicted 8-Hour Ozone Concentration in Grid Cells Near Monitor (ppb)	Normalized Bias	Fractional Bias	Normalized Error	Fractional Error
9/13/99	55.70	49.97	-9.59	-10.49	10.85	11.73
9/14/99	60.54	55.51	-7.69	-8.39	9.68	10.32
9/15/99	75.59	68.27	-9.22	-9.94	9.65	10.36
9/16/99	76.50	70.20	-7.51	-8.19	9.44	10.07
9/17/99	84.58	75.31	-10.58	-11.33	11.00	11.75
9/18/99	86.86	77.16	-11.11	-12.02	11.11	12.02
9/19/99	89.31	83.39	-6.39	-6.96	8.79	9.26
9/20/99	81.58	77.53	-4.89	-5.47	7.58	8.11

Figure 28. Scatter plot of observed and predicted daily maximum 8-hour ozone concentrations at Central Texas monitors. Predicted values are based on daily maximum ozone concentrations within a 7x7 array of grid cells ‘near’ each Central Texas monitor. Quantiles are shown as well as the correlation coefficient.

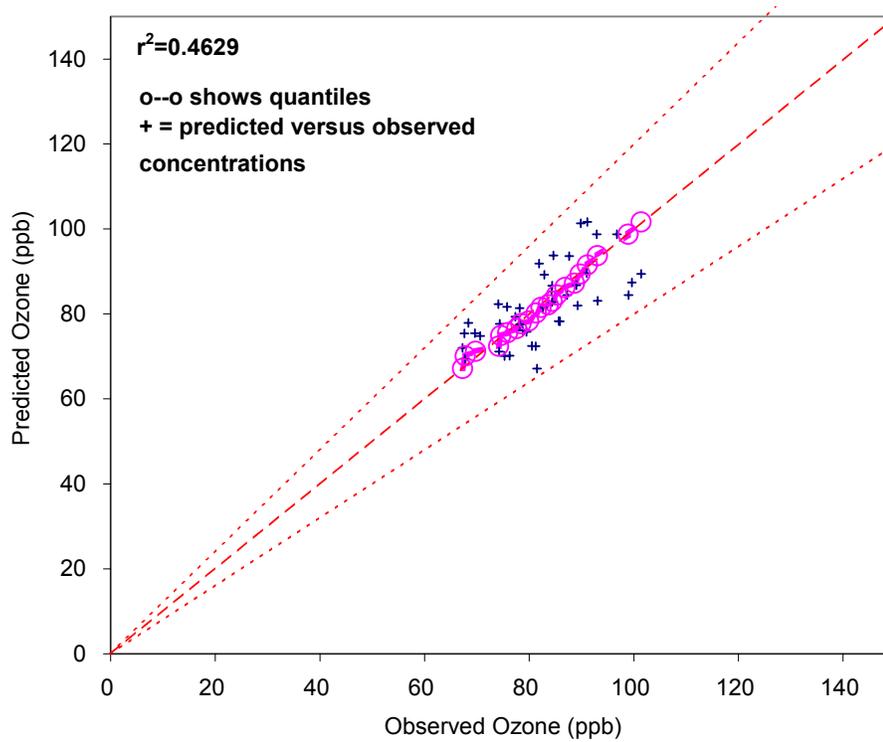


Figure 29. Scatter plot of observed and predicted daily maximum 8-hour ozone concentrations at Central Texas monitors. Predicted values are based on the daily maximum ozone concentration within a 7x7 array of grid cells ‘near’ each Central Texas monitor that is closest in magnitude to the observed daily maximum. Quantiles are shown as well as the correlation coefficient.

