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A Performance Analysis of the CMAQ Model and Its Sensitivity to Ozone Precursors in East Tennessee

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To the Graduate Council:

I am submitting herewith a thesis written by Karthikeyan Ramaswamy entitled "A Performance Analysis of the CMAQ Model and Its Sensitivity to Ozone Precursors in East Tennessee." I have examined the final electronic copy of this thesis for form and content and recommend that it be accepted in partial fulfillment of the requirements for the degree of Master of Science, with a major in Environmental Engineering.

Terry L. Miller, Major Professor

We have read this thesis and recommend its acceptance:

Wayne T. Davis, Joshua S. Fu

Accepted for the Council:

Dixie L. Thompson

Vice Provost and Dean of the Graduate School

(Original signatures are on file with official student records.)

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Accepted for the Council:

Anne Mayhew

Vice Chancellor and Dean of Graduate Studies

(Original signatures are on file with official student records.)

**A Performance Analysis of the CMAQ Model and Its
Sensitivity to Ozone Precursors in East Tennessee**

A THESIS PRESENTED FOR THE MASTER OF SCIENCE DEGREE
THE UNIVERSITY OF TENNESSEE, KNOXVILLE

KARTHIKEYAN RAMASWAMY
MAY 2005

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ABSTRACT

This paper presents the results of sensitivity analyses and its effect on ozone concentrations in East Tennessee. The objective of this research was to conduct a sensitivity analysis on ozone precursor emissions. In this research, the Models-3/Community Multiscale Air Quality (CMAQ) and Sparse Matrix Operator Kernel Emissions (SMOKE) models were utilized to predict base case ozone concentrations based on 1999 National Emission Inventory (NEI) in East Tennessee from August 27th to September 9th, 1999. The modeling domain consisted of a three tiered nested domain with grid resolutions of 36 km, 12 km and 4km. The 4 km domain covered the entire State of Tennessee. Performance analysis of the CMAQ model followed by sensitivity analyses of ozone precursors were conducted to determine the possibility of attaining the federal 8-hr ozone standard in East Tennessee. The results showed that substantial NO_x reductions and moderate VOC reductions are needed in mobile and point sources.

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CHAPTER 1

INTRODUCTION

1.1 Overview of Ozone

Ozone (O₃) is a highly reactive gas composed of three oxygen atoms. Ozone has the same chemical structure irrespective of its location in the atmosphere. Ozone occurs naturally in the stratosphere approximately 10 to 30 miles above the earth's surface which is considered to be beneficial as it forms a layer that protects life on earth from the sun's harmful ultraviolet rays. In the lower atmosphere, ozone is considered harmful [1]. This ground level ozone is a colorless and odorless gas that acts as a powerful respiratory irritant and is harmful to people with respiratory disease, senior citizens and children [2]. Ozone often mixes with other species like sulfate aerosols in large-scale pollution events [3] to form urban smog.

Ground level ozone is created by a chemical reaction between oxides of nitrogen (NO_x) and volatile organic compounds (VOCs) emitted from natural and anthropogenic sources. The primary sources of NO_x and VOCs are exhaust from motor vehicles, electric utilities, and other industrial, commercial and residential sources that burn fuels, or emit gasoline vapors, and chemical solvents. [1]

High-level ozone is associated specifically with greater solar radiation and higher temperatures which further intensified with stagnant atmospheric conditions that suppress vertical mixing in the atmosphere [4].

1.2 Air Quality Modeling

An Air Quality Model is useful to local and state agencies for making regulatory decisions on air quality management, as well as to research scientists for performing atmospheric research [6]. Air Quality models contain a set of mathematical equations and use the computer program to simulate the transport, physical transformation and chemical reactions of pollutants after they are released into the atmosphere. Based on the input variables, the model will mathematically simulate the atmospheric conditions, predict pollutant concentrations in the air and the amount of pollution deposited on the ground from the air [7]. They are also necessary to predict how air quality in a region will be affected by economic and population growth, and by the strategies to reduce pollution emissions [5].

The results of models are based on specific inputs such as

- Meteorological conditions (like temperature, cloud cover and wind speed),
- Physical characteristics of the pollution source (like height of a smoke stack) and
- Surrounding topography or terrain [5]

Among the various air quality models, photochemical grid models are essential to states and local agencies for air quality planning and development of state implementation plan (SIP) for regions that are not in compliance with the National Ambient Air Quality Standards (NAAQS) for ozone [8].

In the CMAQ photochemical model, a community or region's atmosphere can be represented as a three-dimensional matrix of grids, packed one on top of another with varying heights. Within each cell, the photochemical model considers the following factors to predict the ozone concentration using its precursors (NO_x and VOCs) emission:

- Advection and the dispersion of pollutants
- Mixing of pollutants upward and downward among layers
- Newly emitted emissions from point, area, mobile and biogenic sources that occur within the cell
- Incoming solar radiation [8]

1.3 Emission Inventory

The emissions inventory database used in this study was the 1999 TDEC inventory. This inventory was developed by the University of Tennessee under the contract with TDEC, to support the regional and urban ozone air quality modeling in Tennessee. With the support from emissions processing models like SMOKE, EMS-95 etc the inventory database is processed to grid-cells. Criteria pollutant emissions in the inventories are typically resolved at the county level, for an average summer day or average annual day. Using the emission-processing tool, emissions are spatially allocated to grid-cells, temporally resolved to hourly estimates and chemically speciated.

1.4 Research Objective

The main purpose of this study was to explore the sensitivity of the CMAQ photochemical model to various control scenarios, to analyze the performance of the model compared to measured ozone concentrations and to determine whether various control scenarios in the Knoxville, TN area may actually result in predicted attainment. The area under study was the East Tennessee air quality region (Figure 1.1). Based on a study conducted by American Lung Association, Knoxville has been recognized as an area with high ozone levels for the fifth consecutive year since 2000. In the annual report released by American Lung Association, Knoxville ranks ninth among the 25 most ozone air polluted cities in the United States (Refer Table 1.1). This rating was based on the number of days the county's air reached unhealthy levels or exceeded the federal 8-hour ozone standard as of 80ppb. The Great Smoky Mountain National Park, located in the East Tennessee region is classified as a Class I region, reported 53 days that exceeded the NAAQS for ozone during the summer of 1999 [11].

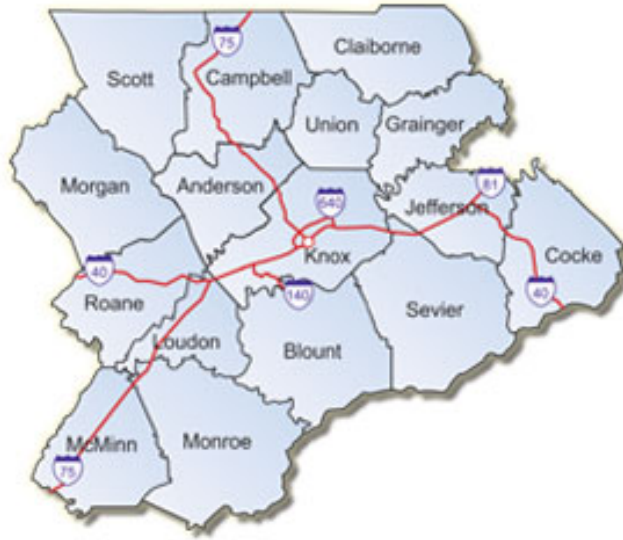


Figure 1.1 Counties in East Tennessee Air Quality Region [9]

Table 1.1 Knoxville ranking among most polluted cities in US

Year	Knoxville ranking among most polluted cities in US
2004	9
2003	9
2002	8
2001	9
2000	12

CHAPTER 2

BACKGROUND

2.1. Background

Ozone concentrations are typically expressed in parts per billion by volume (ppbv), which represent the volume fraction of air molecules represented by ozone. It is formed at ground level by chemical reaction between volatile organic compounds (VOCs) and oxides of nitrogen (NO and NO₂), commonly reported as NO_x. Some of the major sources of NO_x and VOCs are motor vehicle exhaust (on-road source and off-road engines), electric utilities and industrial emissions.

Based on the new scientific health studies conducted by U.S. Environmental Protection Agency (EPA) in 1997, the national standard for ground-level ozone was revised from 120 ppb 1-hour "peak" standard to 80 ppb 8-hour "average" standard [12]. All Air Quality Regions (AQR) in Tennessee have attained the National Ambient Air Quality Standards (NAAQS) for all criteria pollutants, including the 1-hour ozone standard, but have not met the 8-hour ozone standard. These non-attainment AQRs are subject to general and transportation conformity requirements.

2.2 Early Action Compact (EAC)

Several counties in East Tennessee are non-attainment for ozone. Non-attainment counties require the development of an implementation plan to reduce NO_x and VOC emissions from vehicles, industrial facilities, and electric utilities [13] [14] to attempt to meet the NAAQS standard.

Strategies to reduce emissions of VOCs and NO_x include the following:

- Reducing NO_x emissions from electric utilities
- Introducing low-emission cars and trucks
- Using reformulated gasoline (RFG) to reduce VOC and NO_x
- Improving or initiating vehicle inspection maintenance (I/M) programs and
- Speed limit reductions on rural interstates to reduce NO_x emissions.

2.3. Health Effects

The American Lung Association of Tennessee estimates that during the ozone season in Knox County alone, about 4706 children, and 20,117 adults, suffer from asthma [16]. Breathing ozone can limit the ability to take a deep breath, and it can react chemically with internal body tissues that come in contact with them. It can cause coughing, throat irritation, affect lung function and worsen asthma attacks. Studies have shown that repeated long-term exposures to moderate levels of ozone can cause reductions in lung

function, shortness of breath and lower resistance to respiratory disease, inflammation of the lung lining, damage lung tissue, and aggravate chronic lung disease (such as asthma or bronchitis) [12]. Medical studies have shown that ozone damages lung tissue and complete recovery may take several days after exposure has ended [16].

Vegetation and Ecosystem: Ozone is also a pollutant of ecosystem concern because it can affect both forests and agricultural crops. Ground-level ozone damages vegetation and ecosystems. It leads to reduced agricultural crops, reduced growth of tree seedlings, and increases diseases and pests. It also damages the foliage of trees and other plants, affecting the site of cities, national parks and forests, and recreation areas [15].

2.4 Sources of Emissions

Ozone is not emitted directly and therefore is a secondary pollutant. Ozone is formed through atmospheric chemical reactions between its precursors (NO_x and VOCs). Therefore, the sources and concentration of ozone's precursors are an important aspect of understanding ozone concentrations [17]. Precursor's annual and daily emissions were estimated from the National Emissions Inventory (NEI) for this study. The 1999 NEI of Criteria Air Pollutants was the source of data used in this study.

2.4.1 Nitrogen Oxides (NO_x)

Anthropogenic NO_x emissions primarily result from stationary and mobile combustion processes. Nitrogen in the fuel source combines with atmospheric oxygen at high temperatures forming NO_2 and NO , the most common species [17]. The primary anthropogenic sources of NO_x include transportation sources, and certain industrial processes. In addition emission from electric utilities burning coal, oil, or natural gas, as well as smaller heating units in commercial and residential properties, account for rest of the NO_x emissions.

Natural sources also account for a small percentage of total emissions of NO_x . Emission from natural sources includes emission from forest fires, lightning and soil microbial activity [17].

In Tennessee, based upon 1999 emission inventories, 41% of the annual NO_x emissions originated from the mobile source, 43% of the annual NO_x emissions from the industrial sector and 16% from the Area sources (Figure 2.1).

The Figure 2.2 shows the 1999 Annual NO_x Emission Distribution in Tennessee. The electric power-generating sector produced about 31% of NO_x emissions. Onroad mobile sources account for about 41% of NO_x emissions. Because diesel fuel causes higher NO_x emissions than gasoline, they account for a larger proportion of NO_x emissions. The spatial distribution of NO emissions in TN is shown in Figure 2.3.

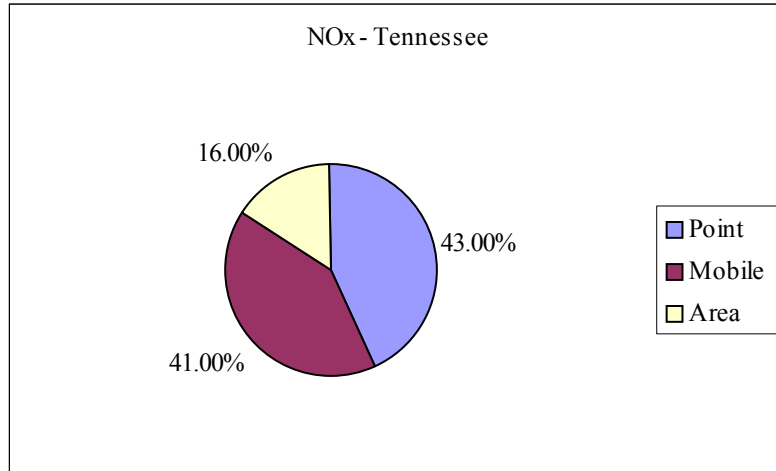


Figure 2.1 1999 Annual NO_x Emissions from Major Sources in Tennessee

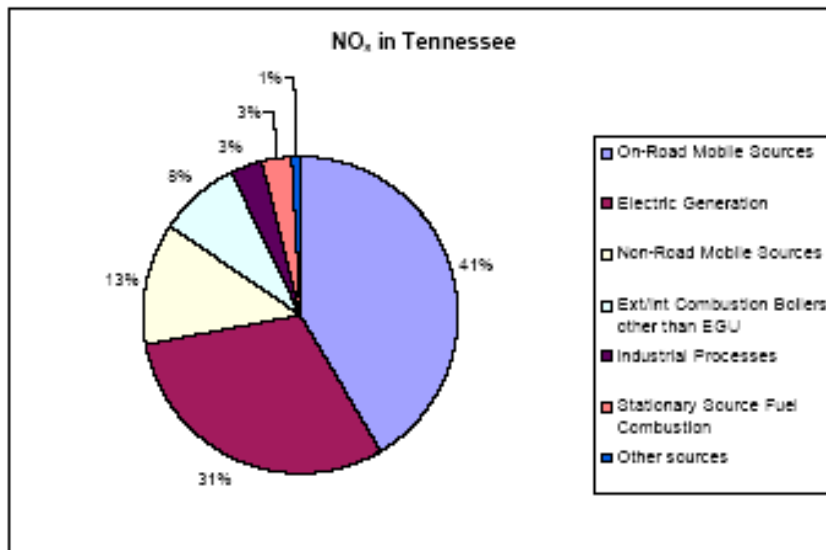


Figure 2.2 1999 Annual NO_x Emission Distribution in Tennessee

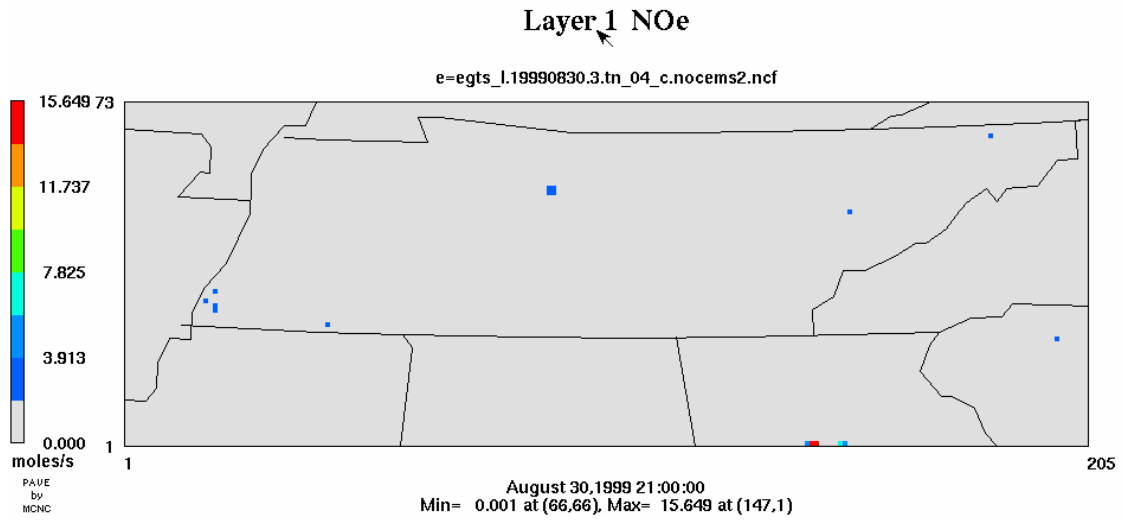


Figure 2.3 Spatial Distribution of NO emissions in TN on 30th August 1999

2.4.2 Volatile Organic Compounds (VOCs)

VOCs are the other precursor involved in ozone formation. VOCs are released in large scale from both combustion and evaporation processes. The largest anthropogenic sources of VOC in Tennessee are known to be solvent utilization and onroad mobile sources; other principal contributors are industrial processes, nonroad mobile sources, solvent use, petroleum refining and distribution and waste disposal etc. The VOCs emission inventory excludes photochemical non-reactive compounds such as methane, ethane and chlorofluorocarbons.

Area source and mobile source produced about 51% and 30% of the total VOC emissions respectively (Figure 2.4). That is, over half of the manmade emissions of VOC are area related. The distribution of these emissions is shown in Figure 2.5.

Natural VOC emissions from vegetation are also important in ozone formation. Being a natural emission, it was not included in 1999 anthropogenic VOCs emissions inventory. A separate emission inventory was prepared for biogenic emission. Biogenic VOCs emissions from vegetation are highest in the warmer growing season when ozone levels are also high. Of these biogenic emissions, Isoprene from deciduous forests and monoterpenes from coniferous forests are the most important VOC compounds involved in ozone formation. Biogenic VOCs emissions are 2.8 times more reactive than most anthropogenic VOC's [17].

2.5. Regulations

In the United States, ground-level ozone is regulated under the comprehensive Clean Air Act (CAA) and it requires the U.S. EPA to set standards for “ozone”. These standards are known as the National Ambient Air Quality Standards (NAAQS) [18]. EPA has developed two NAAQS standards for ozone:

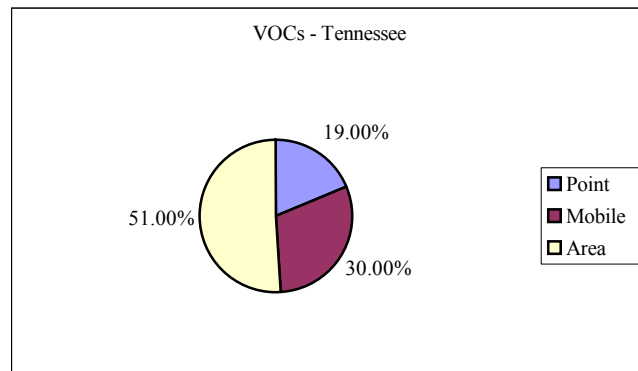


Figure 2.4 1999 Annual VOC emissions from Major sources in Tennessee

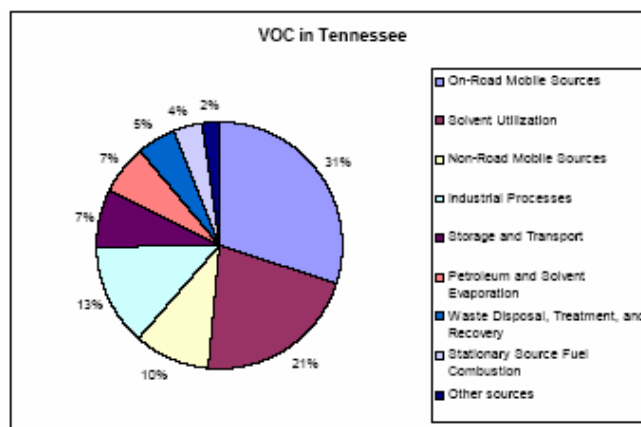


Figure 2.5 1999 Annual VOCs Emission Distribution in Tennessee

- The standard which is intended to protect public health is the primary standard.
- The standard which is intended to prevent damage to the environment and property is the secondary standard.

Air Quality Regions (AQR) that do not meet the primary standard are called nonattainment while areas that meet the primary standard are called attainment [19].

In 1997, EPA ruled out and replaced the previous one-hour standard (125ppb) with a new eight-hour standard (85ppb) to protect public health against longer exposures to the ozone [26]. The AQR is in violation of ozone standard if the average of the annual fourth highest of daily eight-hour maximum over a three-year period is above 85ppb. The EPA enforced the eight-hour standard in 2004. An AQR will meet the new eight-hour standard when the three-year average of the fourth-highest daily maximum eight-hour concentration measured at each monitoring site is less than 85 parts per billion. [20]

2.6 Emission Inventories

2.6.1 Point Sources

Point source emissions are generated from stack emissions. Point source emissions include emissions from major industrial and non-industrial stationary equipment like power plants, commercial boilers, electric utility boilers, turbine engines, wood and pulp processors, industrial surface coating facilities, refinery and chemical processing operations, and petroleum storage tanks and hazardous waste incinerators [22]. Predominant Point sources like electrical utilities and industrial boilers are major emitters of nitrogen oxides (NO_x) - accounting for about 43% of total releases in Tennessee. Point sources contribute less of total VOCs. Insignificant point sources are included in the area

source inventory. Area sources that may fall under the point source definition are piping leaks, industrial wastewater treatment ponds and tank farms [23].

The inventory contains the coordinates of the stacks or release points so point source locations are known. General temporal profiles are used to group certain industries and processes by source classification code (SCC), which assumes that a certain type of process emits a given percentage of its daily emissions during a certain hour.

Continuous Emission Monitoring System (CEMS): CEMS data are real emission data. The most accurate method for determining the amount of emissions produced by a point source is with continuous emissions monitoring. CEMS measures and records actual emissions during its period of operation and the data can be used to estimate emissions for different operating periods. Some major point sources use CEMS that are permanently installed at a source to generate data 24-hours a day. Mass emission rates can be computed from the CEMS concentration data provided the air volume through the monitor is known. CEMS are typically used to measure stack gas concentrations of NO_x, CO₂, CO, SO₂, and total hydrocarbons (THC) [27]. The NEI (average emissions) point source inventory provides only average hourly emission rates of all major pollutants from all point sources in the USA.

Other methods of estimating emissions include stack testing, equipment vendor test data and material balances. Facilities must report these emissions to the local or state agency in tons per year or tons per day for the calendar year [22].

2.6.2 Mobile Sources

Mobile sources are broadly classified as

- On road sources including sources such as cars, trucks and buses and
- Nonroad sources include sources (off-road equipment [22]).

The contribution from these two classes of mobile sources to air pollution is very significant.

Highway emissions are calculated using the MOBILE6 model, which was developed by the Environmental Protection Agency (EPA). MOBILE calculates an emission factor for mobile sources using a set of complex mathematical equations that require several user input values. Vehicles are classified into eight vehicle classes with MOBILE generating an emissions factor for each class and a composite emissions factor representing all classes [22].

An emissions factor is generated for each vehicle class from MOBILE. The factor is then used with the appropriate vehicle miles traveled (VMT) estimates developed for that selected area. This combination determines the contribution of emissions from mobile sources in a city, county, or state.

Nonroad mobile sources: As the name suggests they are not associated with highway vehicles but with a wide variety of sources being used off the road using internal combustion engines. Ships, airplanes, agricultural and construction equipment, Lawn mowing, recreational boating, and locomotives are examples of major nonroad mobile sources that emit significant amounts of NO_x, VOCs, and carbon monoxide (CO) [22].

EPA's computer model is used to calculate most aircraft emissions from various engine types and landing/takeoff cycles. Actual fuel usage and track mileage are applied to determine locomotive emissions. Ship and barge traffic data are used to calculate emissions from marine vessels [22].

2.6.3 Area Sources

An area source consists of many sources too small to be treated as individual point sources. While the emissions from individual sources are relatively small, collectively they contribute a significant amount of emissions - particularly where large numbers of sources are located in heavily populated areas. Area sources include sources like dry cleaners, gas stations, and auto body paint shops [24]. Area sources often lack locational data and site-specific emissions data. For this reason, emissions are reported at the county level in X tons of pollutant released per square mile. The emissions are spatially allocated based on various surrogates. A surrogate is a readily available geographic substitute such as population that can be used to locate area source emissions spatially [22].

The category also includes commercial buildings (heating and cooling units; surface coatings), residential buildings (fire places; surface coatings) and fuel combustion. Waste disposal in the form of open burning, landfills and wastewater treatment are significant area sources. Area source emissions are calculated by various methods depending on the type of data available for each category. Based on categories available, area source inventories generally report emissions collectively in categories rather than by individual source.

2.6.4 Biogenic Sources

Biogenic emissions are particularly important because different types of trees and crops emit different types of VOCs and their emissions depend strongly upon the temperature and solar radiation to which the leaves are exposed. The largest emitters of VOCs are oaks, pines, sweet gums, eucalyptus, and poplars. Fragrant monoterpenes are emitted by pines, sycamores, and eucalyptus [22].

Many factors that affect the biogenic emissions are

- Species composition
- Leaf biomass density
- Land use/land cover (LULC) map
- Meteorological variables

Biogenic VOC emissions are estimated in a particular modeling domain using a computer model called Biogenic Emissions Inventory System—Version 2 (BEIS2) that takes into account all the factors mentioned above [25].

2.7 Review of Current Studies on CMAQ Performance and Its Sensitivity Analyses

P. Georgopoulos et al. (1999) presented studies on evaluation of the performances of a CMAQ in predicting ambient ozone concentrations over the Northeastern U.S. The study revealed that the correlation between the simulated and observed values is slightly better for fine grid compared to the coarse grid simulations. The study summarized that the performance of CMAQ in predicting ozone with both fine and coarse grids is generally consistent with the EPA's recommendation of MNGE (Mean Normalized Gross Error) and MNB (Mean Normalized Bias) for ozone predictions are 35% and 15%, respectively. The mean normalized bias, often just called the bias, is given by:

$$\text{Mean Normalized Bias (MNB)} = \frac{1}{N} \sum_1^N \left(\frac{\text{Pred.} - \text{Obs.}}{\text{Obs.}} \right) \cdot 100\%$$

Where N is the number of observations

Mathematically, the bias is derived from the average signed deviation of the concentration residuals and is calculated using pairs of estimates and observations.

The mean normalized gross error is:

$$\text{Mean Normalized Gross Error (MNGE)} = \frac{1}{N} \sum_1^N \left(\frac{|\text{Pred.} - \text{Obs.}|}{\text{Obs.}} \right) \cdot 100\%$$

Where N is the number of observations

The gross error quantifies the mean absolute deviation of the concentration residuals. Gross error is a robust measure of overall model performance and provides a useful basis for comparison among model simulations across different air basins or ozone episodes [32].

Further the study by P. Georgopoulos stated that the model predictions appeared to be generally consistent with observations, even though the predicted values for the lowest percentile seem to have a minimum of about 20ppb while the observed values were close to zero. The author attributes this to be caused by the fact that CMAQ simulations represent averages over large areas and cannot capture localized effects [28].

C. Hogrefea, et al presented a similar paper based on the evaluation results of the modeling system used to simulate ozone air quality over the eastern United States. It was

mentioned that the comparison of observed and predicted spatial patterns of daily maximum ozone concentrations showed the best performance in predicting patterns for average and above-average ozone concentrations. The author suggested that the MM5/CMAQ system is a suitable tool for the simulation of summertime surface temperature and ozone air quality conditions over the eastern United States [29].

Jinyou Liang et al conducted a study based on the comprehensive field monitoring campaign of the 2000 Central California Ozone Study (CCOS). CMAQ and CAMx (Comprehensive Air-quality Model with extensions) models were employed to simulate the ozone concentration for July 31- August 2, 2000 episode. Jinyou Liang et al determined that the domain-averaged surface ozone is higher in CAMx than CMAQ at all hours and surface NO_x concentrations in CMAQ were less during the daytime and higher during the nighttime than CAMx. The results suggest that CMAQ predicted higher peak ozone than CAMx in areas influenced by forest fires and under predicted ozone in the Bay Area but performed better than CAMx in Sacramento and the San Joaquin Valley. They concluded that ozone was over predicted with CMAQ, especially when observed ozone was lower than 40 ppb and under estimated when observed ozone was higher than 80 ppb. Studies showed that ozone precursors (NO_x, NMHCs, and HCHO) were under predicted overall but still CMAQ met the U.S. EPA model performance criteria for ozone in the Bay Area [30].

Ralph E. Morris et al, applied CMAQ and the CAMx modeling systems to the July 1995 NARSTO-Northeast ozone episode that occurred in the northeastern United States. The author declared that

- CMAQ+MM5 estimated the early morning rise in ozone concentrations reasonably well.
- CMAQ+MM5 also estimated the afternoon fall in ozone and nighttime ozone levels better than CAMx+MM5.
- CMAQ+MM5 estimates the average observed afternoon ozone concentrations slightly better than CAMx/RAMS.

And based on their grid resolution sensitivity tests on CMAQ, they reported the following key findings for reductions of 50% VOCs and 50% NO_x emissions:

- NO_x controls result in widespread estimated ozone reductions across the Northeast
- NO_x controls occasionally results in ozone increases (in some cities like New York City).
- SAPRC97 chemistry is more VOCs sensitive than the CB-IV mechanisms [31].