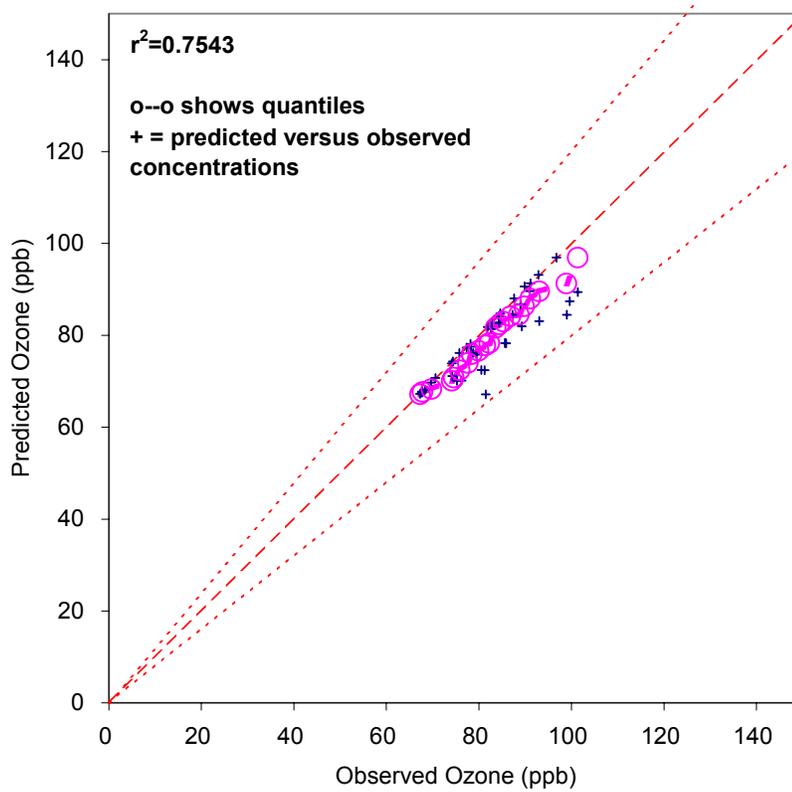
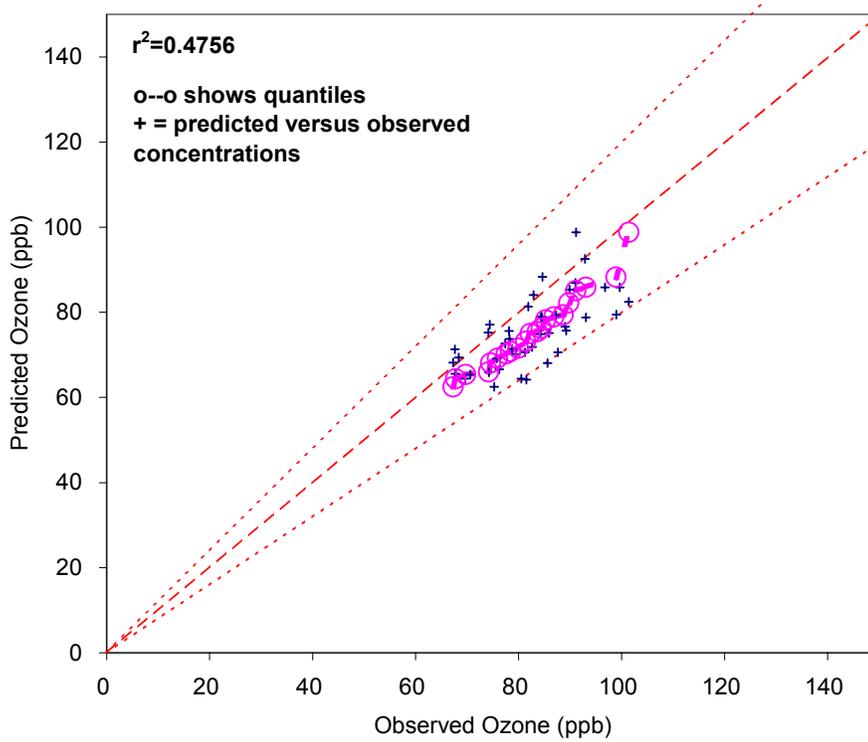


Figure 30. Scatter plot of observed and predicted daily maximum 8-hour ozone concentrations at Central Texas monitors. Predicted values are based on a bilinear interpolation of daily maximum ozone concentrations around each Central Texas monitor. Quantiles are shown as well as the correlation coefficient.



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