CHAPTER 3

METHODOLOGY

This part of the document describes the methodology used to test the sensitivity of the CMAQ model for different emission reduction scenarios. Ozone reductions are needed to attain the National Ambient Air Quality Standards (NAAQS) for ozone in East Tennessee. The purpose of this study is to evaluate CMAQ model performance for different emission rates and to perform sensitivity analyzes to observe the effect of ozone precursor's on ozone formation. Comparisons of predicted daily maximum 8 hour ozone concentrations were made with actual measured ozone concentrations at 8 air monitoring stations in East Tennessee.

To determine the technical feasibility of attaining the 8-hr standard, and to identify the best precursor reduction strategies for moving towards attainment, it is necessary to understand the precursor's sensitivity or relationship in ozone formation. Ozone formation rate depends upon ozone precursor emissions rates. Because these precursor relationships ultimately govern the response of ozone concentrations to changes in local VOC and NO_x emission rates, their determination is essential in designing an effective ozone abatement strategy [33]. Thus to acquire the comprehensive knowledge of ozone precursors sensitivity, a photochemical model was employed. The CMAQ, (Third Generation Model) a photochemical model developed by USEPA to have good precursor sensitivity associated with ozone formation was employed for this study.

To address the objective of this study the following steps were performed:

- Analyzed the performance of the model
- Developed emission inventories for various scenarios, and
- Modeled ozone with CMAQ for various scenarios to determine whether the scenarios actually result in reductions in ozone and achievement of NAAQS.

Each of these steps is discussed in detail in the following sections.

3.1. Episode and Monitors

To analyze the performance of the model, eight monitoring stations were chosen to represent East Tennessee. Table 3.1 shows the locations, AIRS identification number, elevation, and the latitude - longitude of each monitoring station in East Tennessee [34]. Real time values from these monitoring stations were used to compare how well the CMAQ model simulated the ozone concentrations that were actually measured at eight ozone-monitoring stations during the episode considered.

Five counties (Anderson, Blount, Jefferson, Knox and Sevier) in East Tennessee are represented by the eight monitoring stations. Hourly ozone concentrations in East Tennessee were predicted for an 11-day episode starting from August 29, 1999 to

Table 3.1 Monitoring Station Information [34]

Station Name	AIRS Identification Number:	Elevation		Latitude: (Degree)	Longitude: (Degree)
Anderson- Melton Lake	47-001-0101	780 ft	237.74 m	35.965078	-84.22323639
Blount-Cades Cove	47-009-0102	1850 ft	563.88 m	35.603043	-83.783615
Blount-Look Rook	47-009-0101	2700 ft	822.96 m	35.631502	-83.94368111
Jefferson-Lost Creek Road	47-089-0002	1017 ft	309.98 m	36.114444	-83.601111
Knox-Rutledge Pike	47-093-0021	980 ft	298.7 m	36.085049	-83.76465806
Knox-Mildred Drive	47-093-1020	1056 ft	321.87 m	36.018344	-83.87614417
Sevier-Cove Mountain	47-155-0101	4150 ft	1264.9 m	35.696531	-83.60985778
Sevier-Clingmans Dome	47-155-0102	6610 ft	2014.7 m	35.562793	-83.49807028

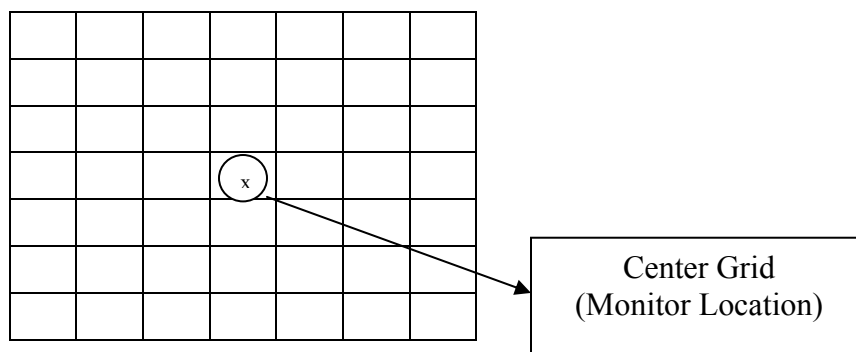


Figure 3.1 7 x 7 Grid Matrix around the Center Grid.

September 8, 1999. A rolling 8-hr average ozone concentration was computed from hourly concentrations and the maximum predicted concentration each day was compared to the maximum 8-hour average monitored concentrations. The predicted maximum 8-hour ozone concentration was chosen from the maximum 8-hour average ozone concentrations predicted in a grid matrix of 7 cells by 7 cells, which encompasses the monitoring grid at the center (Refer Figure 3.1).

3.2. Emission Inventory

For this study we used the 1999 National Emission Inventory (NEI) [35] as the base case emissions to support the performance evaluation modeling as well as for sensitivity modeling. The base year emissions were used for producing modeled concentrations of episode days that can be compared to monitored concentrations for the model performance evaluation. The base year inventory consisted of emissions from point, area, biogenic and mobile sources. This emission inventory included emissions of NO_x , VOC, CO, NH_3 , SO_2 , PM_{10} and $\text{PM}_{2.5}$ in tons/day and in tons/year. These emission inventory files were processed using emission-processing tools (SMOKE [36]). Each of these files was processed individually before they were merged together.

3.2.1. Area and Biogenic Sources

Biogenic emissions and area source emissions were held fixed for all modeling runs while point and mobile emissions were changed to reflect the changes that could possibly arise for various sensitive analyses.

3.2.2. Mobile and Point Sources

Emissions from point and mobile source emissions were reduced for all sources in the modeling domain. Modified inventories were processed using SMOKE for various emission control strategies and multiple CMAQ sensitivity runs were conducted based on these control strategies.

The eleven control strategies that were employed in this study are:

- Run1: Base case using average emission in 11 layers (Base case)
- Run2: Both NO_x and VOC emissions from mobile sources were reduced by 100%
- Run3: Both NO_x and VOC emissions from point sources were reduced by 100%
- Run4: NO_x emissions from mobile sources were reduced by 15%
- Run5: NO_x emissions from mobile sources were reduced by 30%
- Run6: NO_x emissions from mobile sources were reduced by 100%
- Run7: NO_x emissions from point sources were reduced by 15%
- Run8: NO_x emissions from point sources were reduced by 30%
- Run9: VOC emissions from mobile sources were reduced by 100%
- Run10: Base case using CEMS data in 11 layers
- Run11: Base case using average emissions in single layer

In each case mentioned above, the inventory was modified to reflect the corresponding changes. An emission processor was applied to process the modified point source inventory and modified mobile source inventory. The processed output was merged with other anthropogenic sources like area and biogenic source emissions and merged output was prepared in a CMAQ accessible format.

3.3. Emission Processing – SMOKE (Sparse Matrix Operator Kernel Emissions)

The emissions data were processed from the National Emissions Inventory (NEI) [35] using MCNC's Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system [36]. NEI provides annual and daily emissions data for area, point, and mobile source categories for seven species: NO_x, VOC, CO, NH₃, SO₂, PM₁₀ and PM_{2.5}. In order for the CMAQ to utilize these data, emission inventory was spatially gridded, temporary resolved and chemically speciated by SMOKE. SMOKE generates hourly precursor's emissions needed by CMAQ for 36km, 12km and 4km grids. The simulations were processed using the meteorological conditions starting from August 29, 1999 to September 8, 1999.

Once the individual emissions were processed, all the emissions were merged to a single output file called merged output. The merged outputs were used for analyzing the distribution of NO_x and VOCs emission and used as an input to CMAQ to predict the ozone concentration [36]. The SMOKE version 1.5 was used to perform the above task.

CEM (Continuous Emission Monitoring) data: SMOKE accesses the 1999 NEI in order to process them. When CEMs data is used, SMOKE replaces the average emissions of large sources with the CEMs data. CEMs data include the actual hourly emission measured in the stack during the time period under study. Two separate CMAQ runs were conducted based on average emission and CEMS and the results of the two CMAQ runs were compared to illustrate the effect of using CEMS data.

3.4. Meteorology

In order to obtain the meteorological inputs for CMAQ simulations, meteorology simulations were performed with the fifth generation Pennsylvania State University/National Center for Atmospheric Research (NCAR) Mesoscale Model (MM5) [38] model for the nested multiscale model domain. MM5 model simulations were performed for two weeks starting from August 29, 1999 to September 8, 1999. The simulations were performed for three nested domains with a grid resolution of 36, 12 and 4km to obtain the meteorology input information needed by CMAQ. Output from MM5 was taken to run the latest version of the MCIP program, which produces the data in a compatible format for CMAQ. The meteorological output from MCIP was used to characterize advection, dispersion, temperatures, humidity and other critical parameters needed by CMAQ. CMAQ model uses the meteorological inputs to accurately simulate the temporal and spatial movement of air parcels that contain ozone and ozone precursors [41].

3.5. Photochemical Modeling – CMAQ (Community Multiscale Air Quality)

The air quality model utilized for this study was US EPA's Community Multiscale Air Quality (CMAQ) model, a component of the Models-3 system and third generation photochemical model [39]. This model was used to perform the alternative sets of simulations of gaseous and aerosol phase air quality dynamics [43] for the 36km, 12km and 4km resolution domain.

This study used the CMAQ model for the evaluation of grid based ozone modeling for two weeks during the summer 1999. CMAQ needs meteorological inputs and National Emissions Inventory (NEI)'s processed emissions. Meteorological inputs were obtained from the MM5 meteorological mesoscale model and emissions were obtained using the MCNC's Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system, respectively (Refer figure 3.2).

A sample of CMAQ simulation is shown below in Figure 3.3. Figure 3.3 shows the maximum 8 – hour ground level ozone concentration on 7th September 1999 at 5pm EST, over the 4km resolution domain. Following the simulation, modeling results are compared with real time measurements to determine how well the model performed.

Following the model performance analysis, various emission reduction strategies were tested to provide insights into how reductions in precursor emissions impact ambient ozone concentrations.

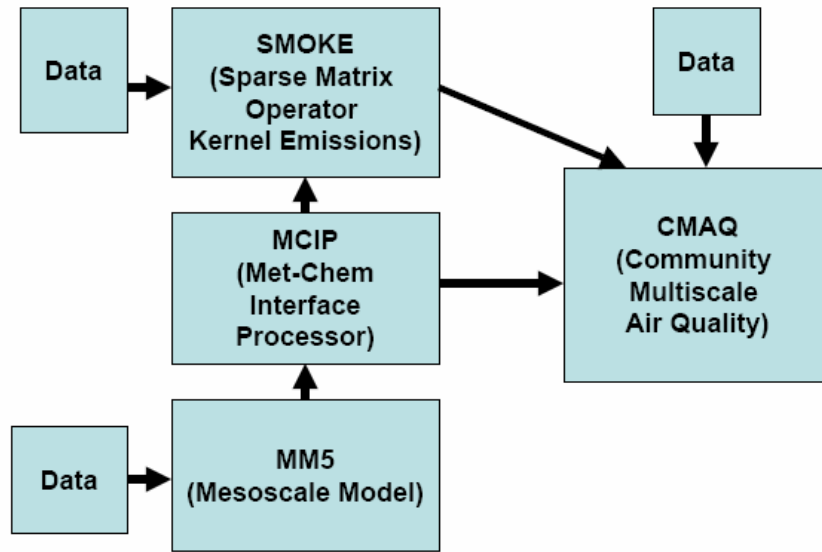


Figure 3.2 Algorithm of Typical Photochemical Modeling

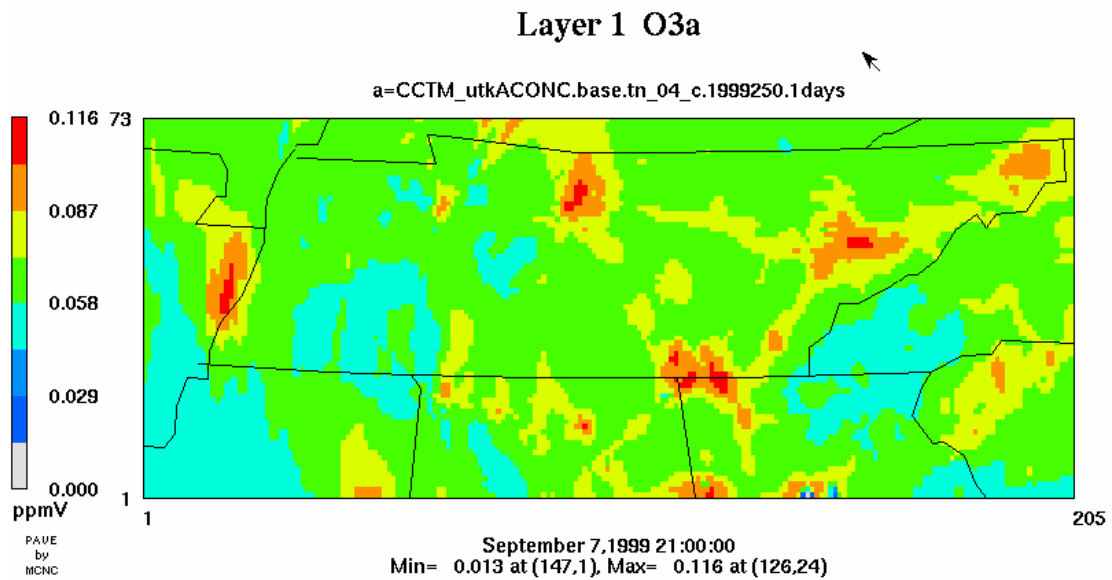


Figure 3.3 Predicted Maximum 8 – hour concentration on 7th September 1999 by CMAQ

3.6. CMAQ Processors

The four processors that were used to perform CMAQ runs are

- Initial condition processor
- Boundary condition processor
- Photolysis processor
- Chemical transport model

3.6.1. Initial and Boundary Condition's Processor

To perform air quality simulations by CMAQ, both initial and boundary conditions of the domain are required. Initial and Boundary conditions are generated by two processors namely ICON and BCON respectively, which are used by the other CMAQ processor namely Chemical Transport Model (CCTM). The ICON processor generates initial concentrations of ozone for every cell in the modeling domain, whereas the BCON processor generates ozone concentrations for the cells immediately surrounding the modeling domain [39], [40].

Default initial and boundary conditions in the CMAQ model were considered for the 36km domain's boundary and initial conditions (Refer Appendix – A3 & A4). ICON processor is needed at the initial stage of a model run to generate initial conditions, which are time independent concentrations for the first day of the episode. For the rest of the episode, ICON processor uses the last hourly concentration of the previous day's output (CCTM file). The initial conditions for start-up of the finer grid are generated using concentrations from the coarse grid [39], [40].

For the CMAQ model run, it is necessary to generate a boundary conditions file for each day of the run. For the course grid, the BCON processor uses the same boundary conditions (ambient condition) for all the days in the episode. When using a nested grid configuration, boundary conditions must generate for all the days in the episode. For the first day run in a fine-resolution grid, model uses the time-varying boundary conditions generated by the BCON processor with input from concentrations from the coarse grid. For the remaining days the episode uses the last hour concentration of the previous day's CCTM file [39], [40].

3.6.2. JPROC Processor

CMAQ uses the JPROC processor to predict the photolysis rates based on vertical ozone profiles, temperature profiles, altitudes and latitudes [40]. Initially, JPROC assumes clear-sky conditions and the CCTM processor then attenuates for cloudiness. It generates a table of photo-dissociation rate constants for the photolytic and gas chemistry reactions, which the CCTM processor uses for predicting the ozone concentration. Photo-dissociation rates are interpolated in CCTM processor to the specified time and location required for modeling.

3.6.3. Chemical Transport Model (CCTM)

The chemical transport model integrates the merged emission output from SMOKE with ICON, BCON, and JPROC processors' output to generate hourly concentration of ozone based on the chemical mechanism used. The chemical mechanism considered in this model was Carbon Bond – IV [42]. This mechanism was selected in order to be consistent with the set up of the SMOKE emission processor output. Eventually the ozone concentrations are resolved temporally and spatially in the domain [42]. Predicted ozone from CCTM was compared with the maximum 8-hour averaged ozone concentration measured at monitor station, located in the region under study.

3.7 Chemical Mechanism

The Carbon Bond-IV Mechanism was developed mainly for urban smog and regional atmospheric modeling. This mechanism was intended to simulate the formation of ozone from its precursor's (NO_x and VOC). It contains a set of inorganic reactions attached to an organic representation based on both explicit and structurally lumped species to convert the ozone precursors to ozone. The Carbon Bond Mechanism contains 35 reactions [42].

3.8. Domain and Vertical Layers

The domain used in this study is shown in Figure 3.4. Eleven layers in the vertical direction and three levels of nested domains with grid resolutions of 36km for the outmost domain; 12km for the intermediate domain and 4km for the innermost domain was used. The outmost domain encompasses the entire eastern United States. The intermediate domain was centered on the states of Tennessee and Kentucky and included portions of the surrounding states including Atlanta, GA. The fine innermost 4km grid domain covered on the entire state of Tennessee and a small area bordering Tennessee (Refer figure 3.4). The parent domain consisted of a 48x42x11 mesh containing 36km grid cells. The intermediate domain consisted of a 94x70x11 mesh of 12km grid cells. The second nested grid consisted of a 205x73x11 mesh containing 4km grid cells.

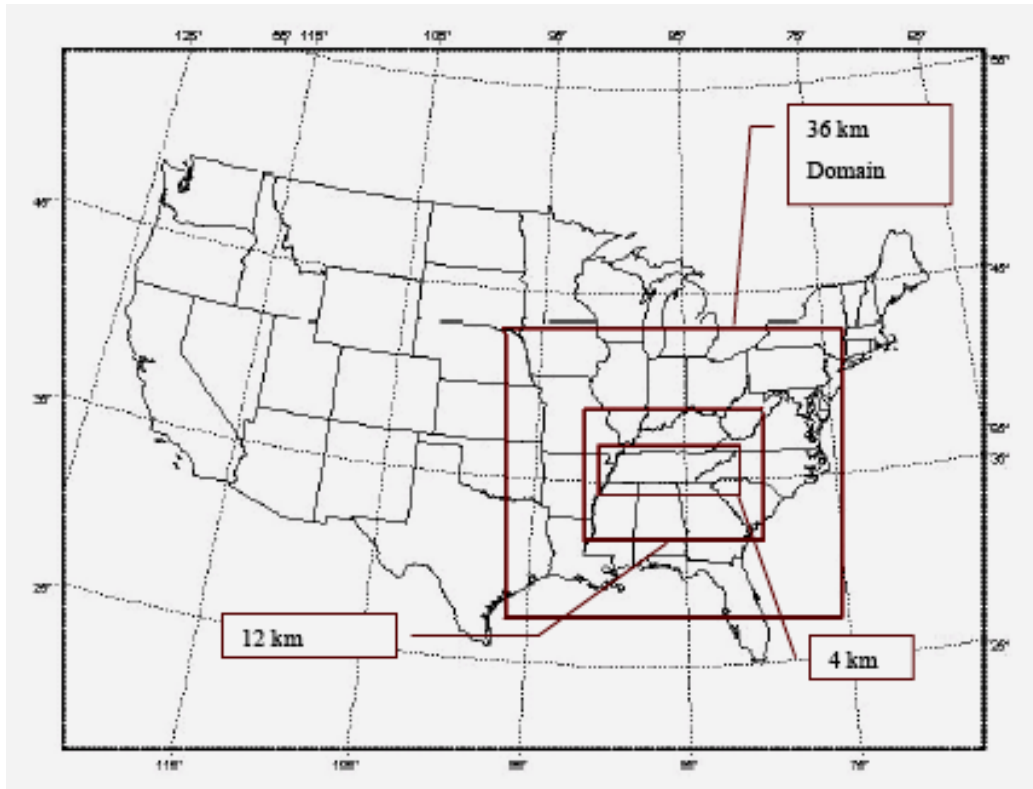


Figure 3.4 Nested Domains

CHAPTER 4

RESULTS

4.1 Analyzing the Performance of the Model

While the primary focus of this research was to determine whether various control scenarios actually result in predicted attainment or achievement of target concentrations, it is important to analyze the performance of the model. For this purpose, the averaged 8-hr ozone concentrations predicted by CMAQ model for the base case were compared to measured concentrations at available monitoring sites.

CMAQ was run for the base case and graphs were developed showing the maximum 8-hr average ozone levels calculated and measured at eight monitoring stations covering a range of urban and rural settings.

4.1.1 Inference Based on Model Output

To compare the model's output to the actual measured value at monitors, both these values were plotted for each day, on the same graph for each location as shown in Figures 4.1 – 4.8.

From the first impression of the graphs, the predictions appeared to be in reasonably good agreement with observation data for all locations. The modeled ozone concentrations were significantly lower than observations for the first part of episode but captured the basic trend of real time data during the 11 day episode at Rutledge Pike (Knox County), Knoxville Mildred Drive (Knox County), Clingmans Dome (Sevier County), Cove Mountain (Sevier County) and Look Rock (Blount County).

Predictions at the Anderson County and Jefferson County sites (Figure 4.1 and 4.4) didn't capture the same trend as the monitoring station but the overall mean ozone concentrations predicted by the models from August 27, 1999 to September 9, 1999 were very similar to the mean observed ozone concentrations (Refer Table 4.1). For the stations at Anderson and Jefferson County, the average bias (-2.78% & 5.33% respectively) was much lower than for the other sites. Knox County performed better than Blount and Sevier County (Refer Table 4.1). For Anderson, Jefferson and Knox County, the second part of the episode from 6th to 8th of September the CMAQ model captured the rising trend with observed data, but over predicted the ozone concentration (Refer Figure 4.1, 4.4 to 4.6).

The CMAQ model over predicted the average 8-hour ozone concentration at Lost Creek Road (Jefferson County) by only 1 ppb (1.5%). For the monitoring stations at Knox and Anderson County, the model under predicted the average 8-hour ozone

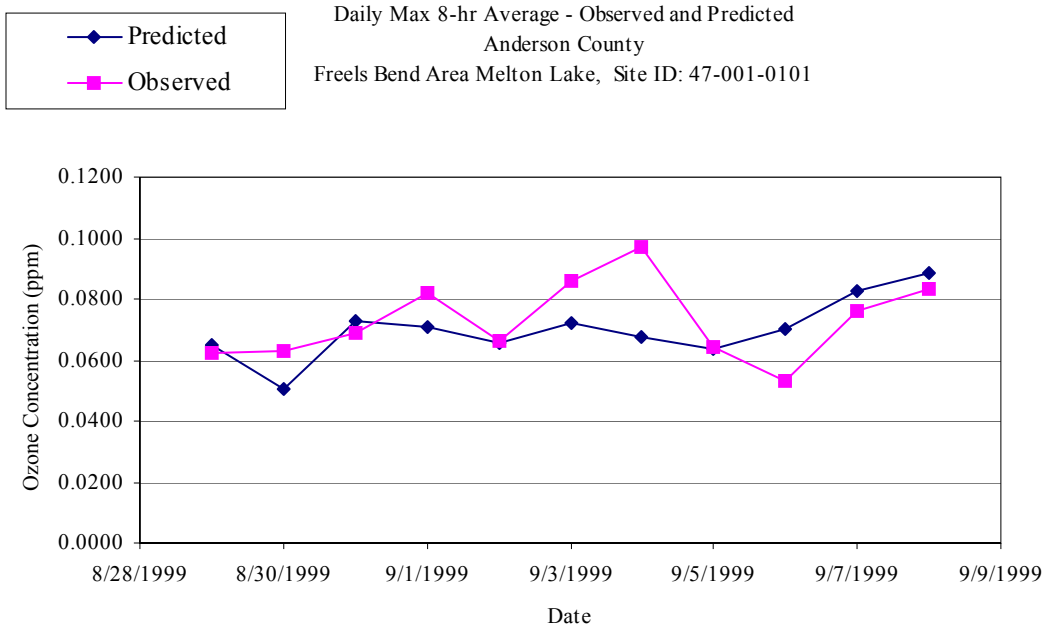


Figure 4.1 Anderson County – Daily Max 8-hr Average – Observed vs. Predicted

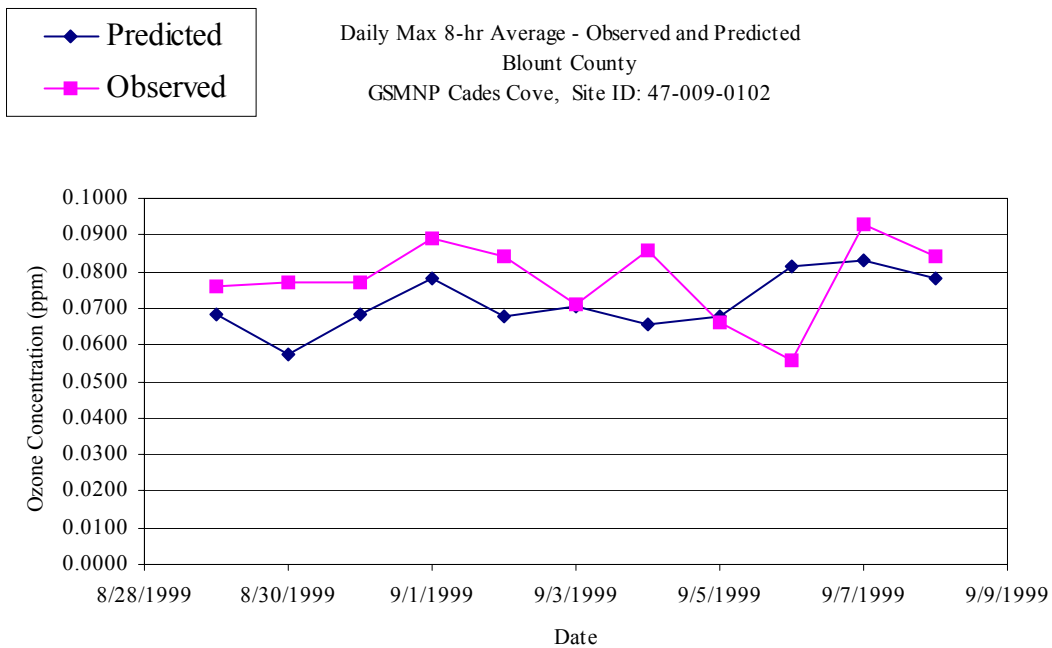


Figure 4.2 Blount County (Cades Cove) – Daily Max 8-hr Average – Observed vs. Predicted

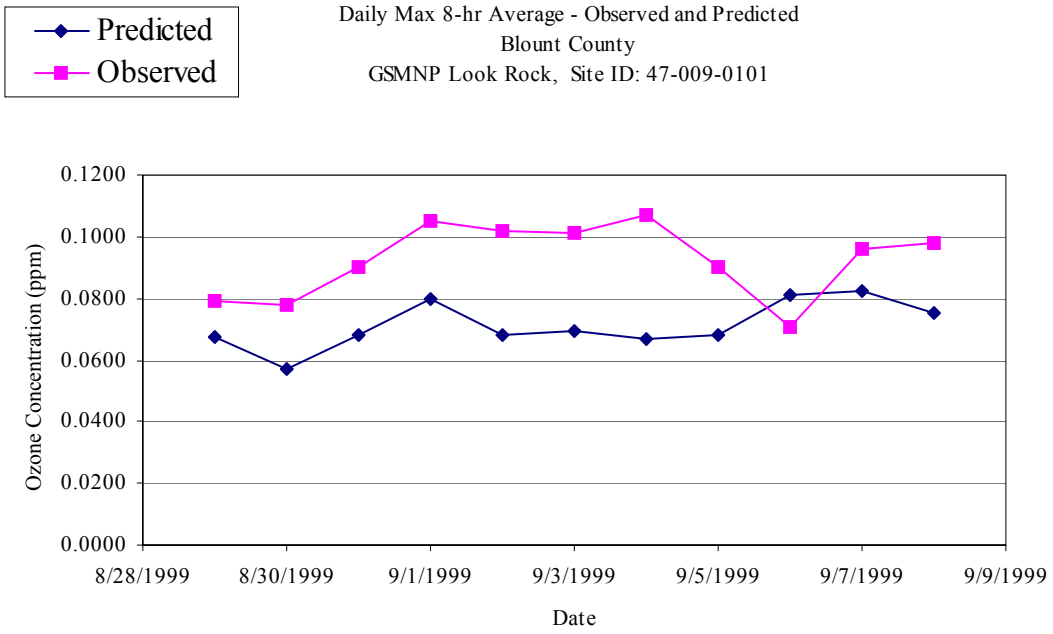


Figure 4.3 Blount County (Look Rook) – Daily Max 8-hr Average – Observed vs. Predicted

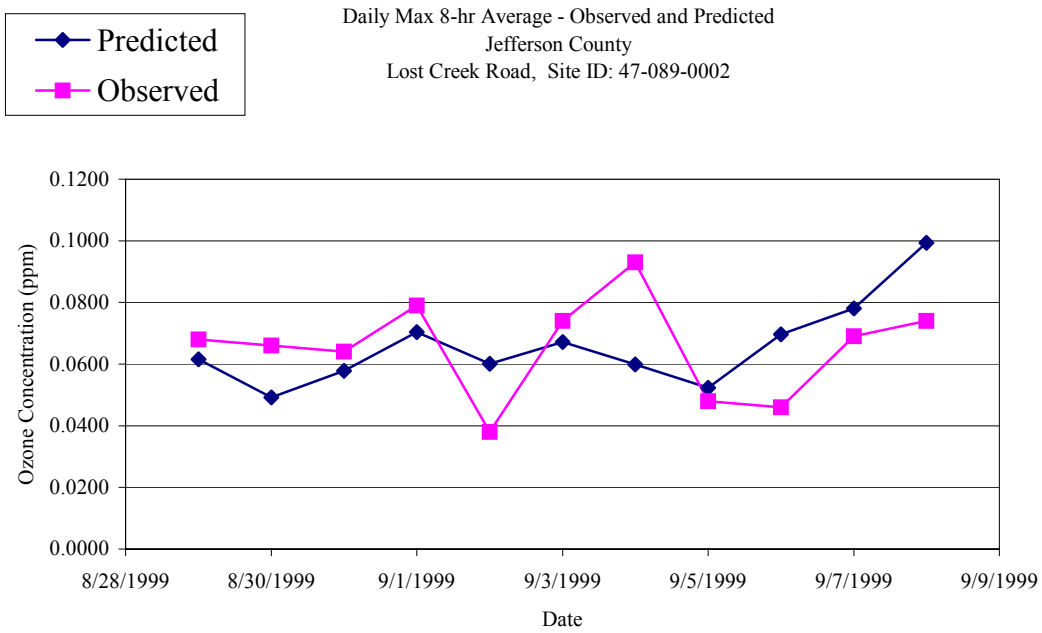


Figure 4.4 Jefferson County – Daily Max 8-hr Average – Observed vs. Predicted

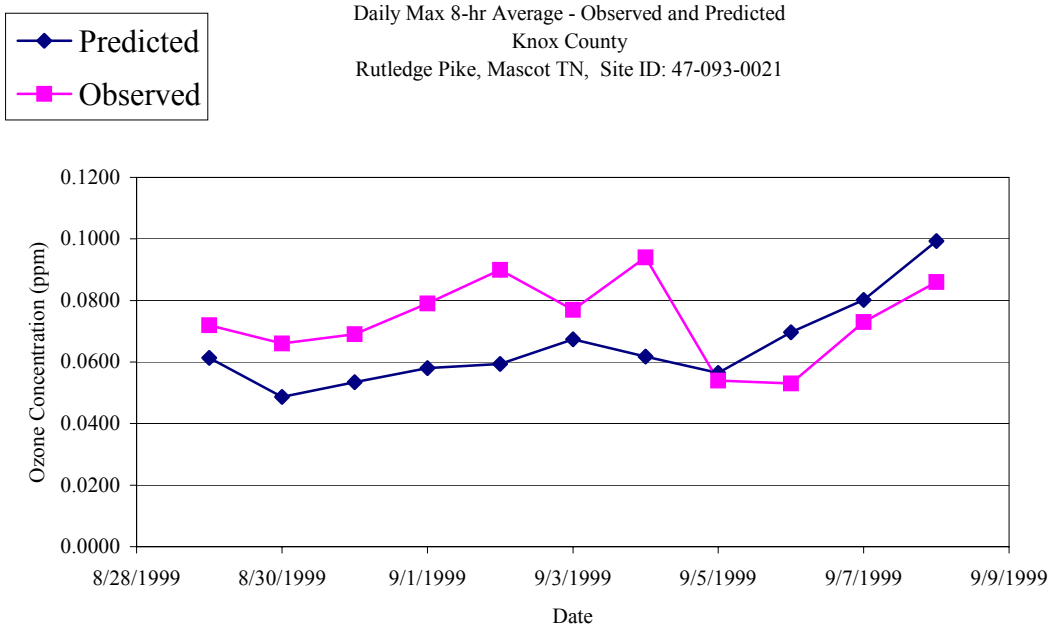


Figure 4.5 Knox County (Rutledge Pike) – Daily Max 8-hr Average – Observed vs. Predicted

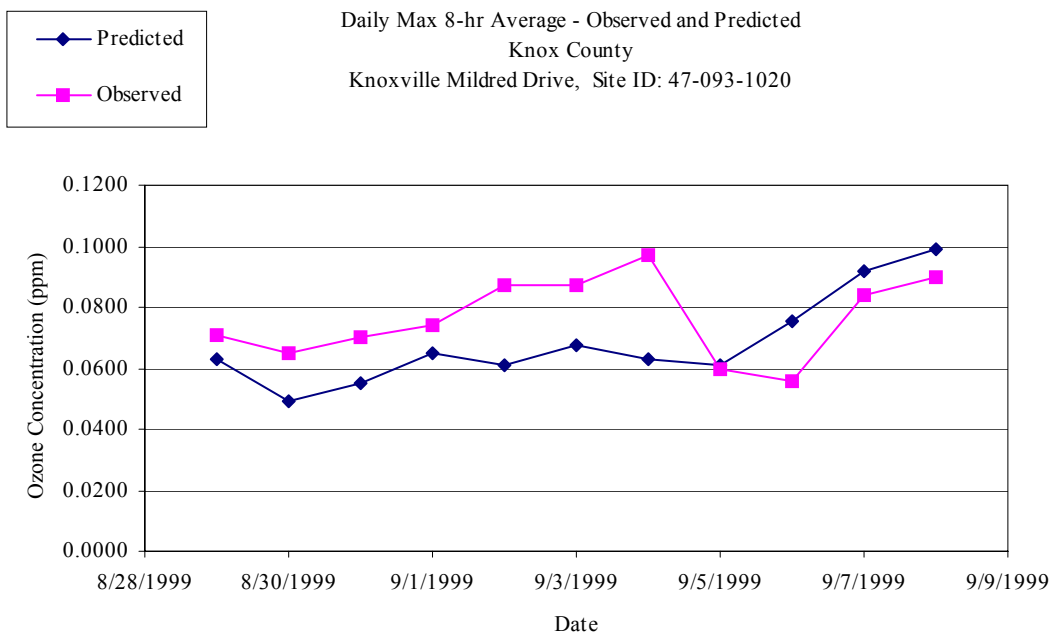


Figure 4.6 Knox County (Middle Drive) – Daily Max 8-hr Average – Observed vs. Predicted

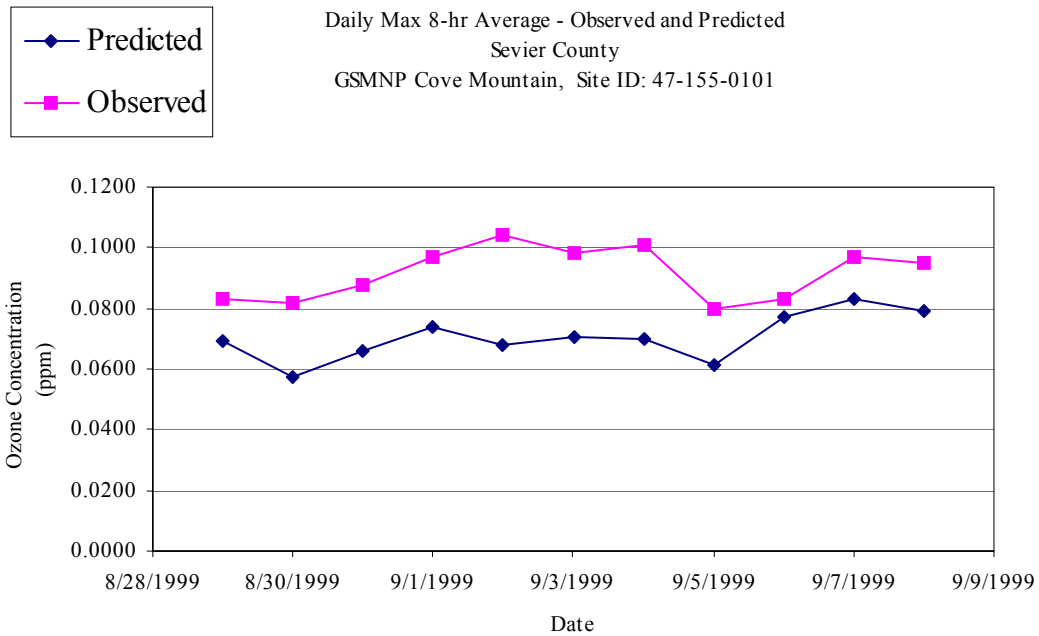


Figure 4.7 Sevier County (Cove Mountain) – Daily Max 8-hr Average – Observed vs. Predicted

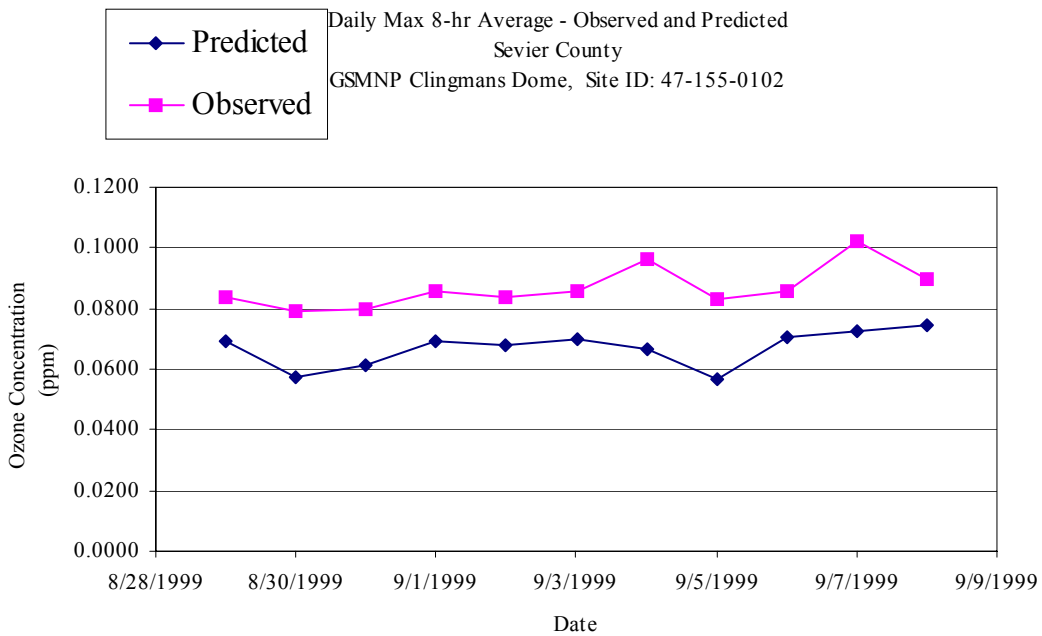


Figure 4.8 Sevier County (Clingmans Dome) – Daily Max 8-hr Average – Observed vs. Predicted

Table 4.1 Overall mean concentrations – Observed vs. Predicted

Station	Predicted Max 8-hr average nearby grids (ppm)	Observed Max 8-hr average at monitor site (ppm)	ppm difference	Average Bias, %
Anderson	0.069	0.073	-0.004	-5.5%
Blount Cades Cove	0.071	0.078	-0.007	-9.0%
Blount Look Rock	0.071	0.092	-0.021	-22.8%
Jefferson	0.066	0.065	0.001	1.5%
Knox-0021	0.065	0.074	-0.009	-12.2%
Knox-1020	0.068	0.076	-0.008	-10.5%
Sevier-0102	0.07	0.092	-0.022	-23.9%
Sevier-0101	0.066	0.087	-0.021	-24.1%

concentrations from 3 to 9 ppb (Refer Table 4.1 and Figure 4.9). The model under predicted the average 8-hour maximum ozone concentration 10% to 12% at Knox County and by 5.5% at Anderson County. Generally CMAQ performed better at Anderson, Jefferson and Knox County compared to the monitors in Blount and Sevier Counties. A high difference was found between the average observed and modeled concentrations for both stations in Sevier County: the maximum difference of 22 ppb was observed at Sevier County when the average concentration predicted by the model was only 70 ppb while the average observed concentration was 92 ppb. Similar differences were observed at Look Rock (Blount County). The above result suggests that the modeled performed poorer at rural elevated locations.

For the episode considered, Figure 4.9 shows the average bias of each monitor. Modeled values under predict the observed values by 9.0% on average for the station at Cades Cove, which is at 1850ft above mean sea level. For the rest of the elevated locations this includes monitors at Cove Mountain (Sevier County), Clingman’s Dome (Sevier) and Look Rock (Blount County), the model under predicted the observed values by nearly 20% on average though the predictions appeared to follow the same day-to-day trend as the observations. (Refer Figure 4.2, 4.3, 4.7 and 4.8).

4.1.2. Analyses Based on EPA’s Bias Limit

A Bias test was conducted to determine if model predictions were within a desired $\leq \pm 20\%$ performance goal. To pass the performance test, modeled daily max 8-hr ozone concentrations should be less than $\leq \pm 20\%$ of observed values at the monitors. To test the model performance, the bias was calculated for all locations. Biases were calculated for each day at all locations. The results are shown in Figures from 4.10 – 4.17. These graphs illustrate that for most of the days in the episode, base case predictions fell within the

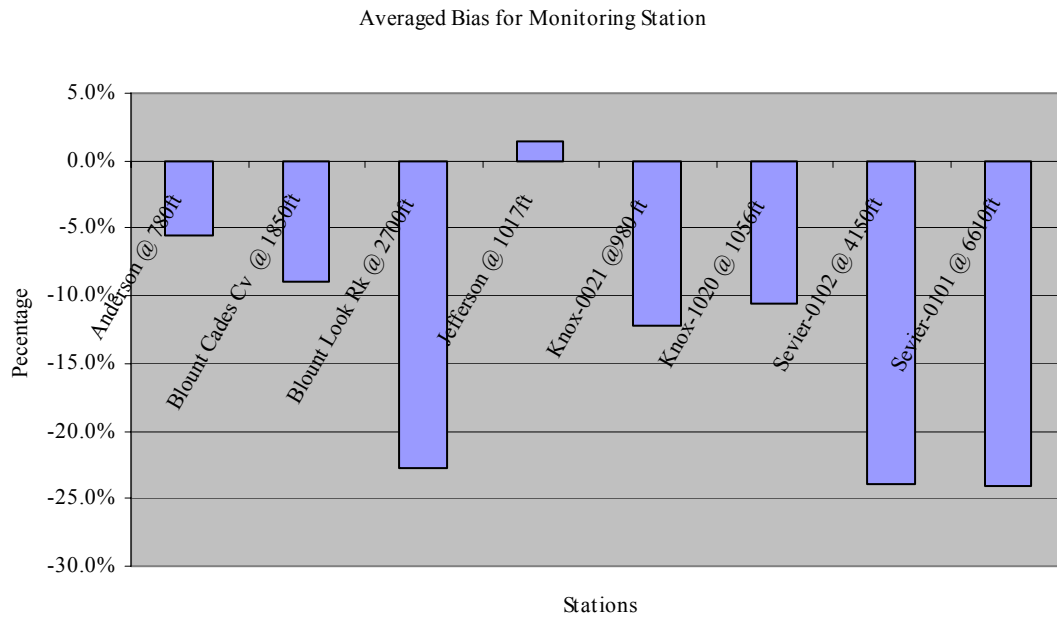


Figure 4.9 Average Biases for Predicted Values at Monitors

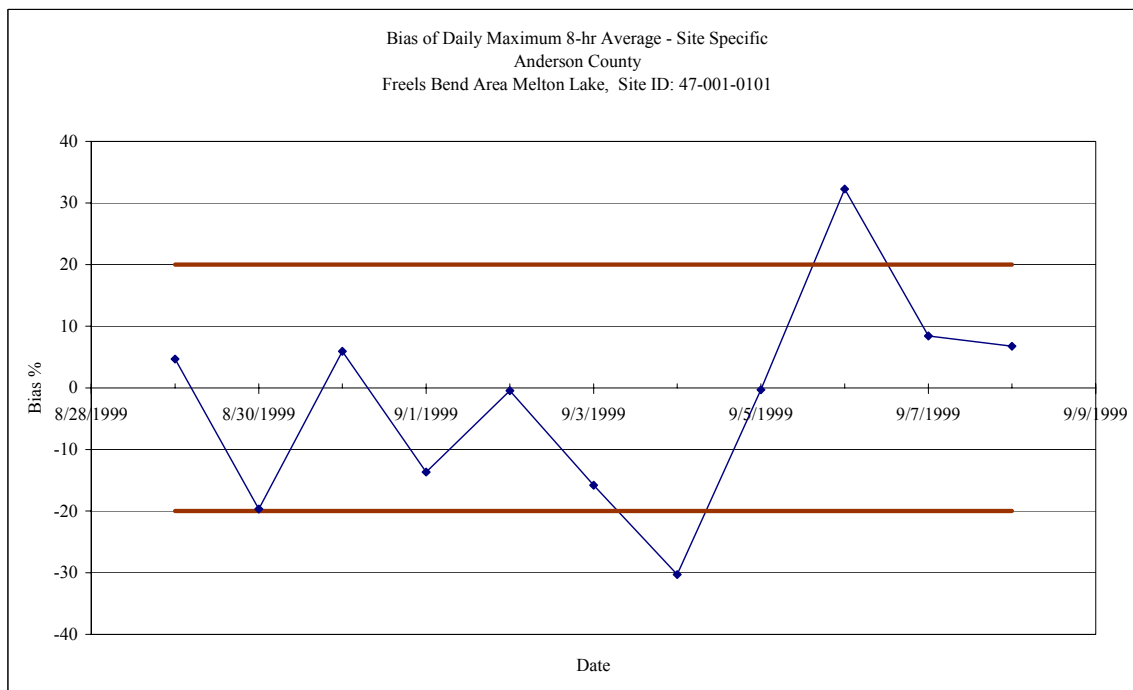


Figure 4.10 Anderson County – Bias of Daily Max 8-hr Average

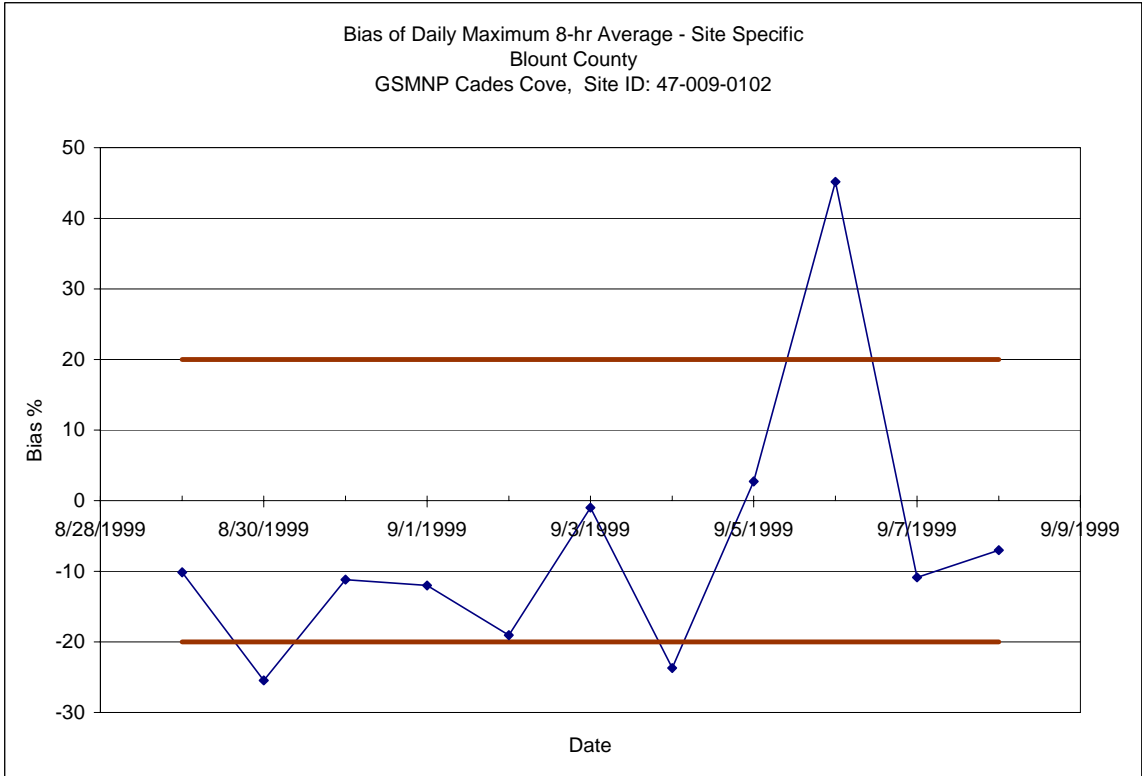


Figure 4.11 Blount County (Cades Cove) – Bias of Daily Max 8-hr Average

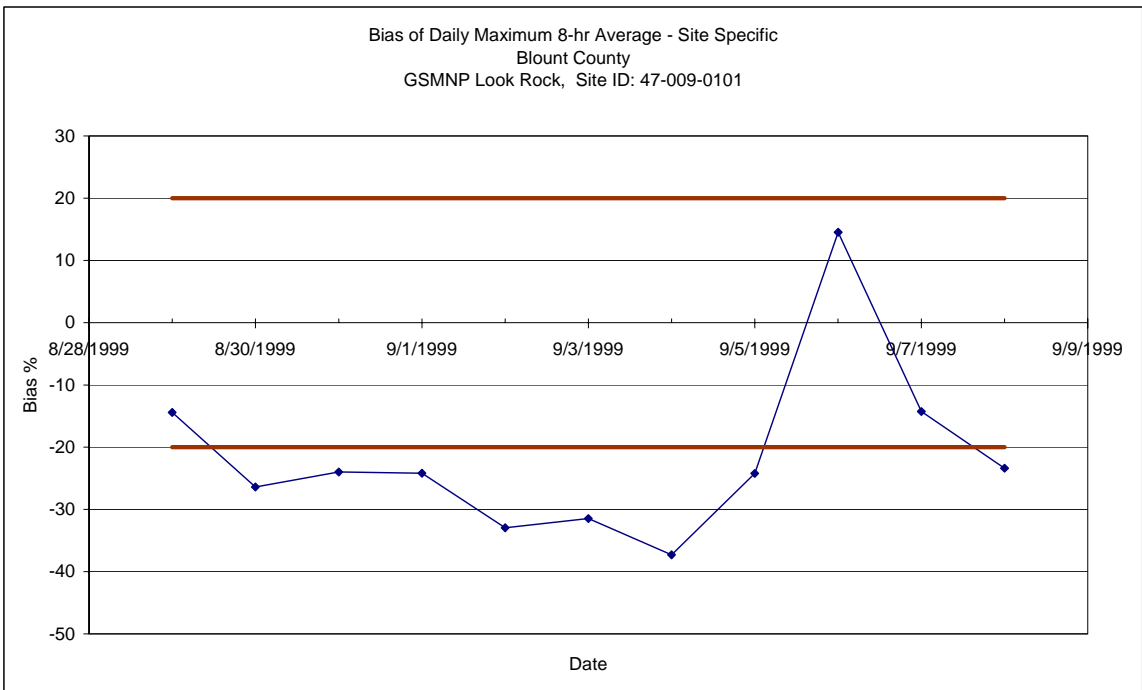


Figure 4.12 Blount County (Look Rock) – Bias of Daily Max 8-hr Average

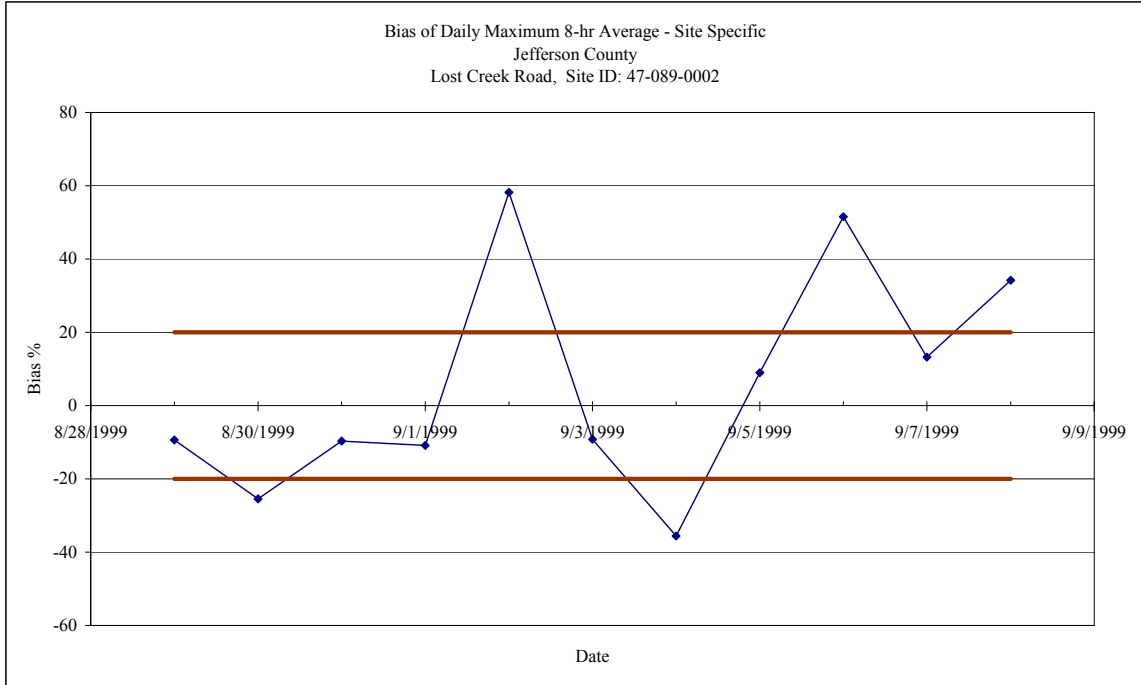


Figure 4.13 Jefferson County – Bias of Daily Max 8-hr Average

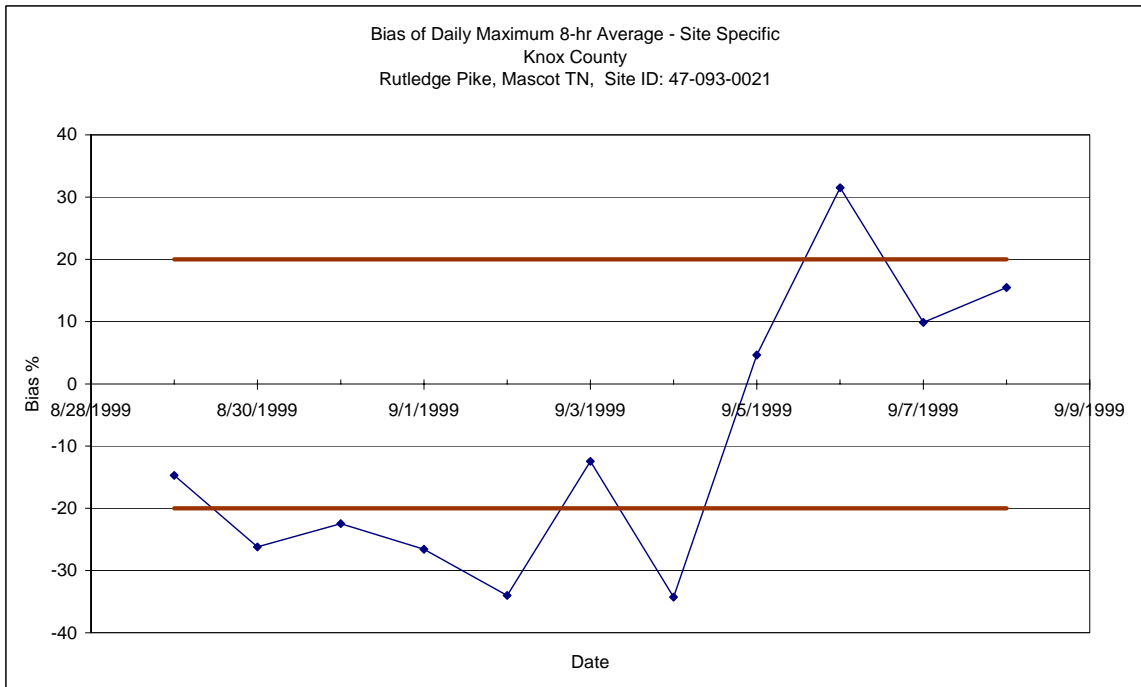


Figure 4.14 Knox County (Rutledge Pike) – Bias of Daily Max 8-hr Average

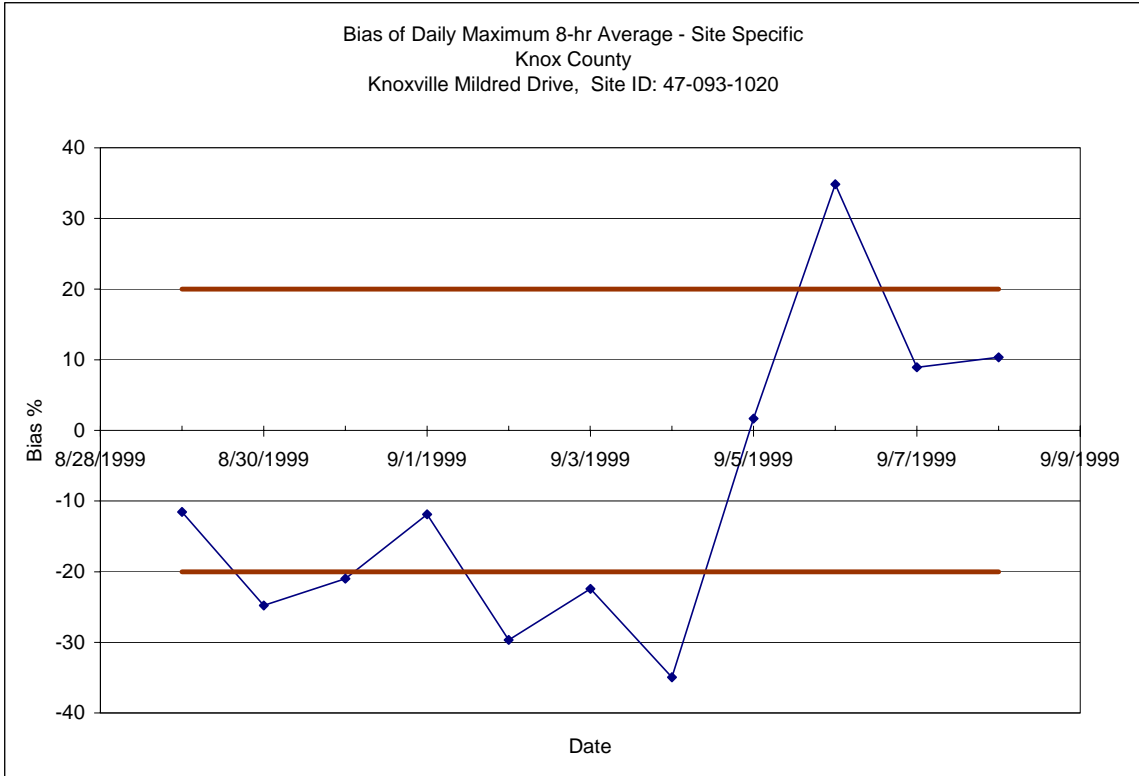


Figure 4.15 Knox County (Mildred Drive) – Bias of Daily Max 8-hr Average

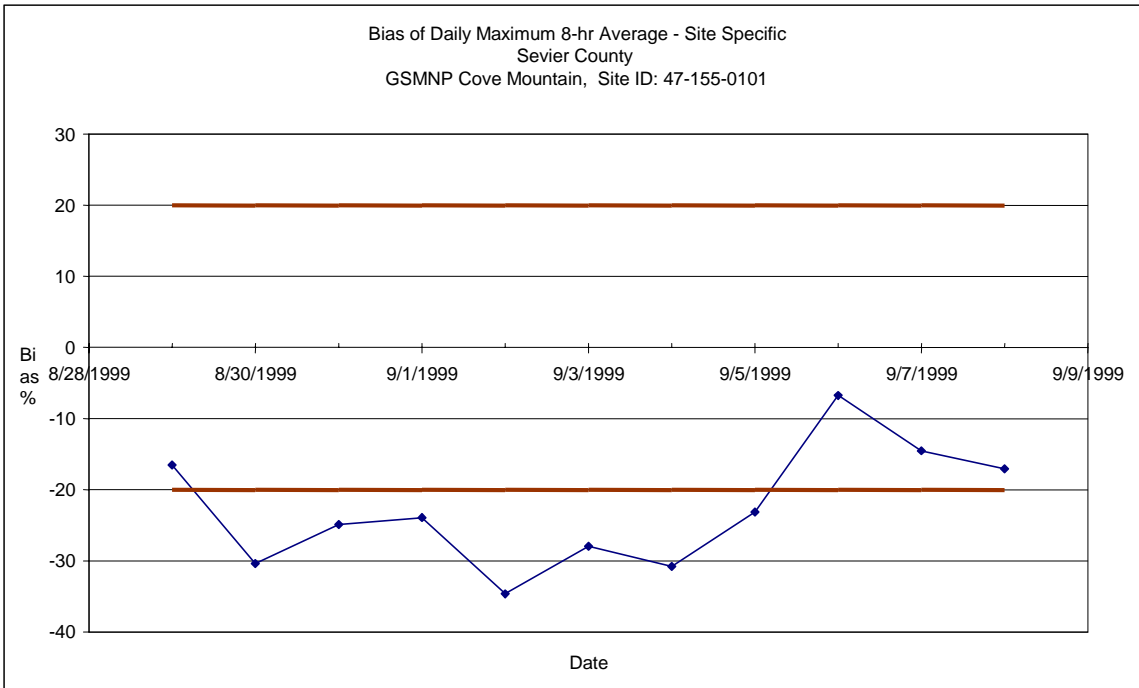


Figure 4.16 Sevier County (Cove Mountain) – Bias of Daily Max 8-hr Average

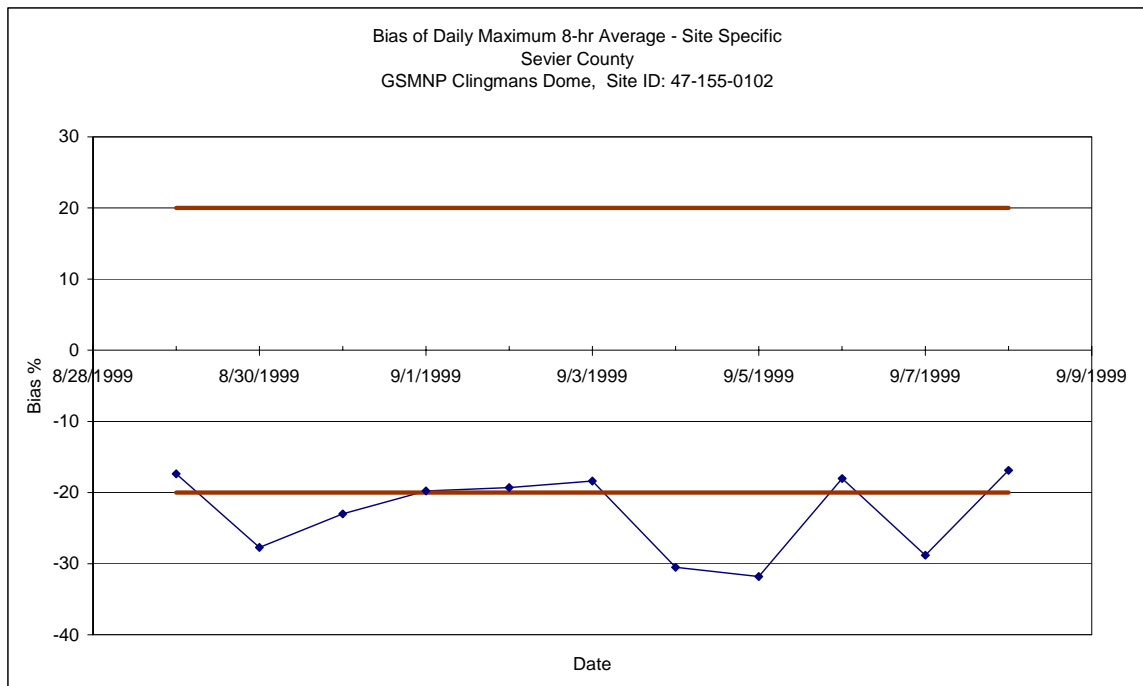


Figure 4.17 Sevier County (Clingmans Dome) – Bias of Daily Max 8-hr Average

EPA’s prescribed bias limit of $<\pm 20\%$ for the monitors at low elevation sites. Most of the days the bias falls out of the bias limit in Blount and Sevier County and again showing that the model under predicts at high elevation ozone monitoring sites.

4.2. Results and Analyses Based on Various Emissions Reduction Scenarios

Based on each scenario, emissions from point and mobile sources were reduced for the complete modeling domain. In each scenario mentioned below, the inventory was modified to reflect the corresponding changes. Biogenic source emissions and area source emissions were held fixed for all modeling runs while point and mobile emissions were changed to reflect the changes that could possibly arise for various emission reduction scenarios. The impacts of reductions in ozone precursor’s emissions throughout the domain were investigated. The results and the summary of each run listed below are given in detail in the following sections.

- Run1: Base case using average emissions in 11 layers (Base case)
- Run2: Both NO_x and VOC emissions from mobile sources were reduced by 100%
- Run3: Both NO_x and VOC emissions from point sources were reduced by 100%
- Run4: NO_x emissions from mobile sources were reduced by 15%
- Run5: NO_x emissions from mobile sources were reduced by 30%
- Run6: NO_x emissions from mobile sources were reduced by 100%

- Run7: NO_x emissions from point sources were reduced by 15%
- Run8: NO_x emissions from point sources were reduced by 30%
- Run9: VOC emissions from mobile sources were reduced by 100%
- Run10: Base case using CEMS data in 11 layers
- Run11: Base case using average emissions in a single layer

The modeled concentrations predicted at the monitors for the cases of 100% reduction in point source emission and 100% reduction in mobile source emissions were plotted and compared to the base case in Figures 4.18 – 4.25. The results for East Tennessee counties for different scenarios are summarized in Tables 4.2 and 4.3. These tables show that the model applied to East Tennessee was more sensitive to reductions in mobile source emissions versus point source emissions. On average 100% reduction in mobile and point source emissions produced about 11.5ppb and 8.4ppb reduction in ozone concentrations respectively.

For Knox-0021, a reduction by 100% in point sources emissions caused almost the same the reduction in ozone as a 100% reduction in mobile source emissions. For Knox County the average percent reductions in ozone concentration for a 100% reduction in point source emissions (11.19% and 10.4%) were closer to the 100% reduction in mobile source emissions (9.49% and 10.62%). This implies that point source emission reductions were as effective as mobile source emission reductions in Knox County.

In the following part of the sensitive analysis, 100% reductions in mobile NO_x emission versus 100% reduction in mobile VOC emission were also analyzed. The purpose of this analysis was to determine whether ozone formation in the region under study is “NO_x or VOC Limited”. If ozone formation is limited by NO_x emissions, reducing the emissions of VOCs may have little or no effect in reducing the level of ozone. A 100% reduction in NO_x emissions from mobile sources caused a significant reduction in ozone, and this reduction in ozone was significantly higher than for the same percent reduction in VOC emissions from mobile sources. But based on concentrations predicted at the monitors for the cases of 100% reduction in mobile NO_x emissions and 100% reduction in mobile VOCs emissions, almost the same amount of reduction in ozone concentrations were observed (See Table 4.2 and 4.3). For the per ton of reduction in each of ozone precursors, NO_x yielded 0.013 ppb and VOCs yielded 0.011 ppb of ozone reduction (also refer figure 4.26 – 4.33). Apparently the region under study is both NO_x and VOCs sensitive. Therefore both mobile source NO_x and VOCs emission reductions can be useful in reducing ozone concentrations. Still it takes a 100% reduction in mobile VOC emissions to yield the same reduction in ozone concentration as a 30% reduction in mobile NO_x Emissions.

Table 4.2 Summary of ozone reduction (in ppb) from base for various scenarios

Location	0% reduction (Base case)	100% reduction in Mobile NO _x and VOCs emission	100% reduction in Mobile NO _x emissions	30% reduction in Mobile NO _x emissions	15% reduction in Mobile NO _x emissions	100% reduction in Mobile VOCs emissions	100% reduction in Point NO _x and VOCs emissions	30% reduction in Point NO _x emissions	15% reduction in Point NO _x emissions
Anderson	0	12.2	11.2	4.3	3.5	4.3	9.6	1.7	1.2
Blount Cades Cove	0	14.2	13.5	5.8	4.9	6.0	9.4	2.9	2.3
Blount Look Rook	0	13.2	12.2	5.4	4.6	5.8	8.7	2.5	2.0
Jefferson	0	9.4	8.2	3.0	2.4	3.4	7.6	2.3	1.8
Knox -0021	0	7.6	6.2	2.7	2.2	3.1	7.3	2.2	1.6
Knox -1020	0	8.7	7.3	2.9	2.3	3.7	7.1	2.2	1.7
Sevier-0101	0	13.9	13.3	5.9	4.8	5.6	9.0	2.8	2.1
Sevier- 0102	0	12.7	12.2	5.7	4.7	5.1	8.5	2.3	1.6
Average	0	11.5	10.5	4.5	3.7	4.6	8.4	2.4	1.8
Tons/day in Tennessee (36km domain)			792.12			427.5			

Reduction of 792.12 tons of mobile NO_x/day yields 10.5 ppb of ozone reduction
 Reduction of 1 ton of mobile NO_x/day yields 0.013 ppb of ozone reduction
 Reduction of 427.5 tons of mobile VOC/day yields 4.6 ppb of ozone reduction
 Reduction of 1 ton of mobile VOC/day yields 0.011 ppb of ozone reduction

Table 4.3 Summary of percent reduction in ozone concentration from base case for various scenarios

Location	100% reduction in Mobile NOx and VOC emission	100% reduction in Mobile NOx emissions	30% reduction in Mobile NOx emissions	15% reduction in Mobile NOx emissions	100% reduction in Mobile VOC emissions	100% reduction in Point NOx and VOC emissions	30% reduction in Point NOx emissions	15% reduction in Point NOx emissions
Anderson	17.43%	16.06%	6.16%	4.95%	6.21%	13.71%	2.47%	1.74%
Blount Cades Cove	19.81%	18.82%	8.14%	6.80%	8.33%	13.17%	4.07%	3.15%
Blount Look Rook	18.48%	17.14%	7.60%	6.42%	8.07%	12.15%	3.48%	2.75%
Jefferson	14.29%	12.50%	4.58%	3.62%	5.17%	11.52%	3.51%	2.69%
Knox - 0021	11.66%	9.49%	4.20%	3.42%	4.81%	11.19%	3.38%	2.50%
Knox - 1020	12.75%	10.62%	4.19%	3.34%	5.47%	10.40%	3.17%	2.42%
Sevier-0101	19.68%	18.82%	8.31%	6.86%	8.01%	12.83%	3.96%	2.95%
Sevier-0102	18.99%	18.28%	8.54%	6.97%	7.67%	12.66%	3.40%	2.42%

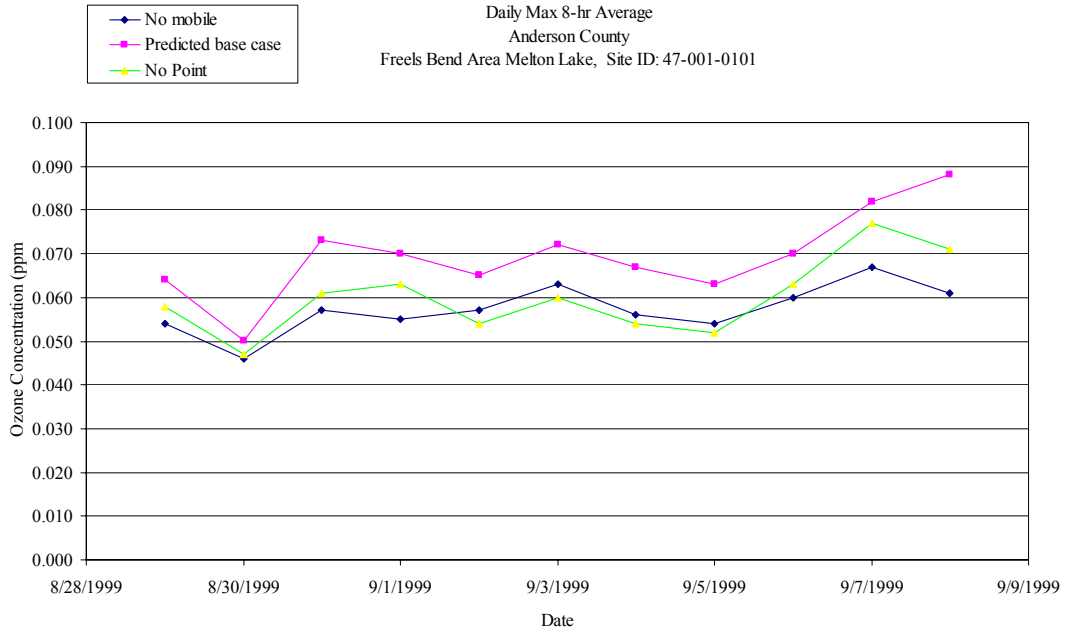


Figure 4.18 Anderson County – Sensitivity analysis – No mobile vs. Predicted base case vs. No point

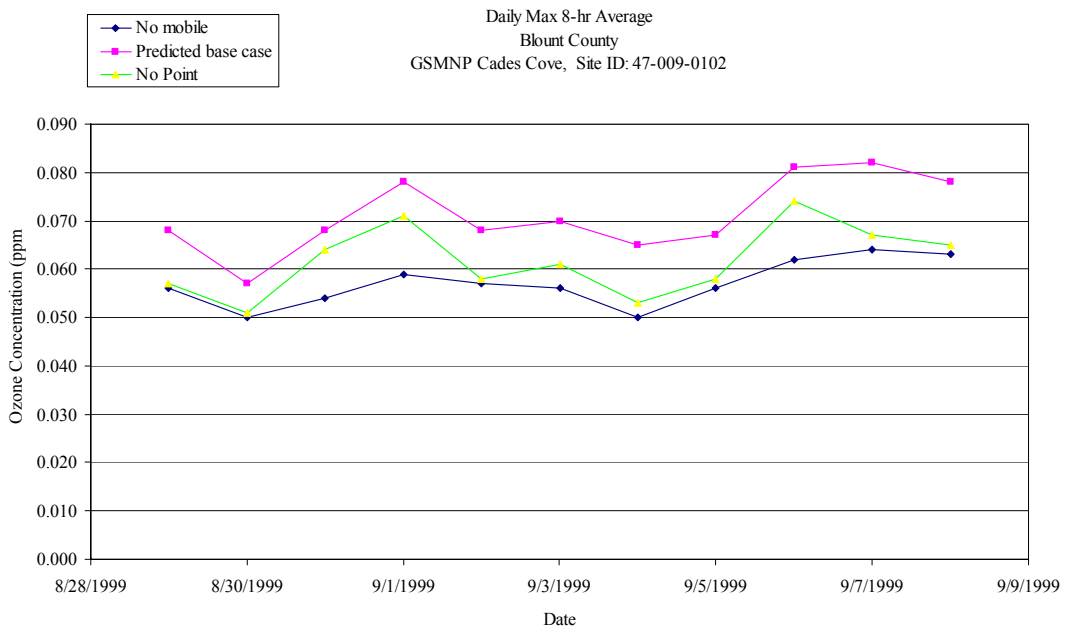


Figure 4.19 Blount County (Cades Cove) – Sensitivity analysis – No mobile vs. Predicted base case vs. No point

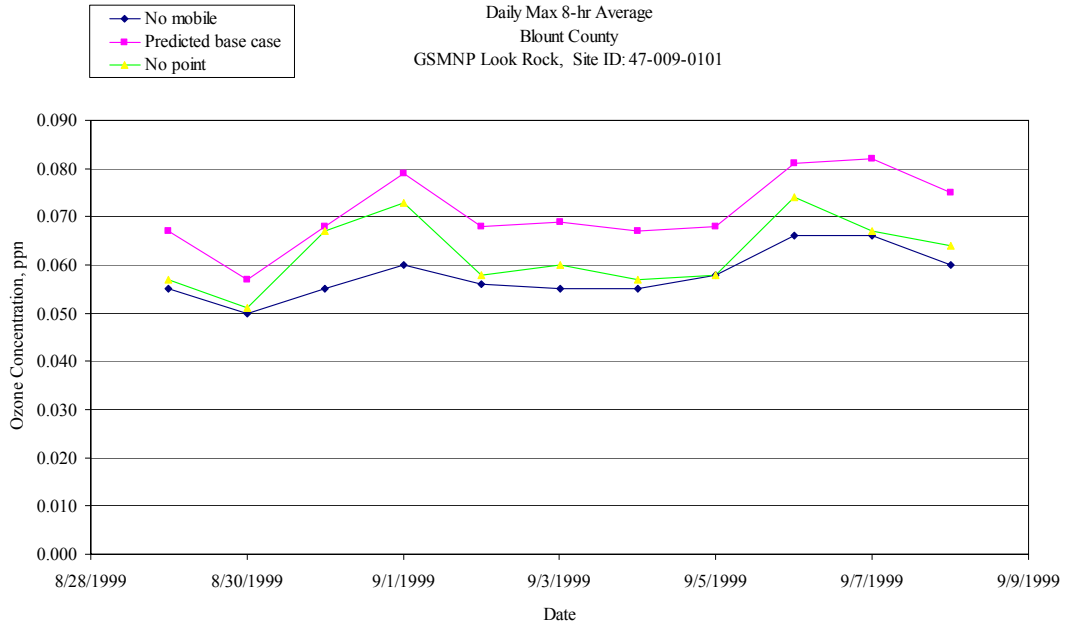


Figure 4.20 Blount County (Look Rock) – Sensitivity analysis – No mobile vs. Predicted base case vs. No point

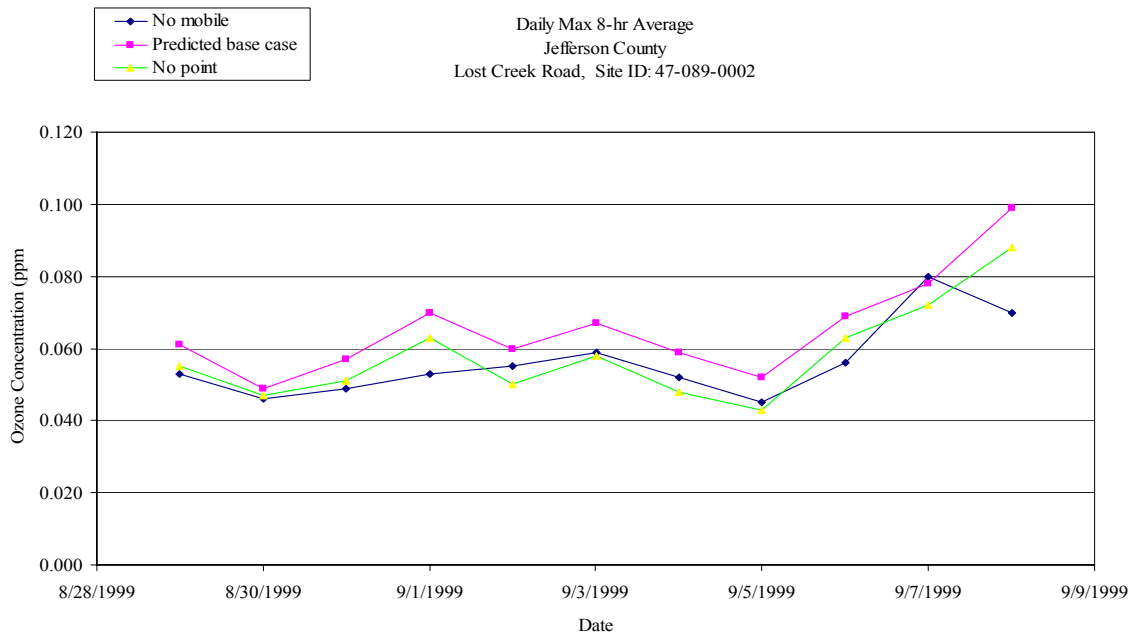


Figure 4.21 Jefferson County – Sensitivity analysis – No mobile vs. Predicted base case vs. No point

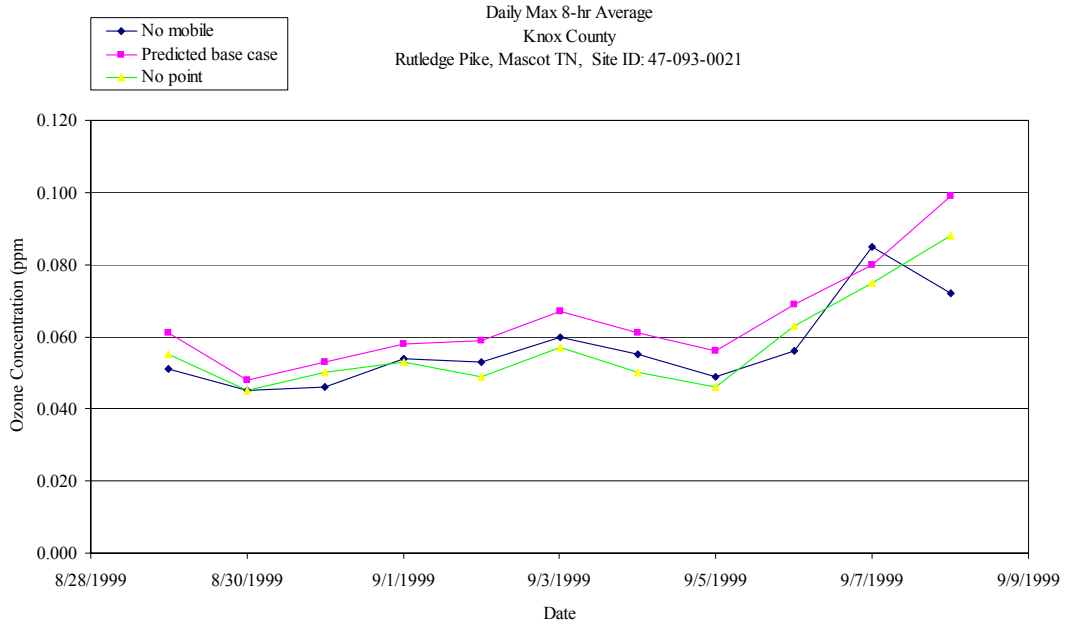


Figure 4.22 Knox County (Rutledge Pike) – Sensitivity analysis – No mobile vs. Predicted base case vs. No point

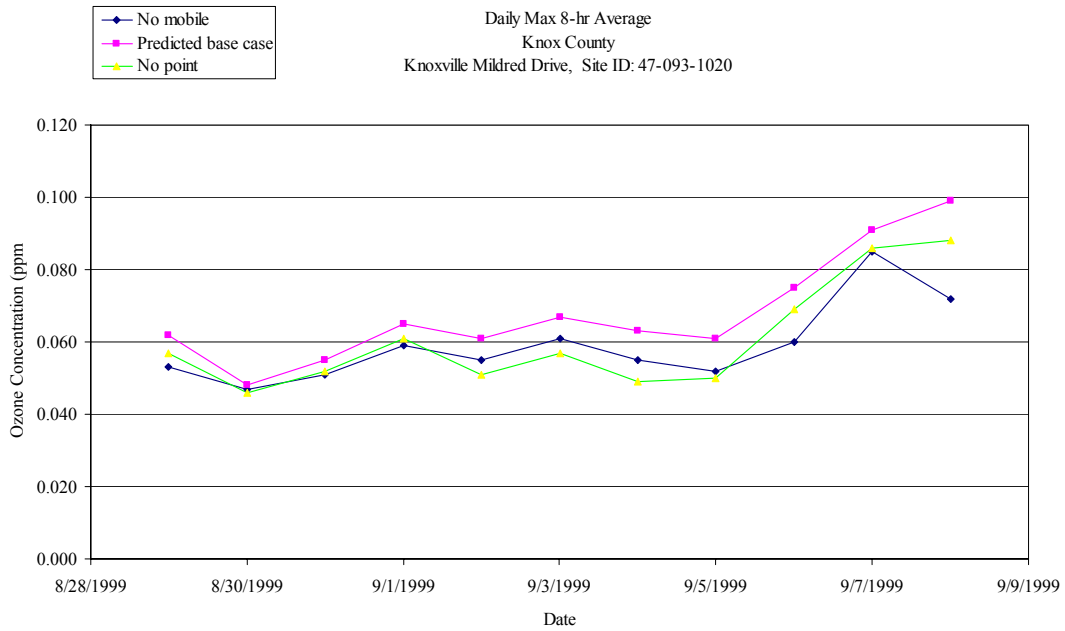


Figure 4.23 Knox County (Mildred Drive) – Sensitivity analysis – No mobile vs. Predicted base case vs. No point

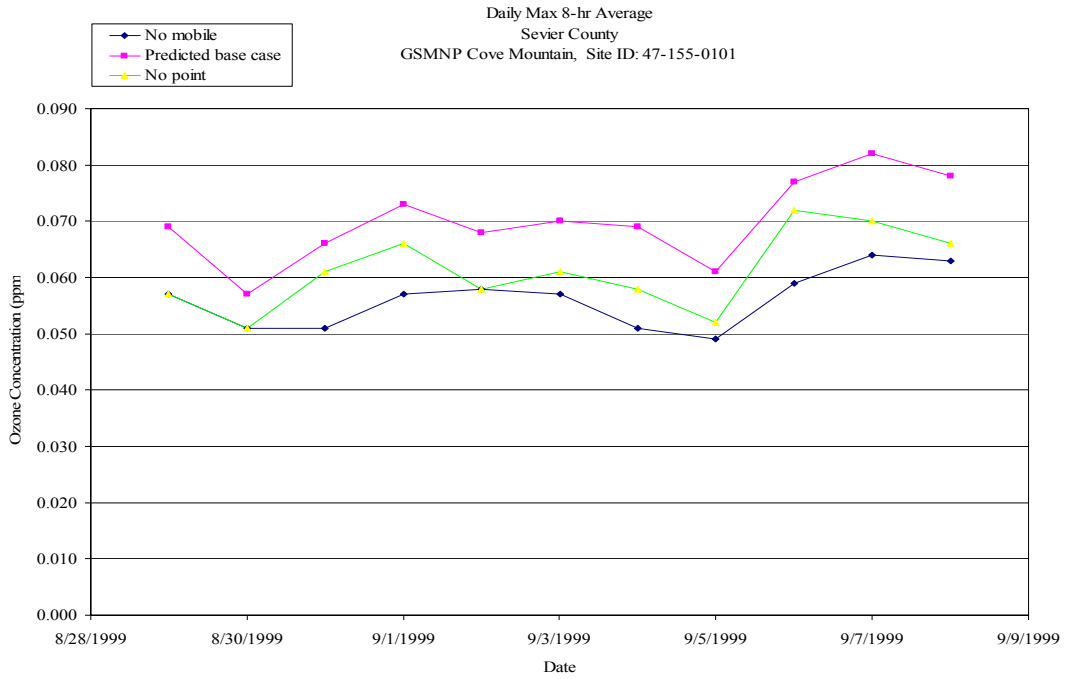


Figure 4.24 Sevier County (Cove Mountain) – Sensitivity analysis – No mobile vs. Predicted base case vs. No point

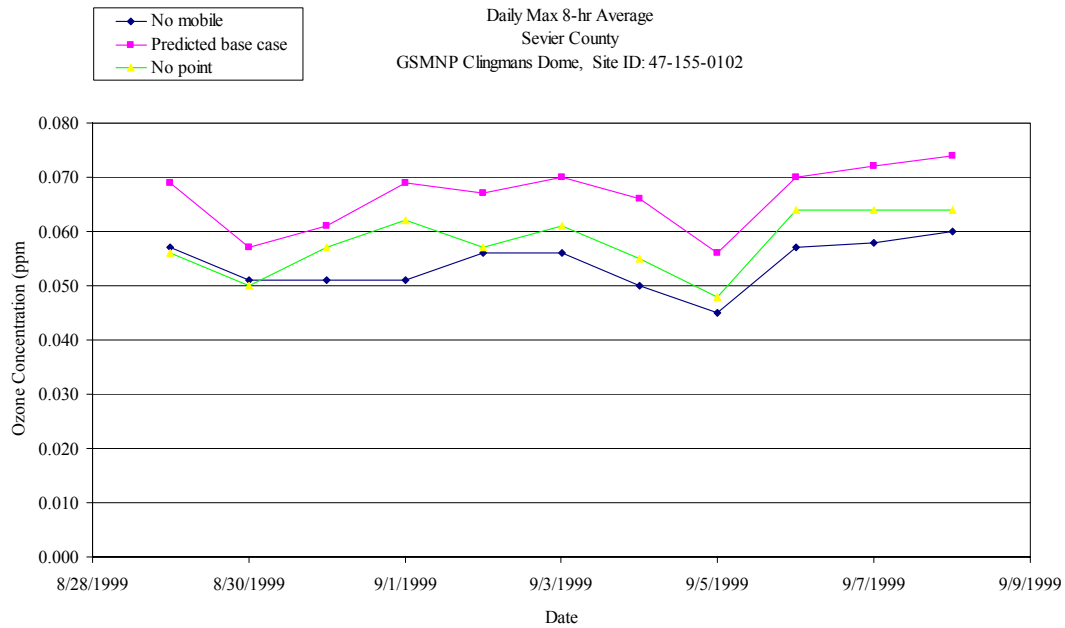


Figure 4.25 Sevier County (Clingmans Dome) – Sensitivity analysis – No mobile vs. Predicted base case vs. No point

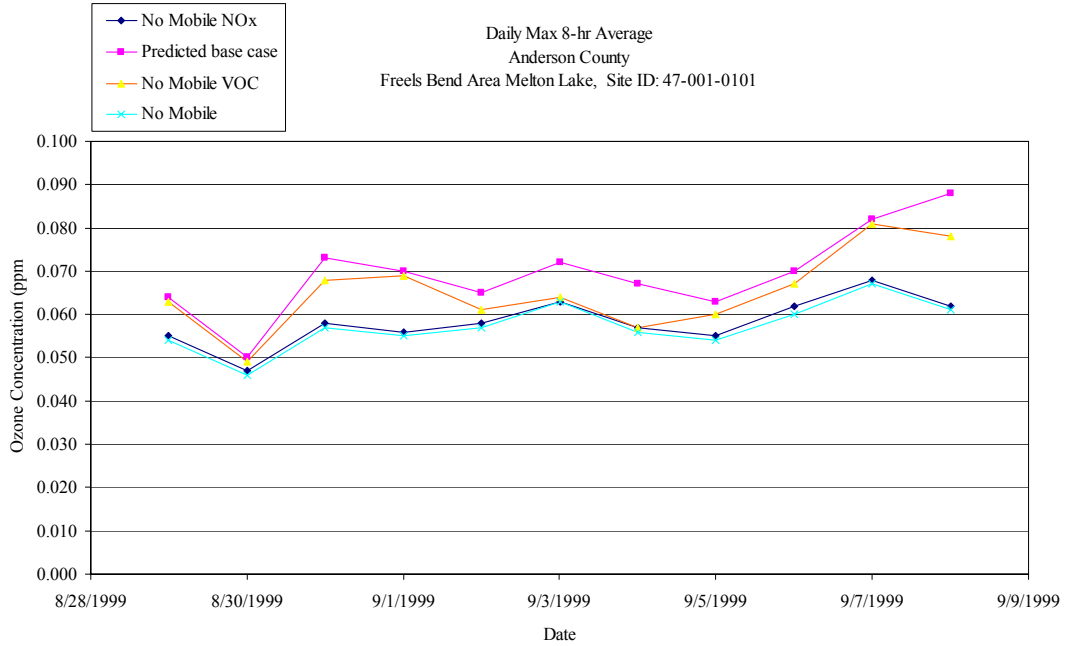


Figure 4.26 Anderson County – Sensitivity analysis – No mobile vs. Predicted base case vs. No Mobile NOx vs. No Mobile VOC

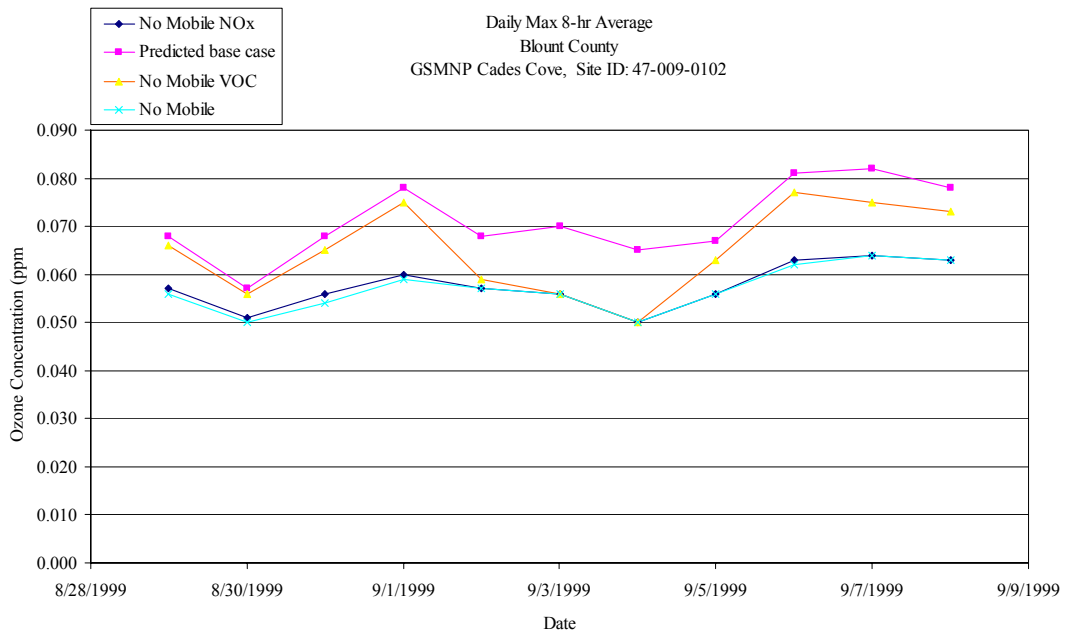


Figure 4.27 Blount County (Cades Cove) – Sensitivity analysis – No mobile vs. Predicted base case vs. No Mobile NOx vs. No Mobile VOC

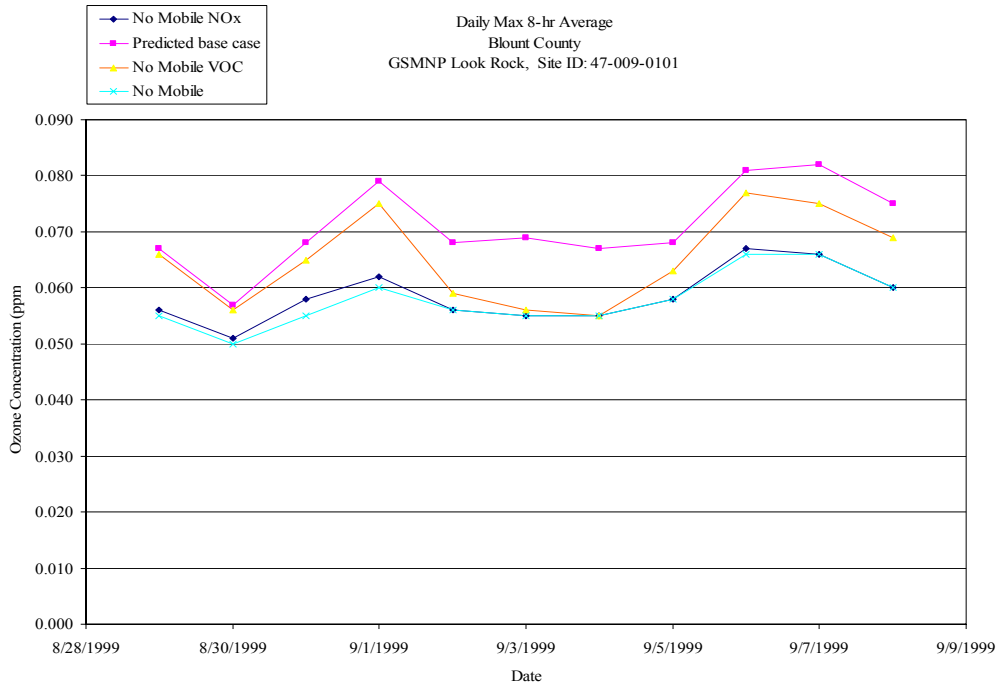


Figure 4.28 Blount County (Look Rock) – Sensitivity analysis – No mobile vs. Predicted base case vs. No Mobile NOx vs. No Mobile VOC

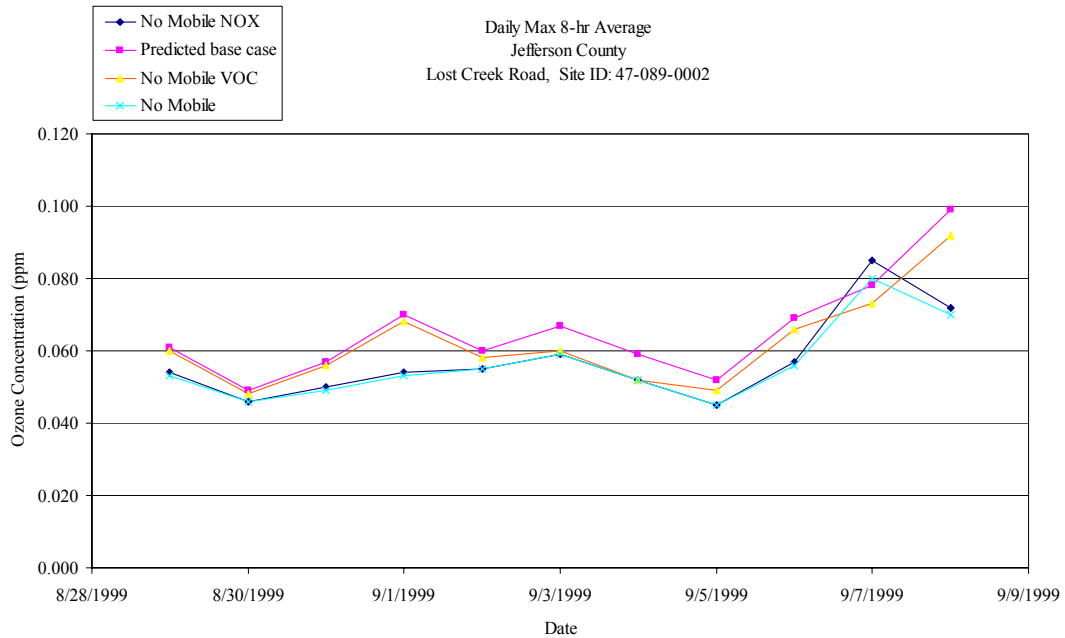


Figure 4.29 Jefferson County – Sensitivity analysis – No mobile vs. Predicted base case vs. No Mobile NOx vs. No Mobile VOC

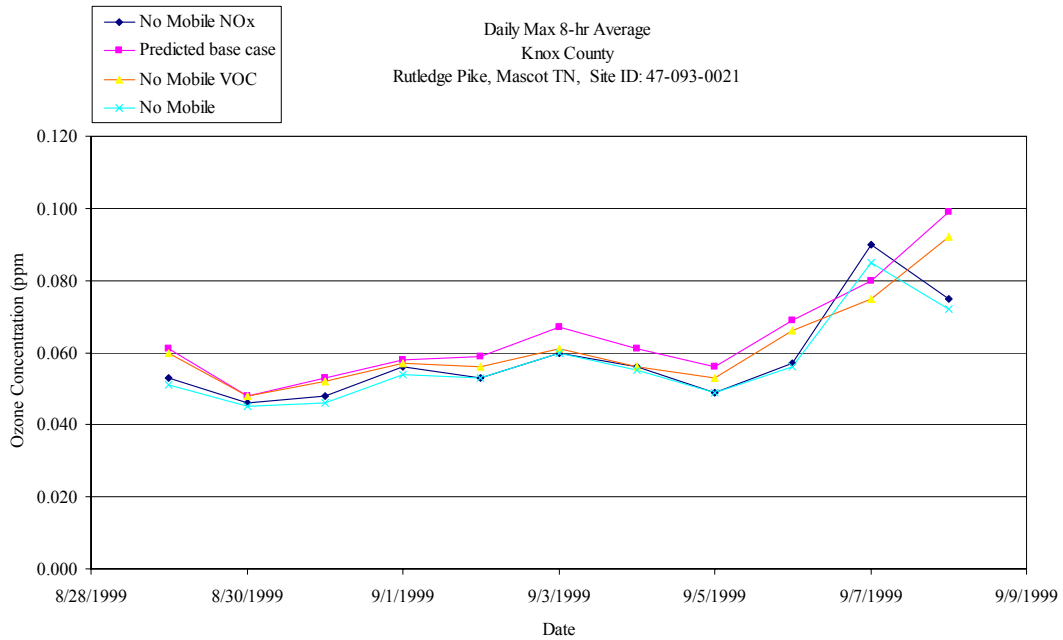


Figure 4.30 Knox County (Rutledge Pike) – Sensitivity analysis – No mobile vs. Predicted base case vs. No Mobile NOx vs. No Mobile VOC

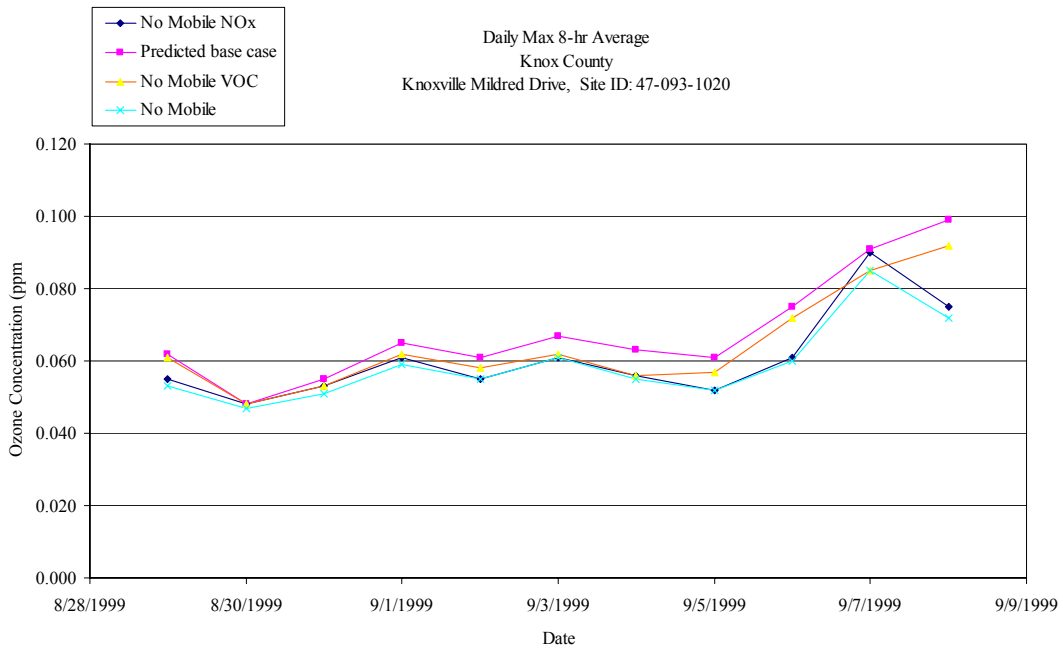


Figure 4.31 Knox County (Mildred Drive) – Sensitivity analysis – No mobile vs. Predicted base case vs. No Mobile NOx vs. No Mobile VOC

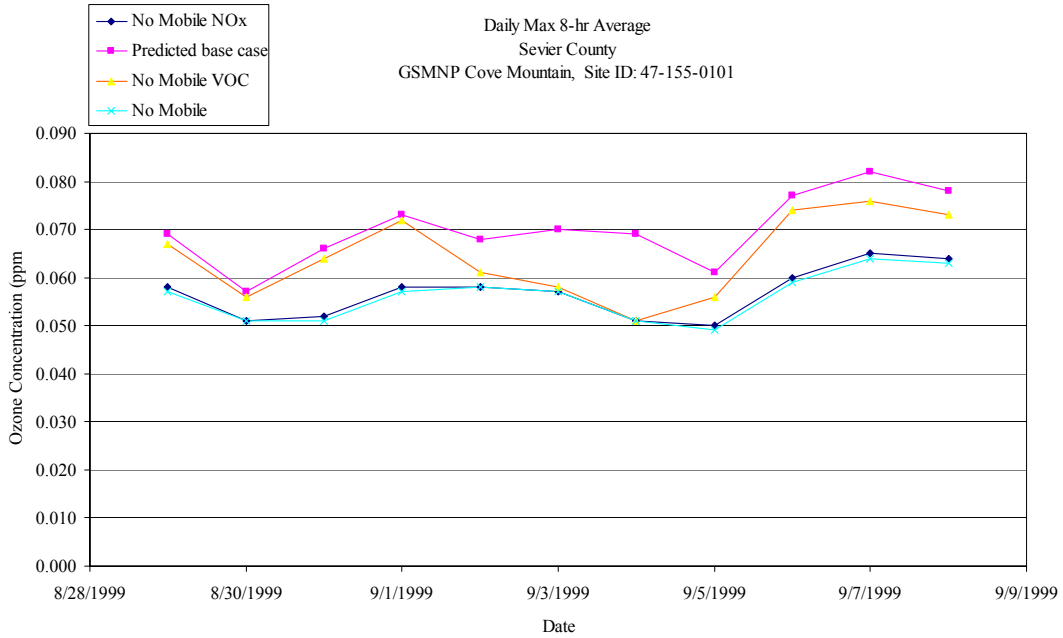


Figure 4.32 Sevier County (Clingmans Dome) – Sensitivity analysis – No mobile vs. Predicted base case vs. No Mobile NOx vs. No Mobile VOC

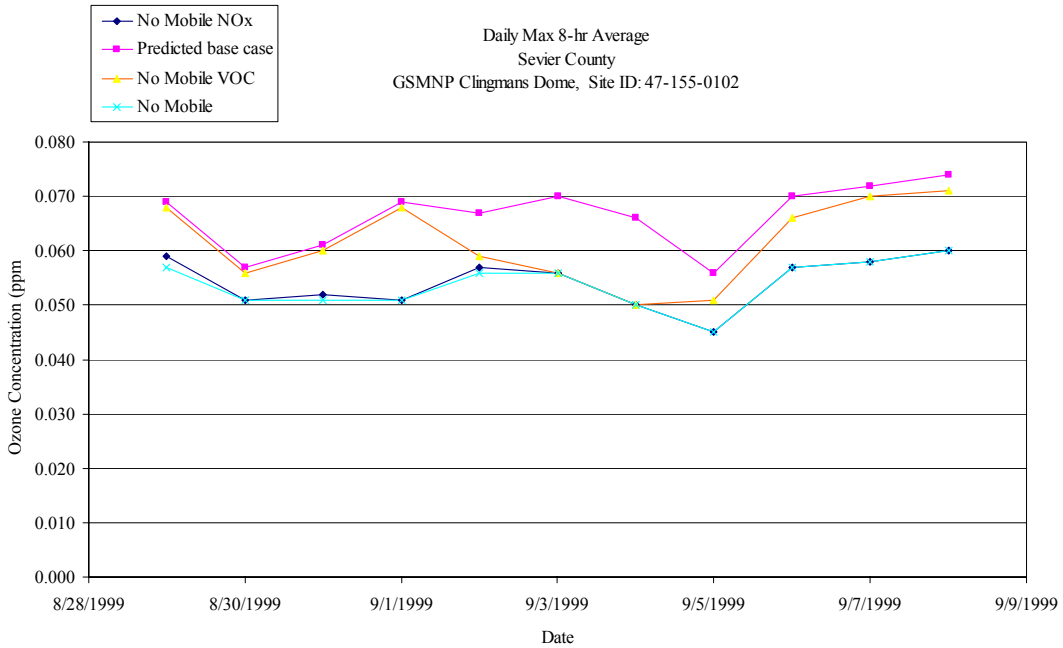


Figure 4.33 Sevier County (Cove Mountain) – Sensitivity analysis – No mobile vs. Predicted base case vs. No Mobile NOx vs. No Mobile VOC

For the rest of the counties (especially rural, high elevation sites), mobile source NO_x emission reductions were more effective than point source emission reductions in lowering ozone levels. As shown in the summary table, a 100% reduction in mobile source NO_x emissions yielded an 18.82% reduction in ozone at Blount and Sevier County sites, while a 100% reduction in point source NO_x yielded near to 13% reduction in ozone. Elevated sites showed a greater reduction in ozone concentrations than low elevation sites. In general, the elevated sites were found to be more sensitive to control strategies than low elevation sites.

Result and analysis for various percent reductions in NO_x Emission from Mobile and Point Sources: To investigate the sensitivity of the model to changes in NO_x emissions, NO_x was reduced by 30% and 15% from mobile and point sources. The results are shown in the Figure 4.34 – 4.49 for each monitor location. The summary table also shows that for Jefferson and Knox County, a 15% reduction in mobile NO_x emissions yields almost the same reduction in ozone as a 30% reduction in mobile NO_x. This suggests that the model is less sensitive to minor reductions in mobile source NO_x emissions. For rest of the counties (elevated/rural sites), the model is more sensitive to minor reduction in mobile source NO_x emissions.

For the episode considered, Figures 4.50 – 4.57 show the overall response of ozone reduction for variable NO_x emission reductions from mobile and point sources. The reduction in ozone with reduction in mobile source NO_x emissions was not necessarily linear. For most sites, a 30 % reduction in mobile NO_x emissions gave a relatively small additional reduction in ozone compared to a 15% reduction in NO_x emissions. A 100% reduction in NO_x emissions always produced the greatest reduction in ozone. See Figures 4.50 – 4.57.

4.3 NEI versus CEMS

Two modeling runs were performed to check the sensitivity of the modeling results for differences in using average emission inputs from large point sources versus using actual emissions taken from the continuous Emissions Monitoring System (CEMS) data. Replacing the NEI point source average emissions with real time data (CEMS data) in SMOKE can be done by selecting the appropriate option. Replacement of CEMS data is controlled based on the SCC (Source Classification Code) and locations of the sources.

To carry out the sensitive analysis of CMAQ to CEMS data versus NEI average emissions, NO_x emission rates were input using CEMS data for one run, and using NEI average emissions in another run. The output results were compared. NO_x emissions in both inventories were speciated to 90% as NO and 10% as NO₂ by SMOKE. The graphs in Figures 4.58 –4.71 show the hourly NO emissions rates from CEMS data compared to NEI average emissions of some major point sources in Tennessee. The 6th of September was Labor Day in 1999 and taken into account as a holiday in the average emissions scenario. Therefore the hourly emission rates of NO were similar to that of Sunday

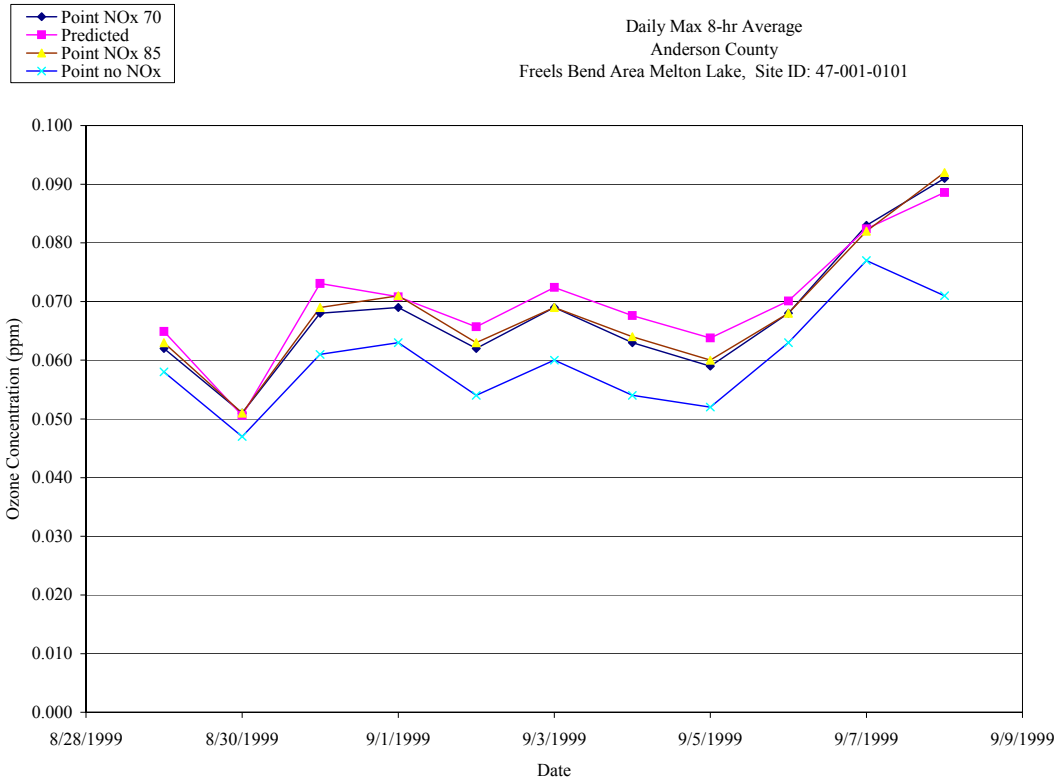


Figure 4.34 Anderson County – Sensitivity analysis – Point with variable NOx

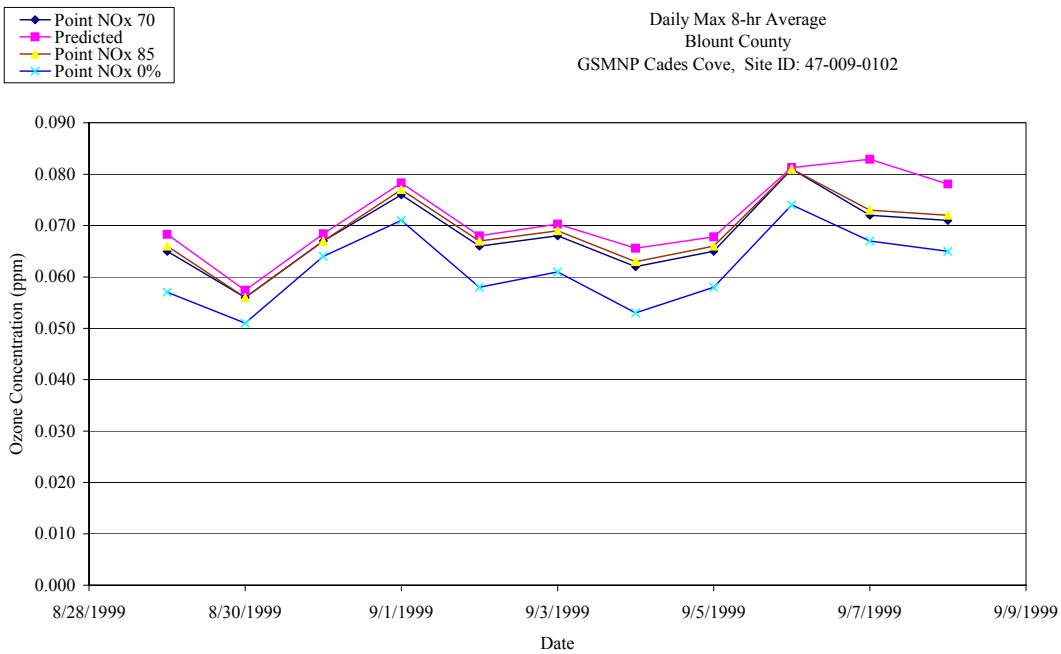


Figure 4.35 Blount County (Cades Cove) – Sensitivity analysis – Point with variable NOx

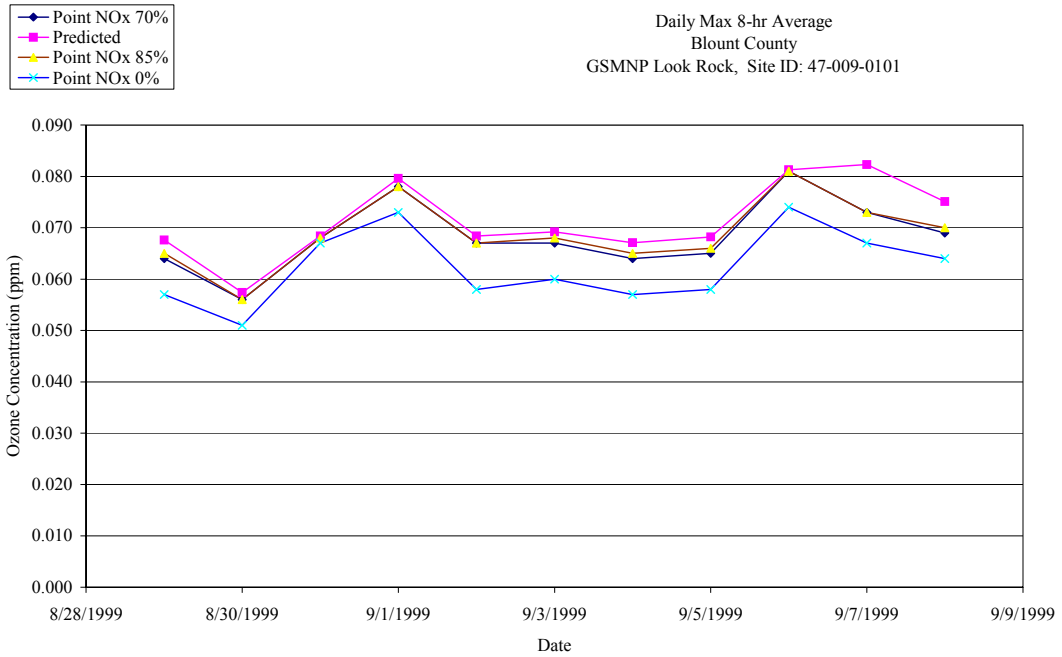


Figure 4.36 Blount County (Look Rock) – Sensitivity analysis – Point with variable NOx

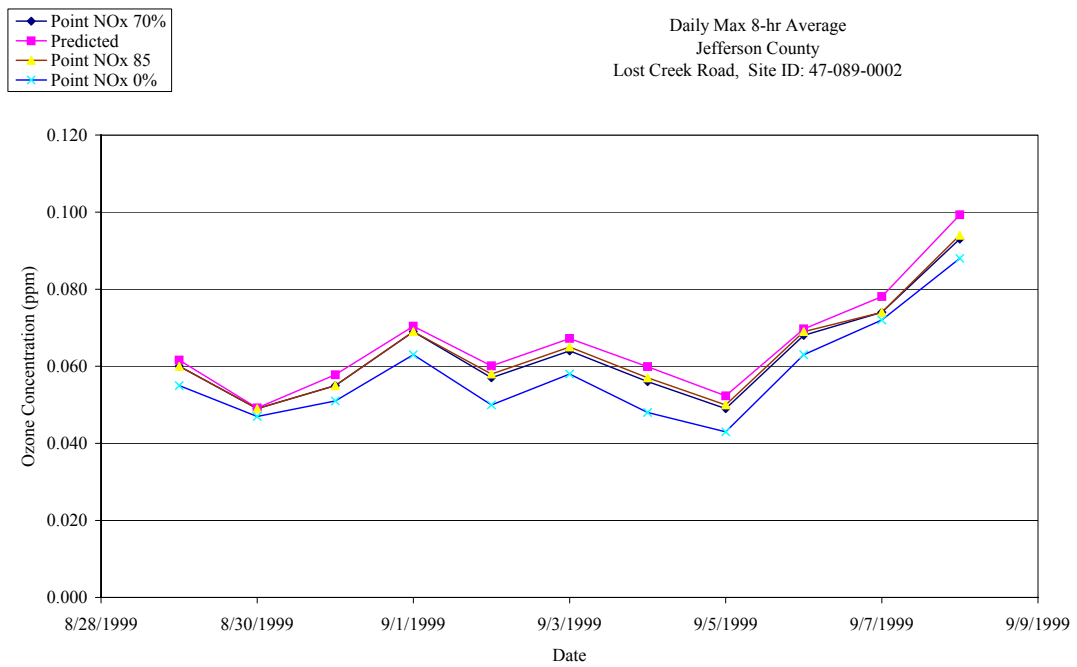


Figure 4.37 Jefferson County – Sensitivity analysis – Point with variable NOx

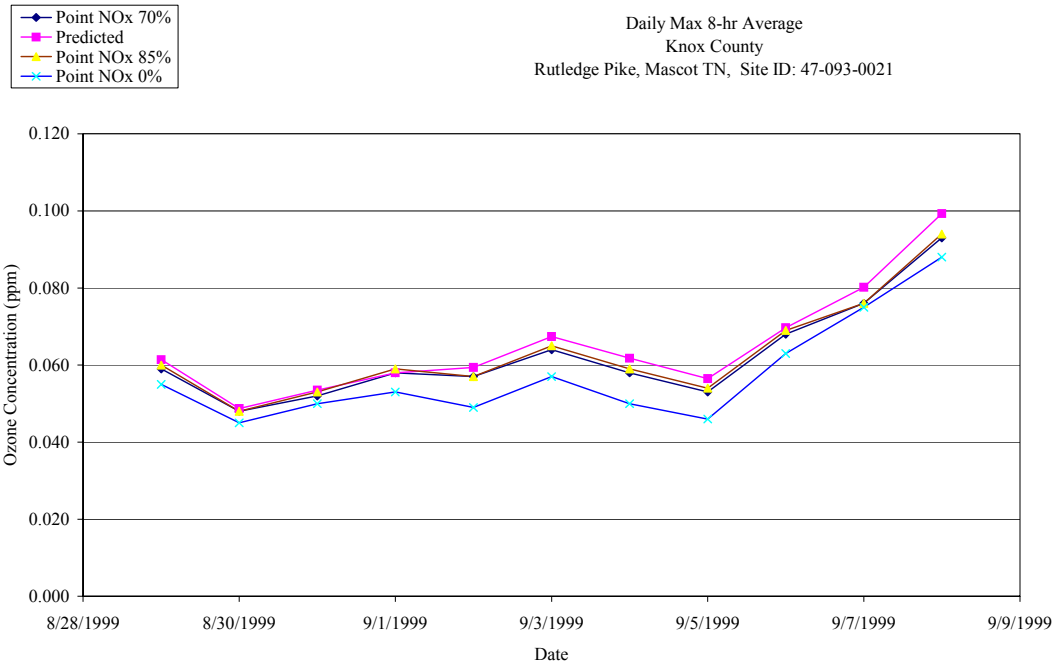


Figure 4.38 Knox County (Rutledge Pike) – Sensitivity analysis – Point with variable NO_x

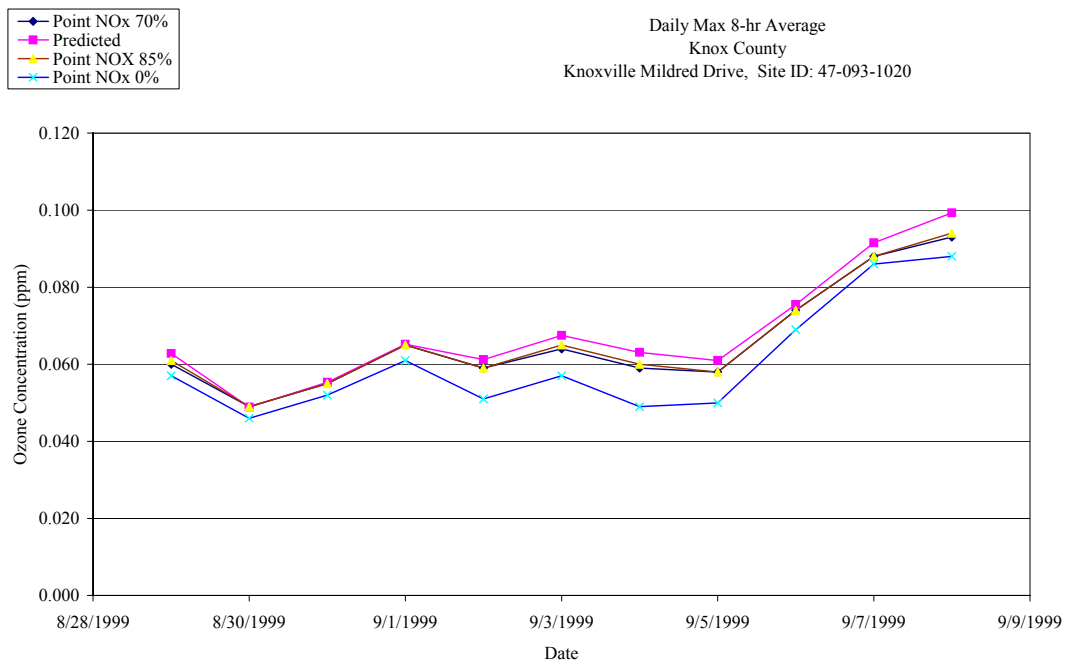


Figure 4.39 Knox County (Mildred Drive) – Sensitivity analysis – Point with variable NO_x

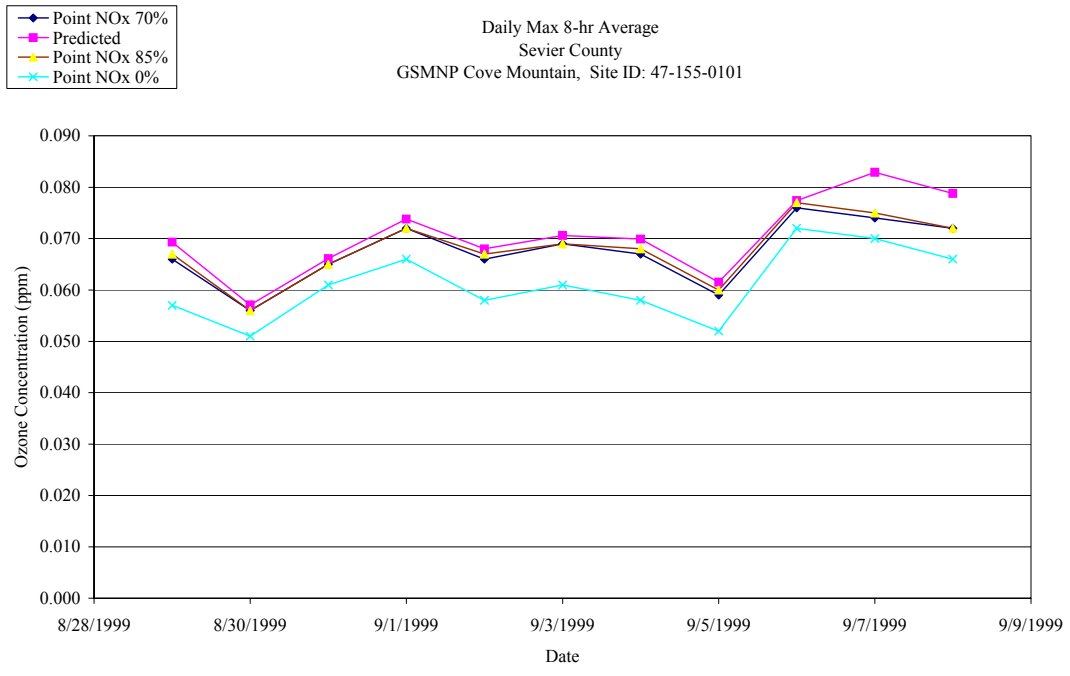


Figure 4.40 Sevier County (Cove Mountain) – Sensitivity analysis – Point with variable NO_x

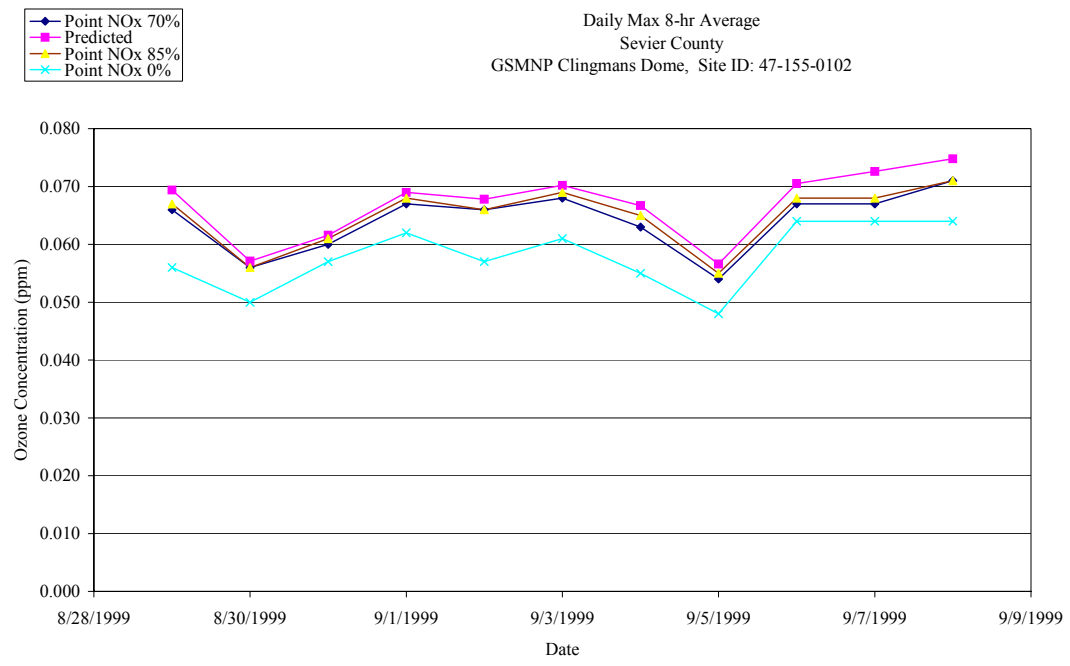


Figure 4.41 Sevier County (Clingmans Dove) – Sensitivity analysis – Point with variable NO_x

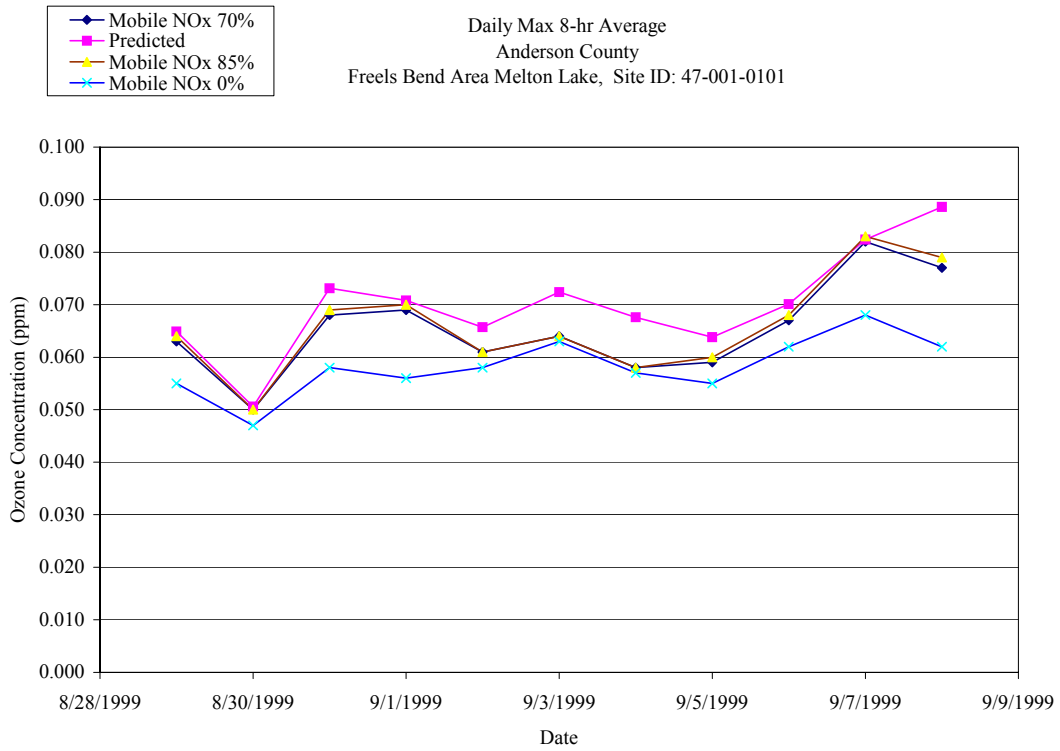


Figure 4.42 Anderson County – Sensitivity analysis – Mobile with variable NOx

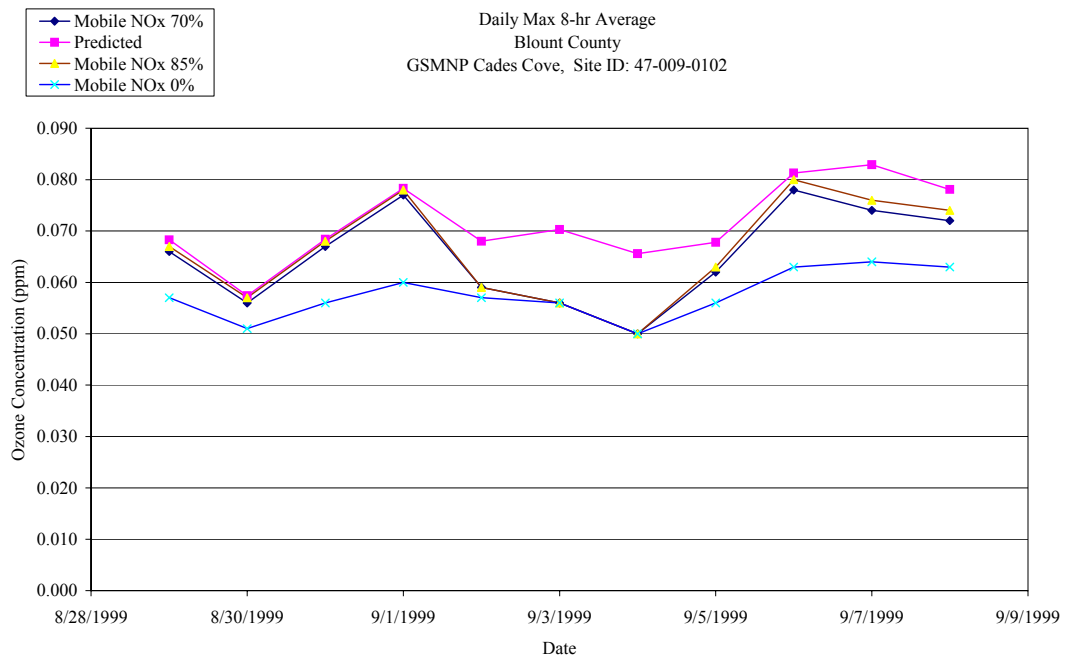


Figure 4.43 Blount County (Cades Cove) – Sensitivity analysis – Mobile with variable NOx

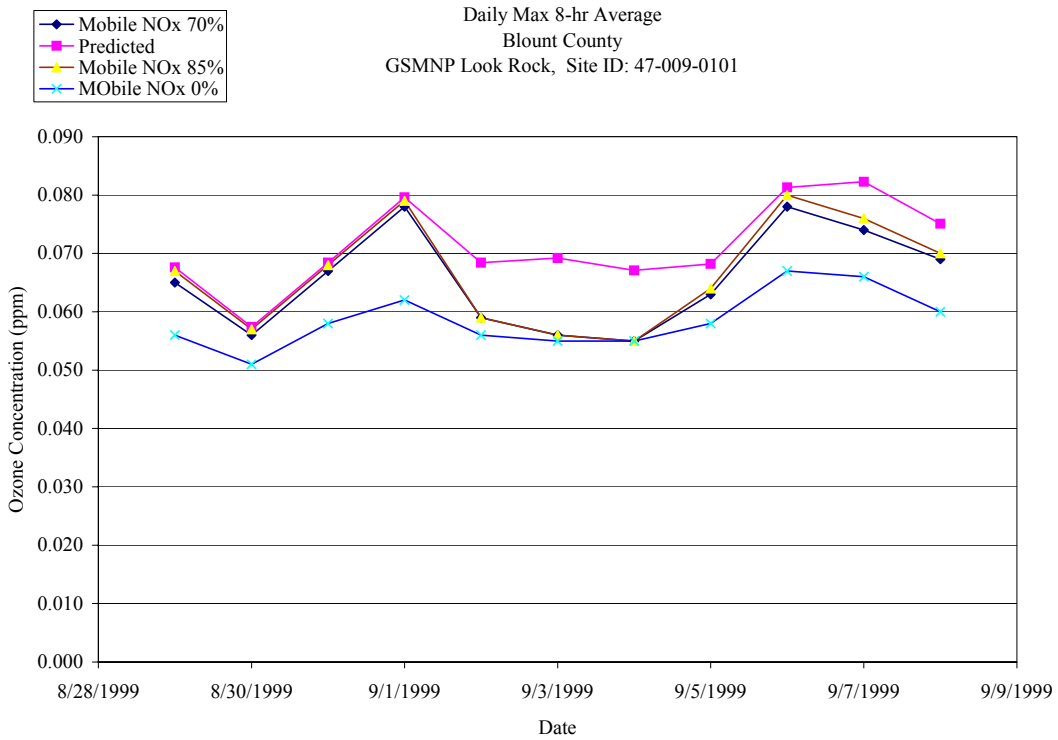


Figure 4.44 Blount County (Look Rock) – Sensitivity analysis – Mobile with variable NOx

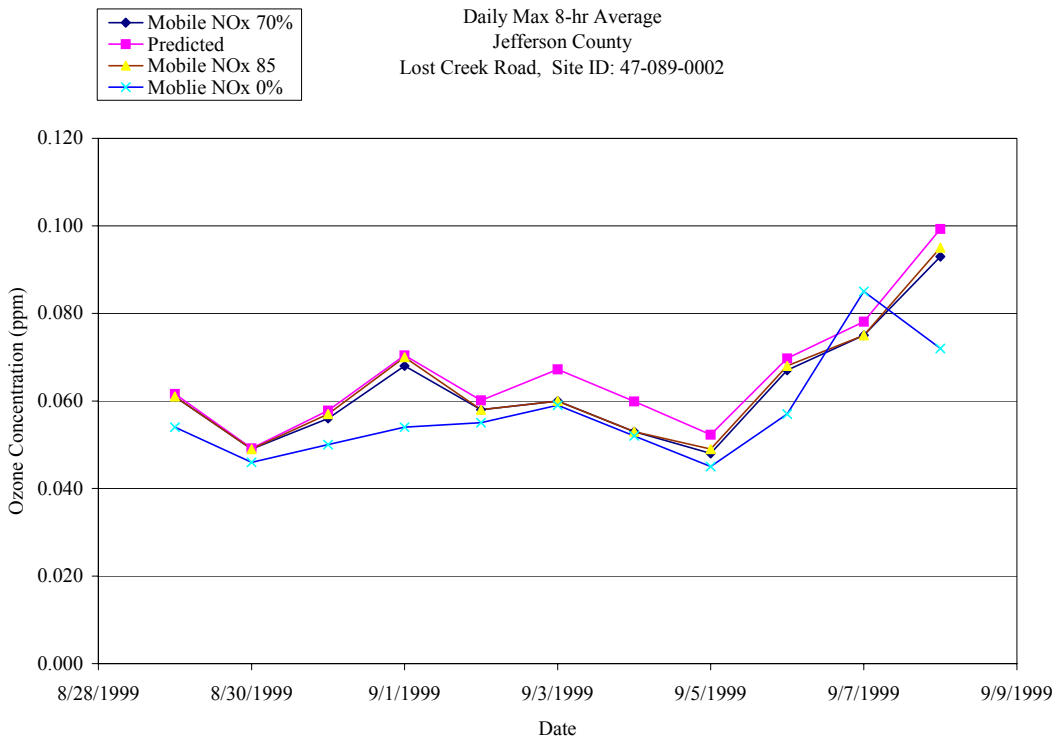


Figure 4.45 Jefferson County – Sensitivity analysis – Mobile with variable NOx

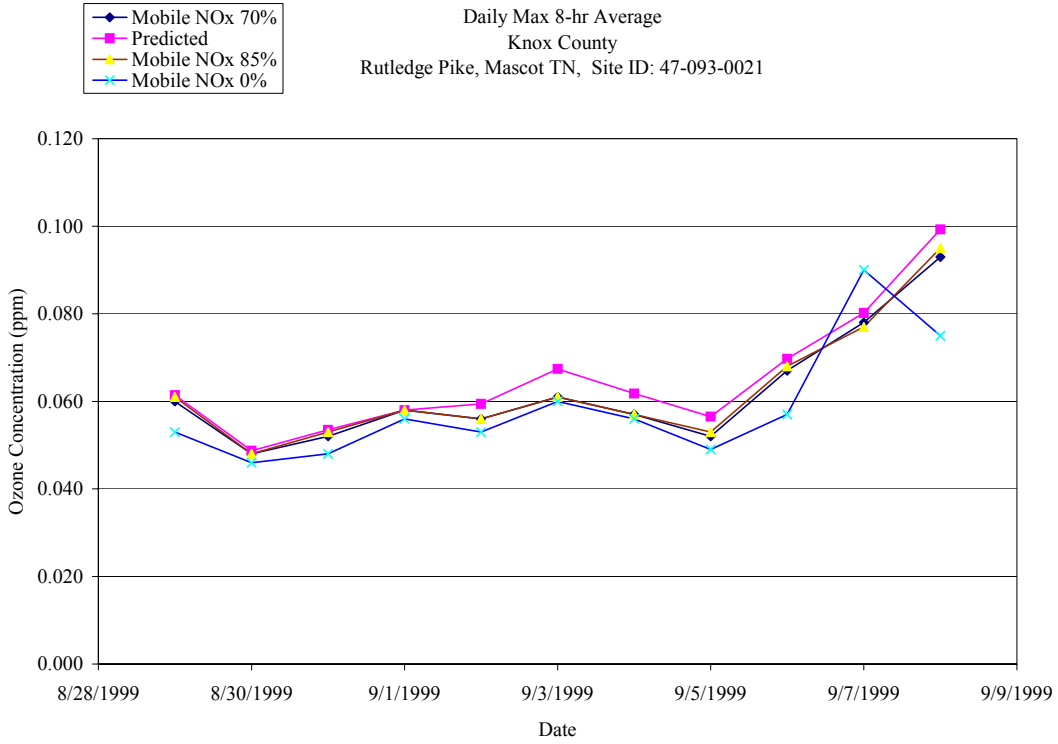


Figure 4.46 Knox County (Rutledge Pike) – Sensitivity analysis – Mobile with variable NOx

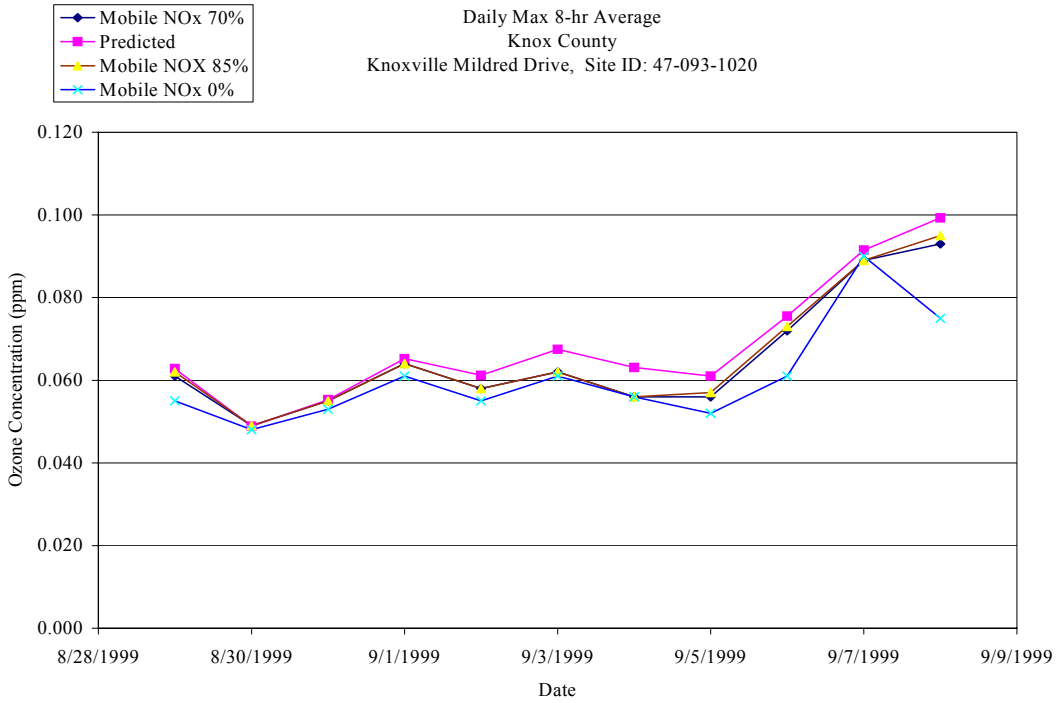


Figure 4.47 Knox County (Mildred Drive) – Sensitivity analysis – Mobile with variable NOx

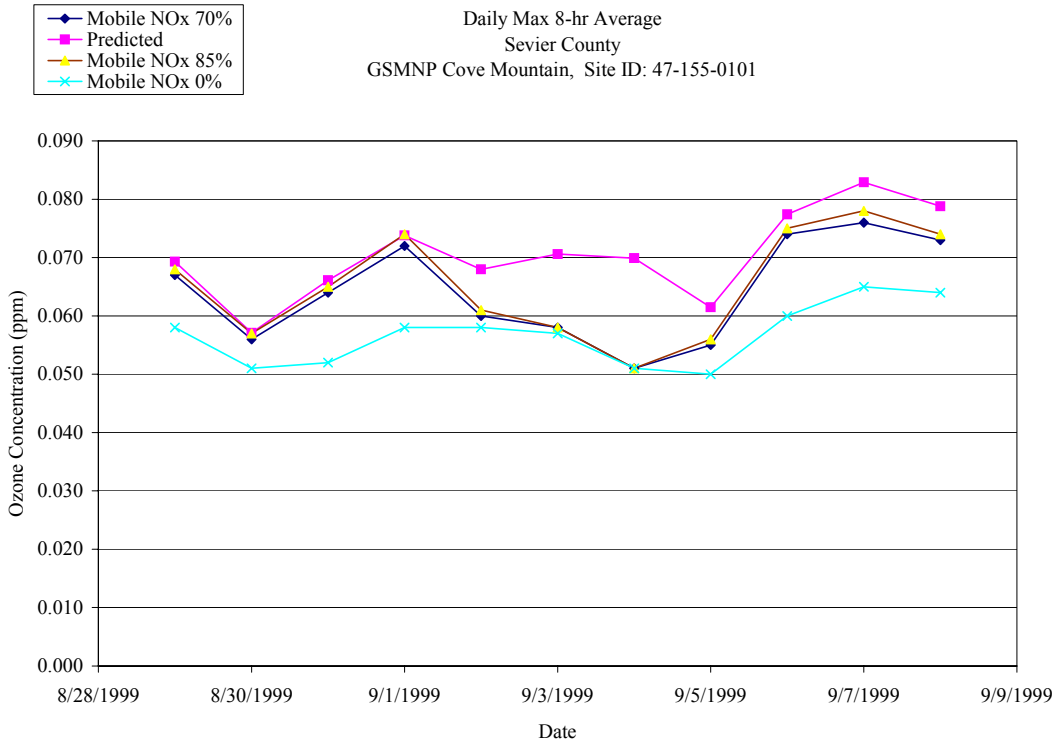


Figure 4.48 Sevier County (Cove Mountain) – Sensitivity analysis – Mobile with variable NOx

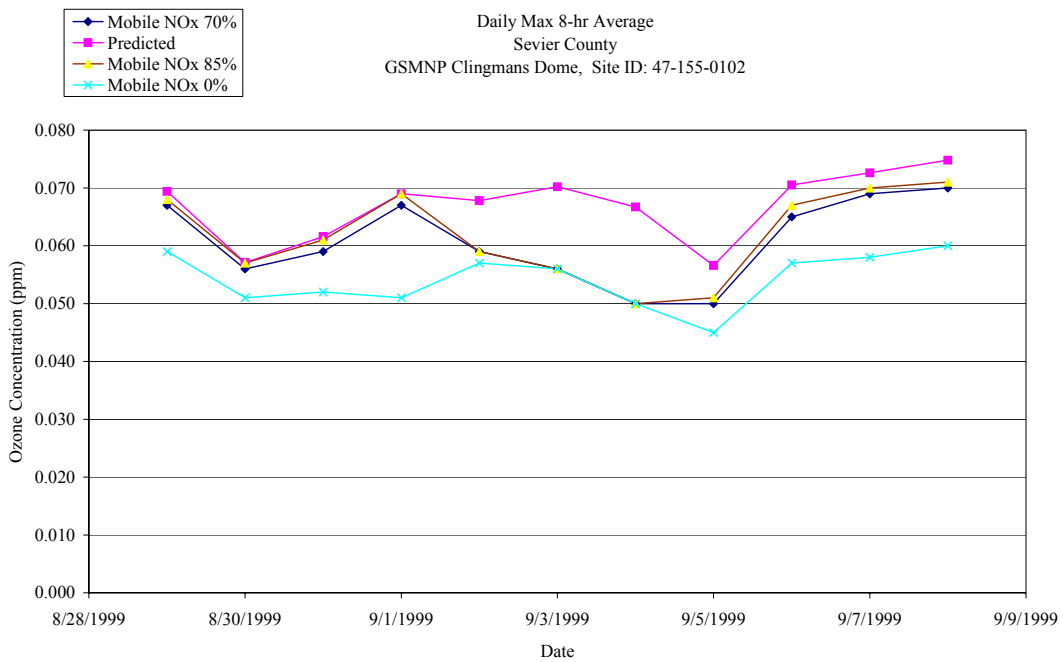


Figure 4.49 Sevier County (Clingmans Dome) – Sensitivity analysis – Mobile with Variable NOx

Various Percent Reduction in Mobile NOx in Anderson

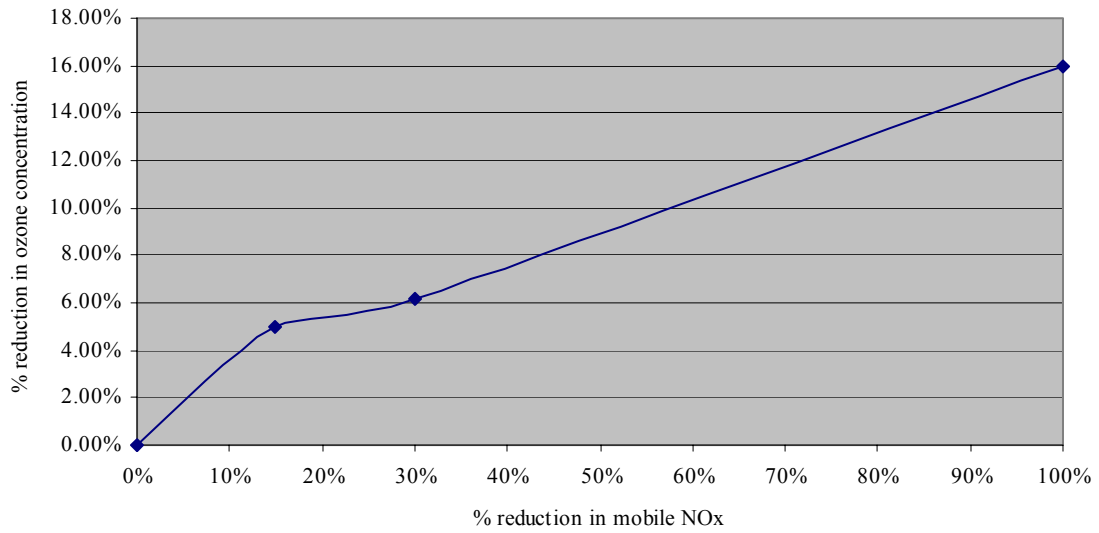


Figure 4.50 Overall Response of Ozone for various percent reductions in Mobile NOx Emission at Anderson

Various Percent Reduction in Mobile NOx in Cades Cove

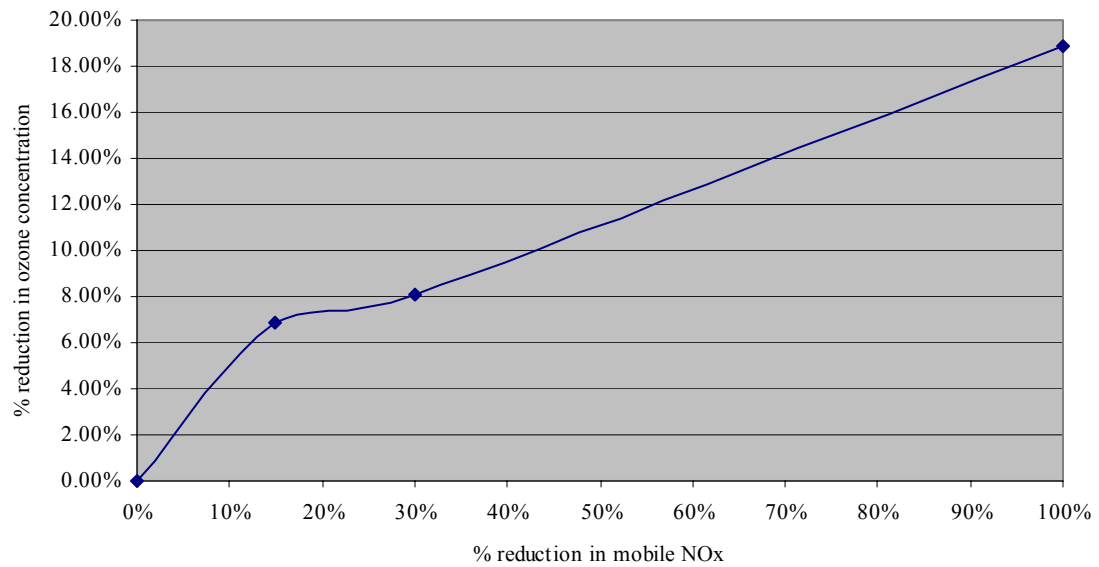


Figure 4.51 Overall Response of Ozone for various percent reductions in Mobile NOx Emission at Cades Cove – Blount County

Various Percent Reduction in Mobile NOx in Look Rock

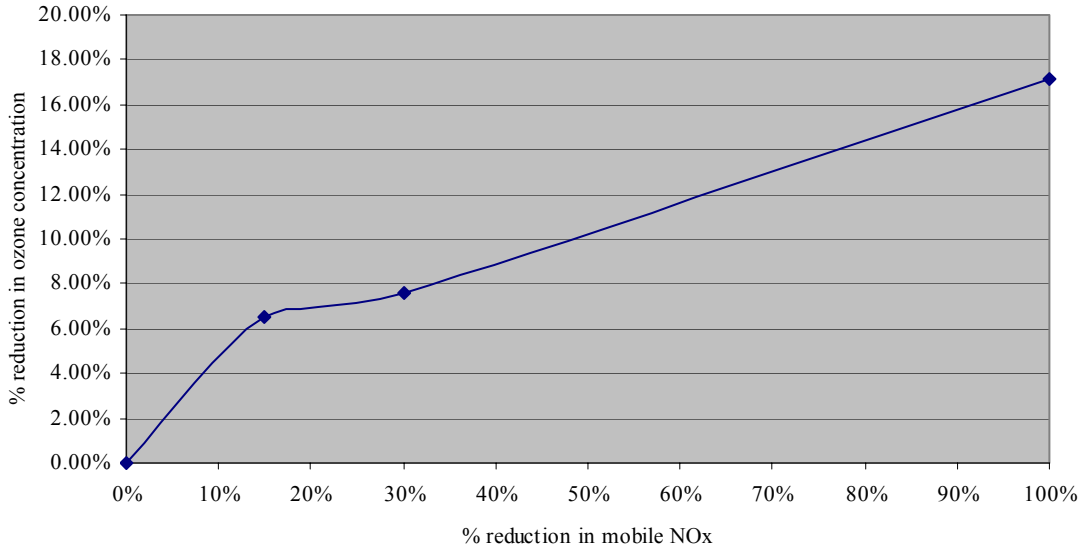


Figure 4.52 Overall Response of Ozone for various percent reductions in Mobile NOx Emission at Look Rock – Blount County

Various Percent Reduction in Mobile NOx in Jefferson

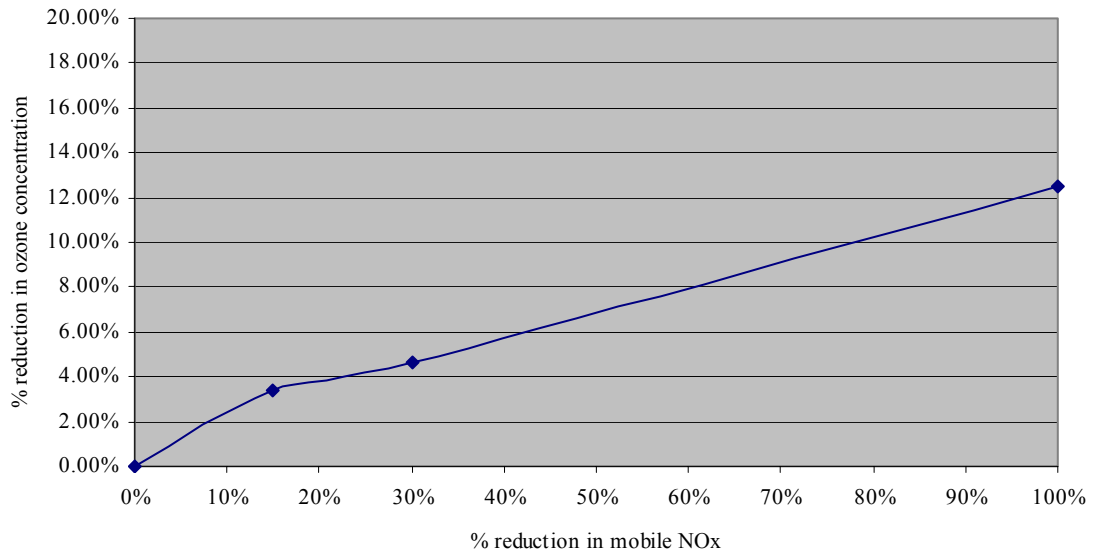


Figure 4.53 Overall Response of Ozone for various percent reductions in Mobile NOx Emission at Jefferson County

Various Percent Reduction in Mobile NOx in Knox-0021

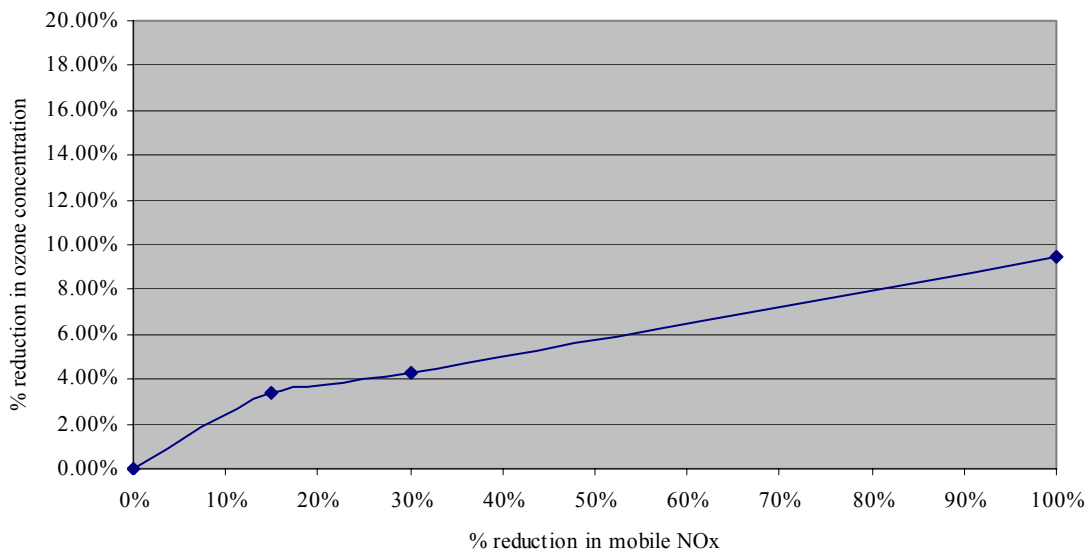


Figure 4.54 Overall Response of Ozone for various percent reductions in Mobile NOx Emission at Knox – 0021

Various Percent Reduction in Mobile NOx in Knox - 1020

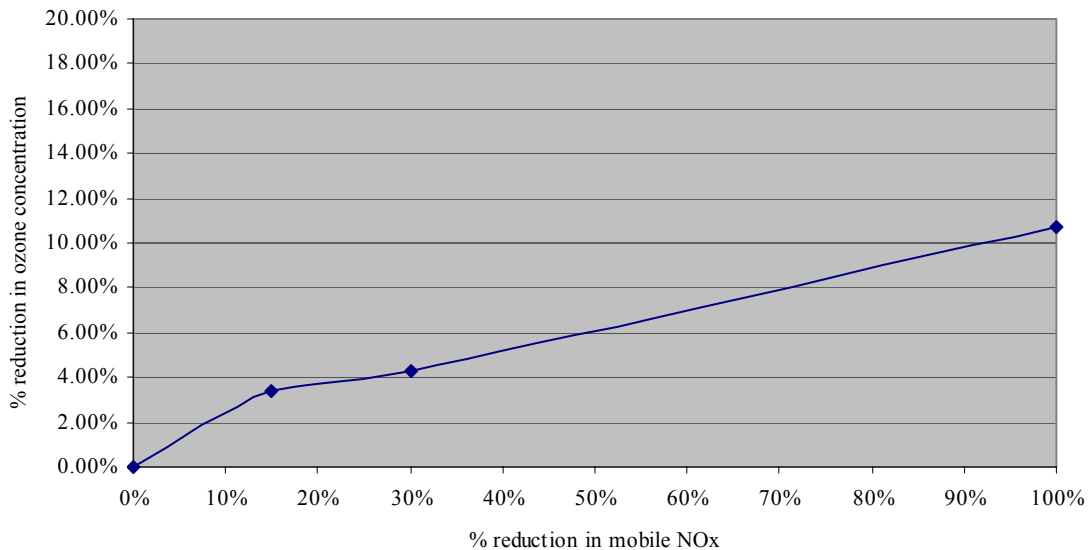


Figure 4.55 Overall Response of Ozone for various percent reductions in Mobile NOx Emission at Knox – 1020

Various Percent Reduction in Mobile NOx in Sev - 0101

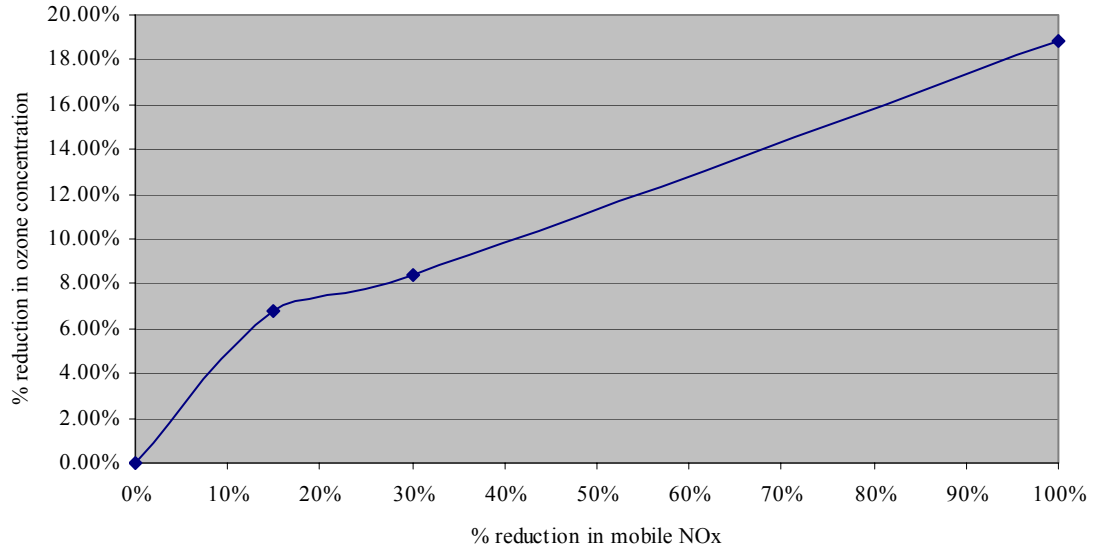


Figure 4.56 Overall Response of Ozone for various percent reductions in Mobile NOx Emission at Sevier - 0101

Various Percent Reduction in Mobile NOx in Sev - 0102

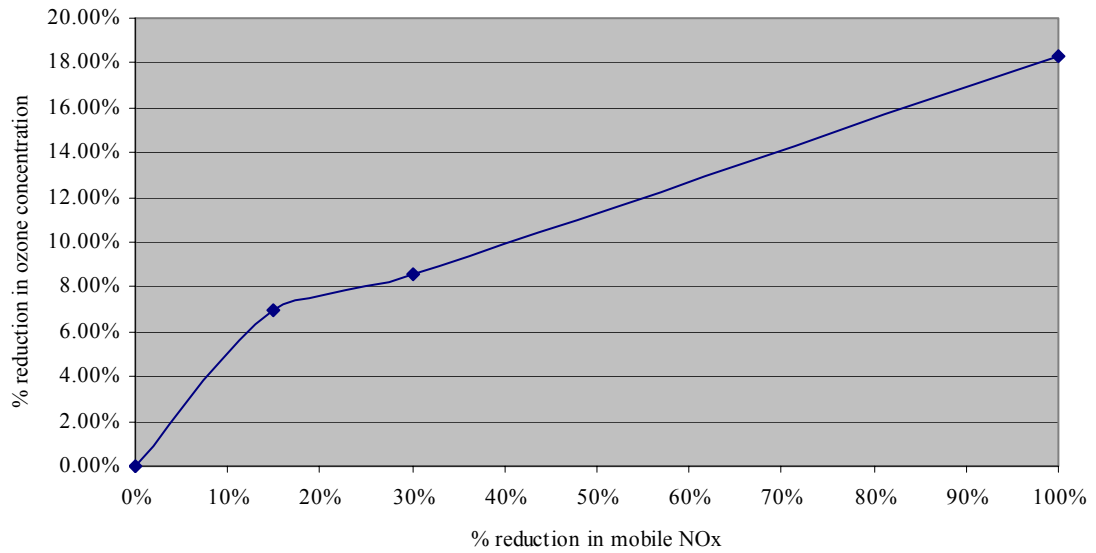


Figure 4.57 Overall Response of Ozone for various percent reductions in Mobile NOx Emission at Sevier - 0102

though it was actually a Monday. A regular hourly pattern in the NEI emissions is visible in all the graphs.

For the TVA Kingston Fossil power plant, (Figure 4.62 & Figure 4.63) the graphs show that the NO emissions from the NEI point inventory were higher than the CEMS data. The opposite was found for the TVA Bull Run power plant (Figures 4.60 & 4.61). It is hard to say which case has higher NO emissions, but these figures confirm that differences in ozone concentrations can occur in CMAQ runs because of differences in NO emissions in the NEI and CEMS inventories. NO emissions in tons/day in each layer were also compared for August 30th and 31st. From Table 4.4 it was found that the NEI exhibited more NO emissions than CEMS in all 11 layers for these two days. On average the NEI NO emissions were 5.33% higher than CEMS emissions. These higher emissions in the NEI were expected to predict higher ozone concentrations but when CMAQ outputs were analyzed it was found that the NEI inventory produced lower ozone concentrations than CEMS at all the monitor locations. The CMAQ model predicted ozone concentrations more accurately using the CEMS emission inventory than the NEI inventory. Table 4.6 shows the average ppb difference between predicted and observed ozone concentrations for the CEMS versus NEI runs. Table 4.6 shows that the average ppb differences between the predicted and observed ozone concentrations were lower for the CMAQ run that used CEMS data than the run using NEI run.

Ozone concentrations were also predicted inputting all NEI emissions in a single layer next to the ground. These ozone concentrations predicted using CMAQ were compared with ozone concentrations from NEI (resolved in 11 layers) and ozone concentrations from CEMS data (resolved in 11 layers). Refer to Figures 4.72-4.79. Table 4.6 shows that the average ppb difference between the predicted and observed ozone concentrations was higher for emissions in a single layer than emissions in 11 layers. CMAQ performed best when the emissions were resolved in 11 layers using CEMS emission data.

Table 4.4 Hourly NO emissions in tons/day in 36km Domain

Layer	30-Aug		31-Aug	
	CEMS	NEI	CEMS	NEI
1	0.3492	0.3614	0.3495	0.3667
2	0.3311	0.3449	0.3168	0.3378
3	0.5193	0.5334	0.4267	0.4505
4	0.2757	0.2975	0.3243	0.3521
5	0.08961	0.094	0.118	0.1287
6	0.01785	0.0178	0.01345	0.014
7	0.0015	0.0017	0.0021	0.0021
8	0.00095	0.001	0.00212	0.0013
9	0.001	0.0011	0.0013	0.0014
10	0.0003	0.0004	0.00089	0.001
11	0	0	0.0007	0.0008
Total Emissions in 11 layers	1.58651	1.6532	1.55586	1.6564
% Increase in NO emissions in NEI	4.20%		6.46%	
Average % increase in NO emissions	5.33%			

Table 4.5 Base Case with CEMS data

Station	Average ppb difference between predicted and observed	Average Bias, %
Anderson	0	0.0%
Blount Cades Cove	4	5.1%
Blount Look Rook	18	19.6%
Jefferson	-4	-6.2%
Knox -0021	6	8.1%
Knox -1020	4	5.3%
Sevier-0101	18	19.6%
Sevier- 0102	18	20.7%

Table 4.6 Average ppb difference between predicted and observed ozone concentrations

Station	NEI in single layer	NEI in 11 layers	CEMS in 11 layers
Anderson	4	3	0
Blount Cades Cove	9	7	4
Blount Look Rook	23	21	18
Jefferson	1	0	4
Knox -0021	11	9	6
Knox -1020	9	9	4
Sevier-0101	24	20	18
Sevier- 0102	22	22	18

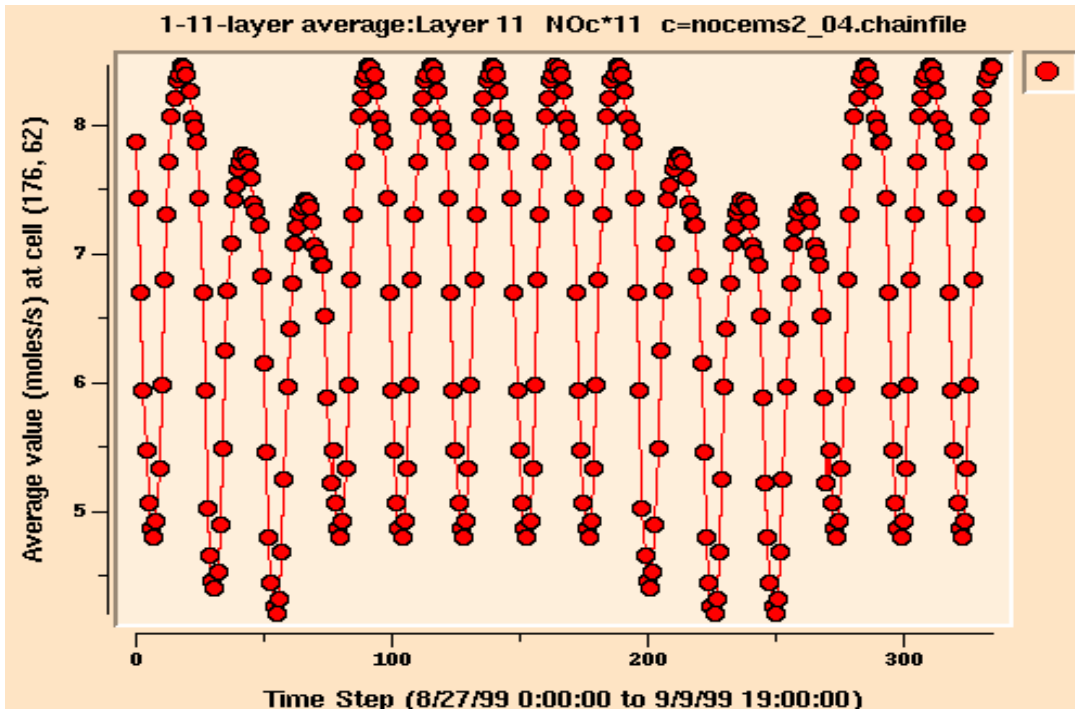


Figure 4.58 NEI Temporal profile of TVA John Sevier Fossil Plant, Hawkins County

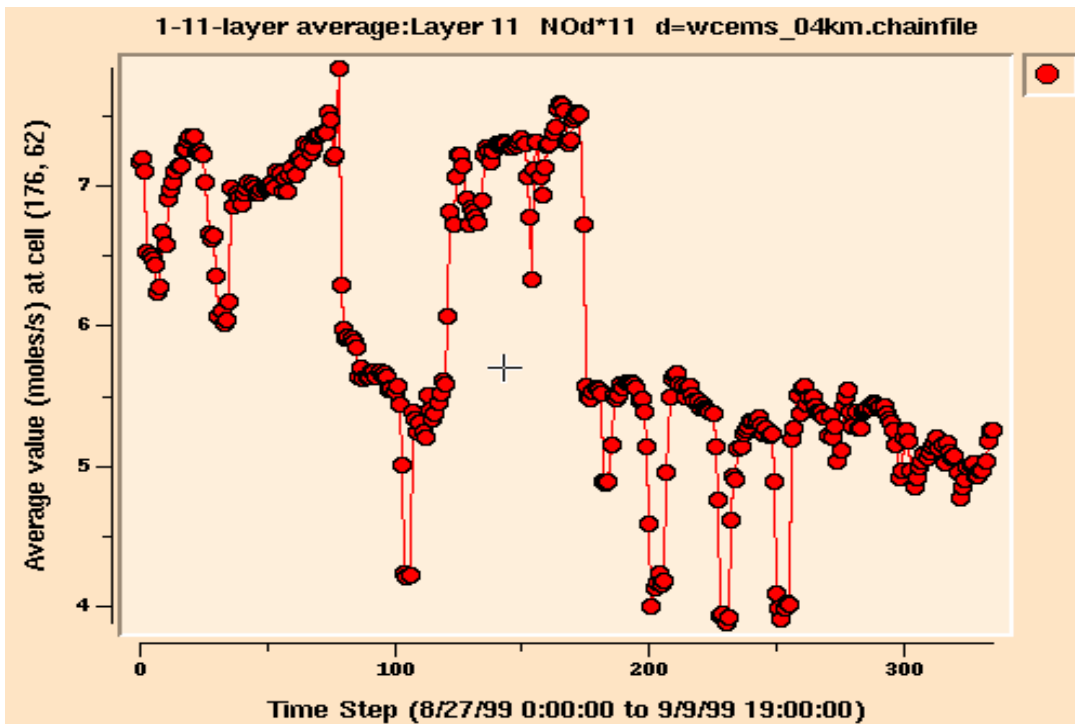


Figure 4.59 CEMS Temporal profile of TVA John Sevier Fossil Plant, Hawkins County

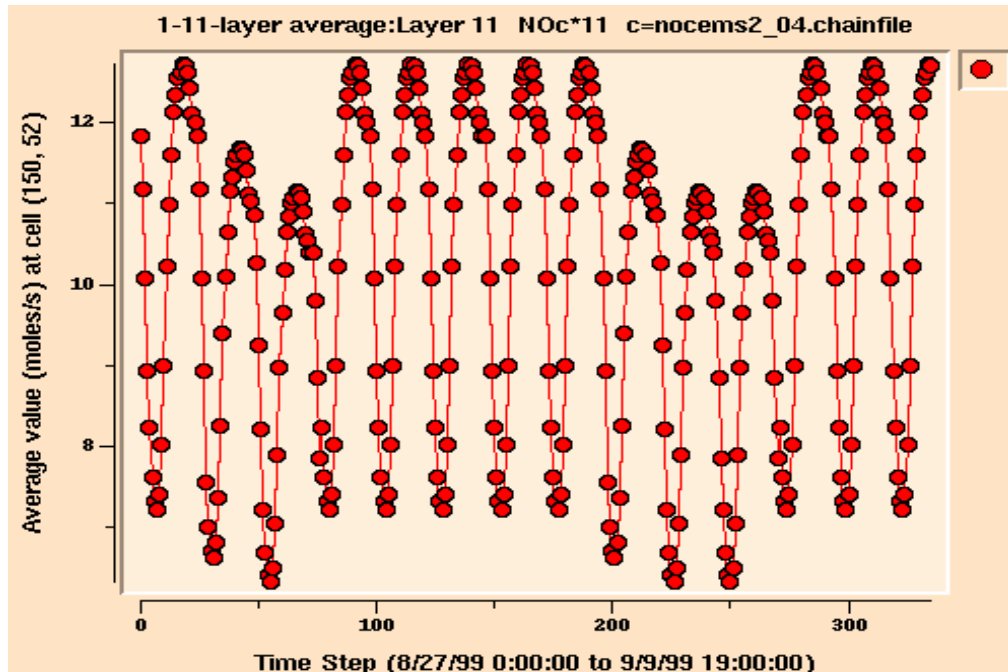


Figure 4.60 NEI Temporal profile of Bull Run Fossil Plant, Anderson County

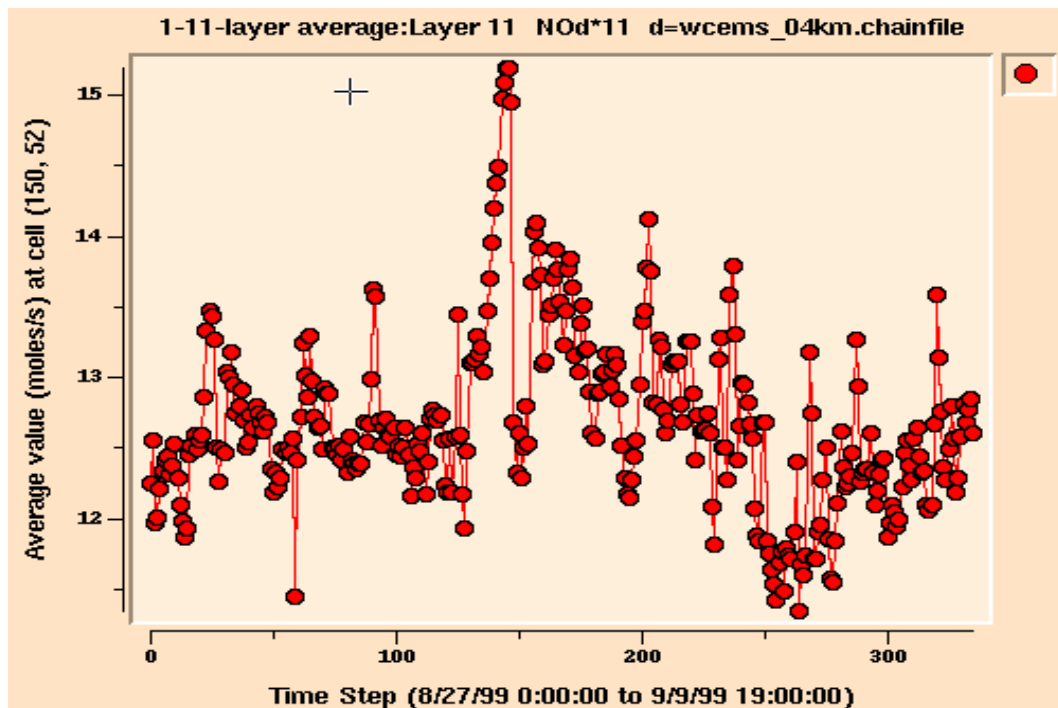


Figure 4.61 CEMS Temporal profile of Bull Run Fossil Plant, Anderson County

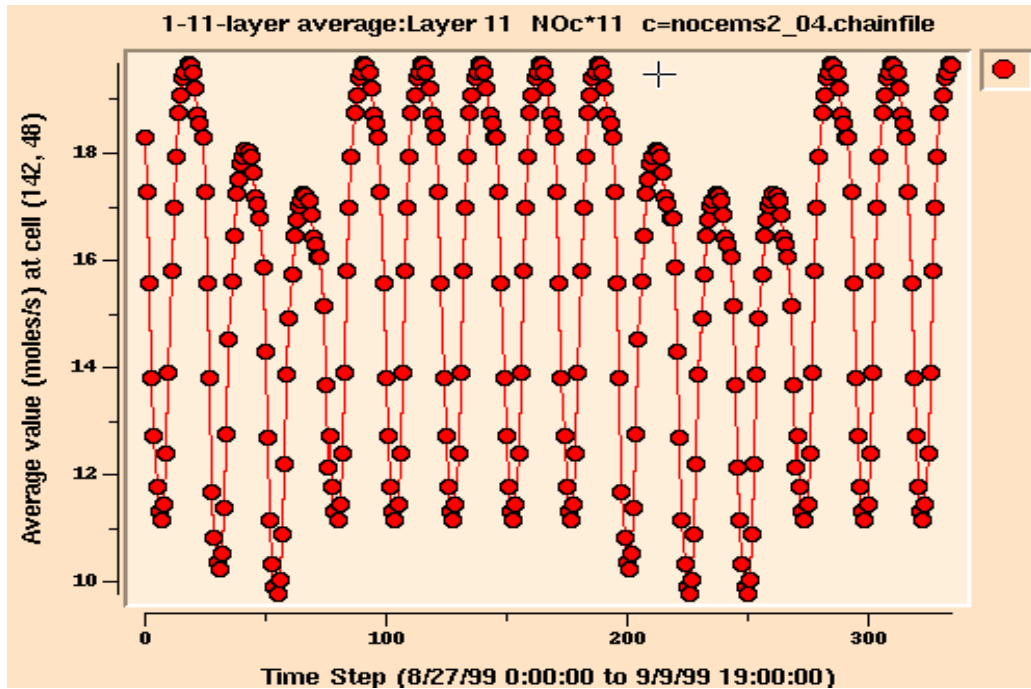


Figure 4.62 NEI Temporal profile of TVA Kingston Fossil Plant, Roane County

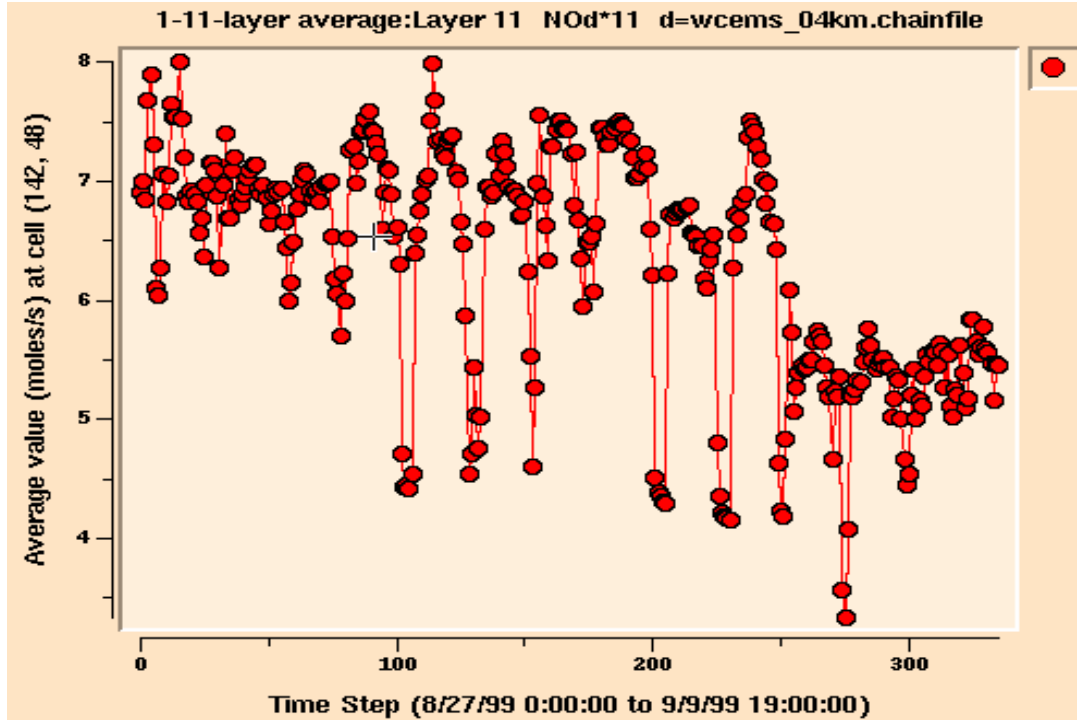


Figure 4.63 CEMS Temporal profile of TVA Kingston Fossil Plant, Roane County

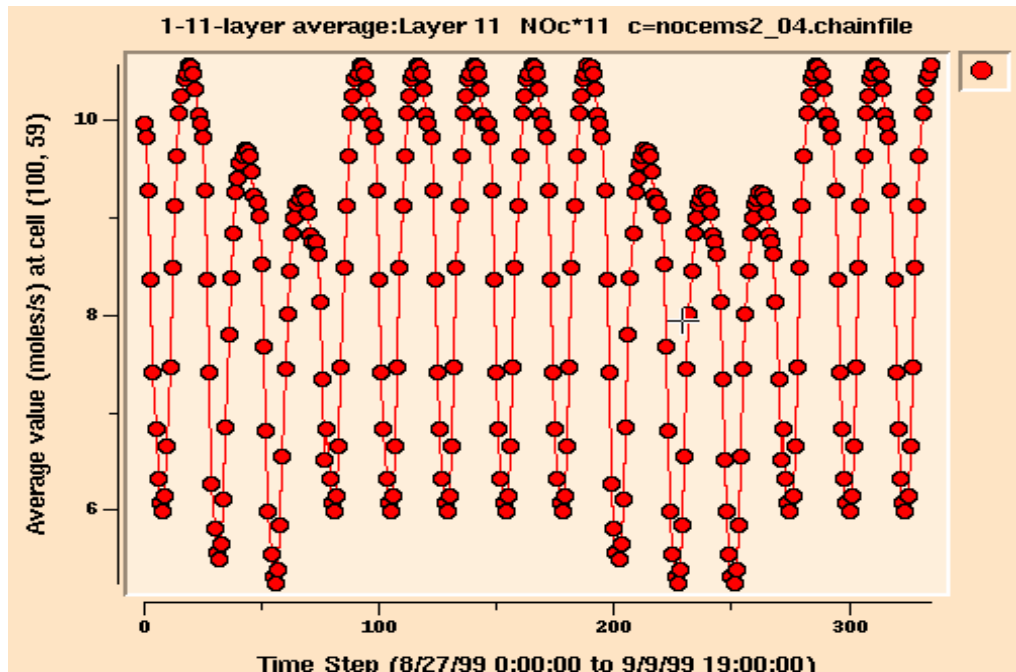


Figure 4.64 NEI Temporal profile of TVA Gallatin Fossil Fuel Plant, Sumner County

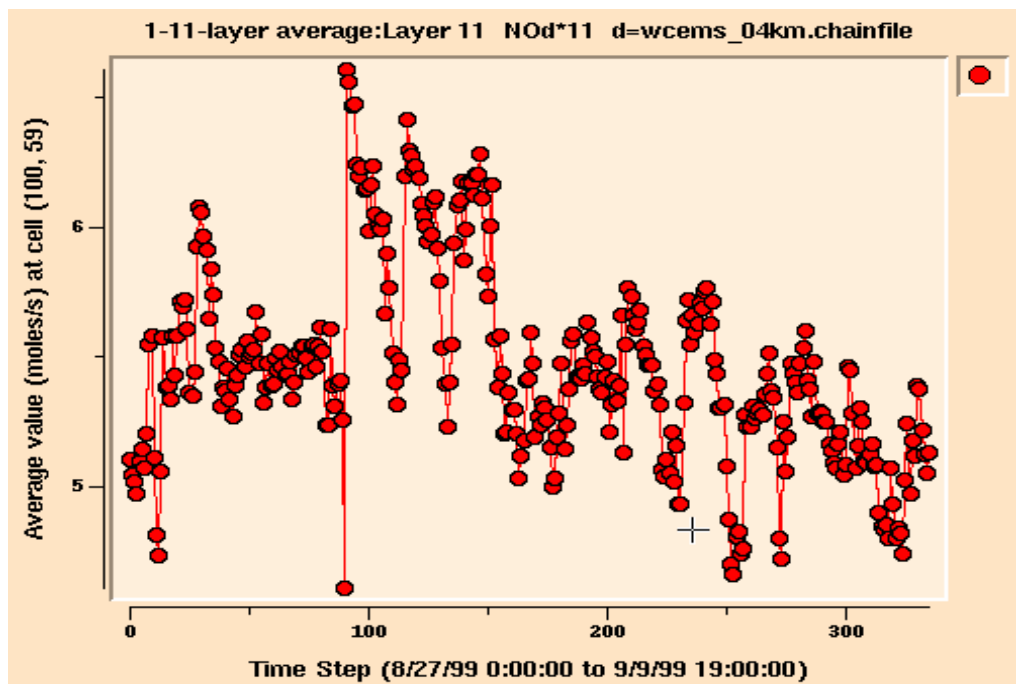


Figure 4.65 CEMS Temporal profile of TVA Gallatin Fossil Fuel Plant, Sumner County

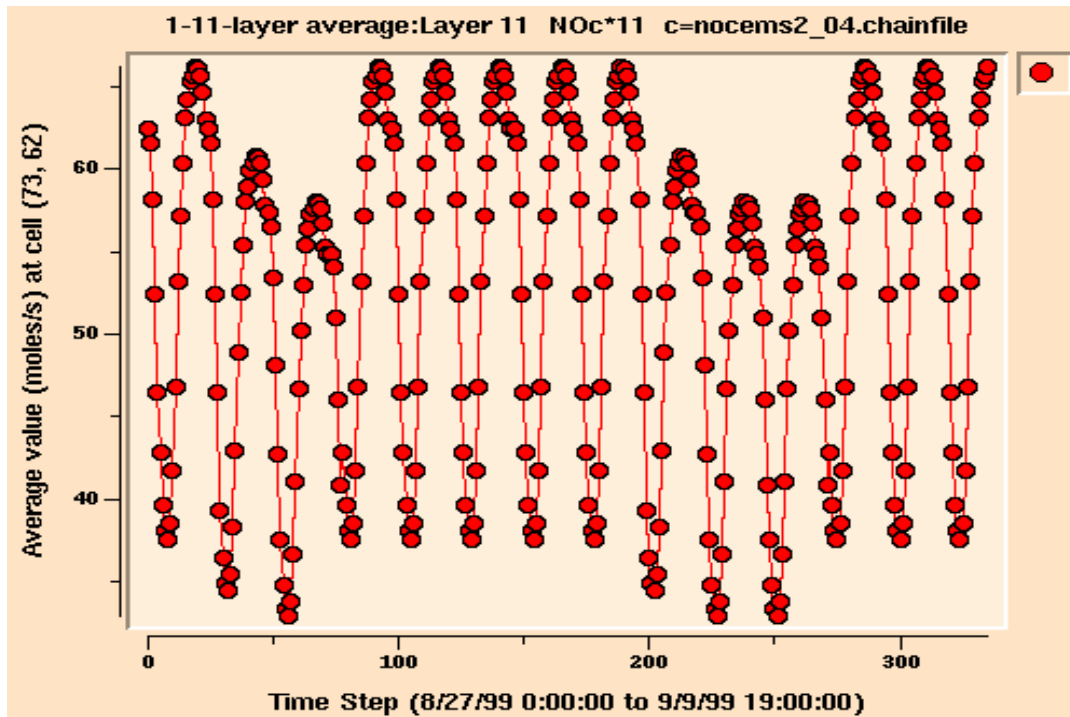


Figure 4.66 NEI Temporal profile of TVA Cumberland Fossil Plant, Stewart County

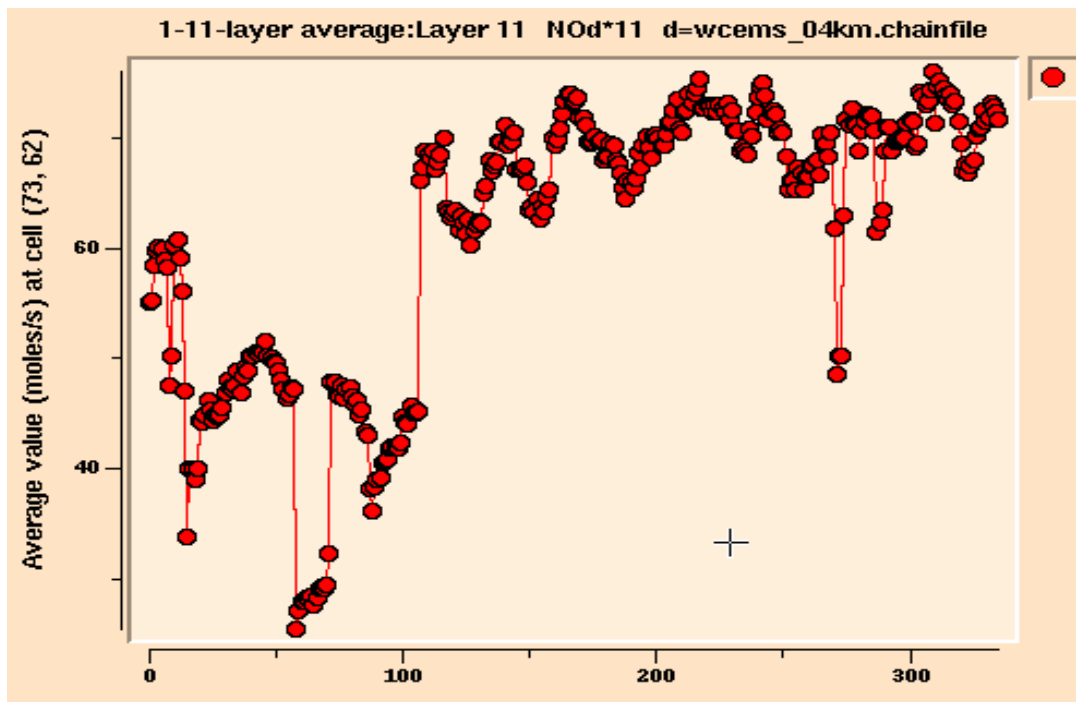


Figure 4.67 CEMS Temporal profile of TVA Cumberland Fossil Plant, Stewart County

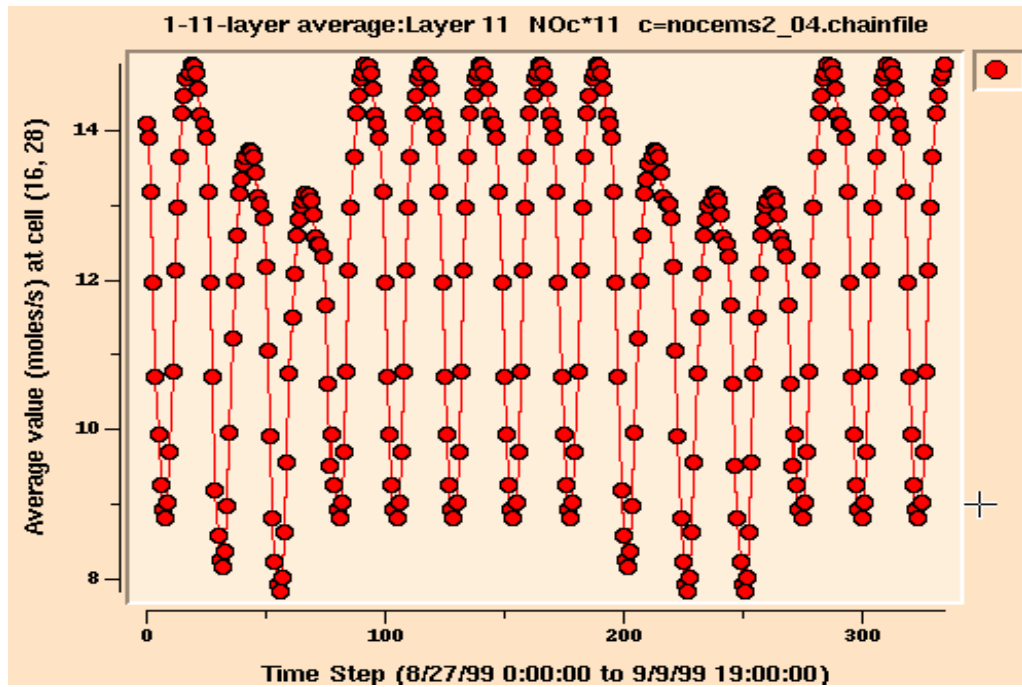


Figure 4.68 NEI Temporal profile of Allen Fossil Plant, Shelby County

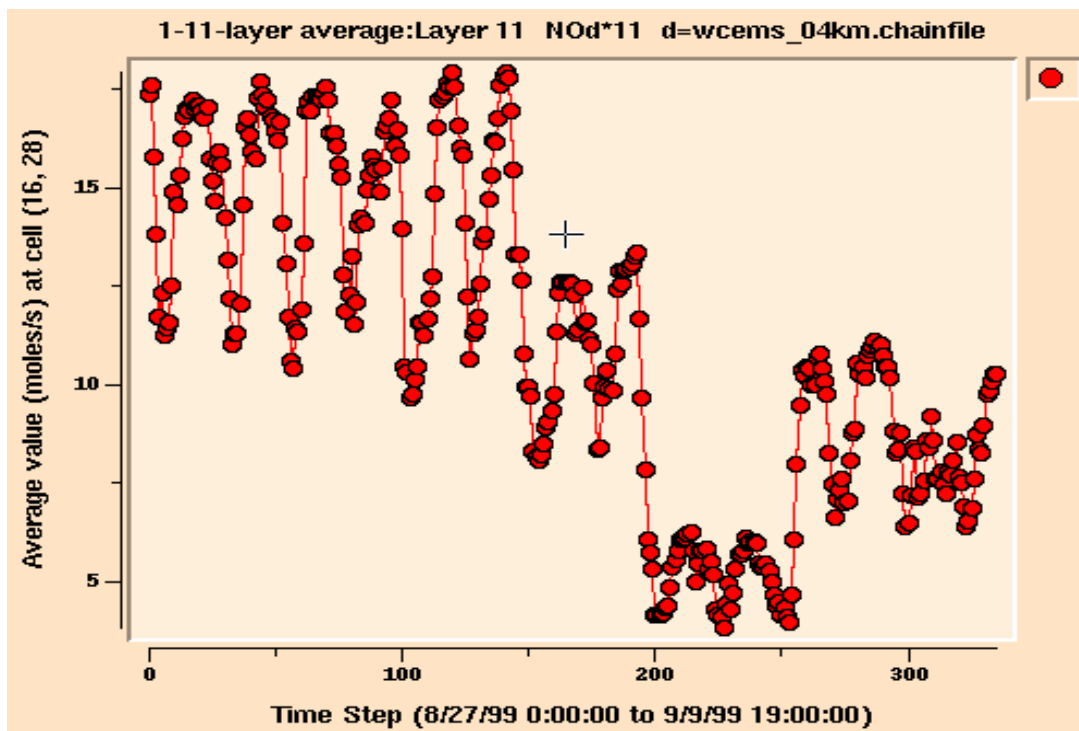


Figure 4.69 CEMS Temporal profile of Allen Fossil Plant, Shelby County

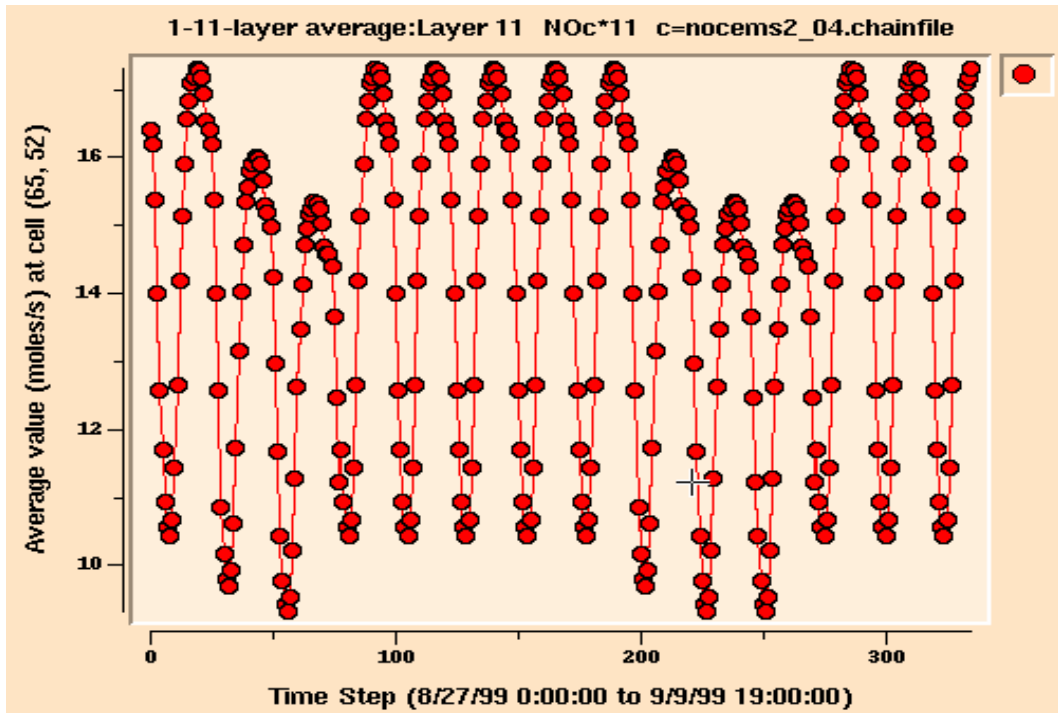


Figure 4.70 NEI Temporal profile of TVA Johnsonville Fossil Plant, Humphrey County

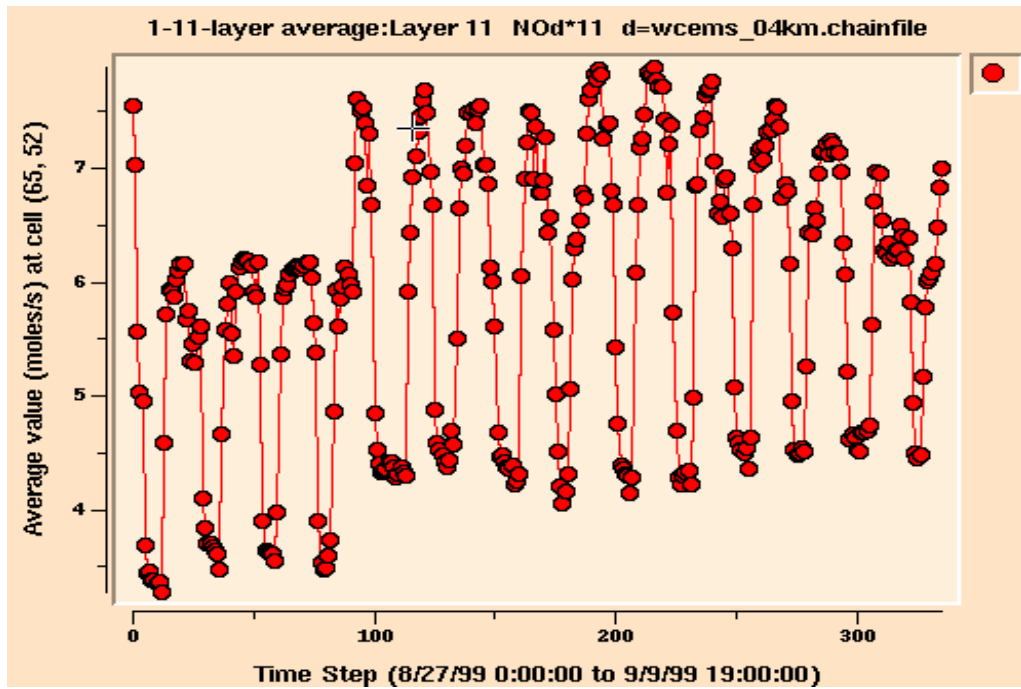


Figure 4.71 CEMS Temporal profile of TVA Johnsonville Fossil Plant, Humphrey County

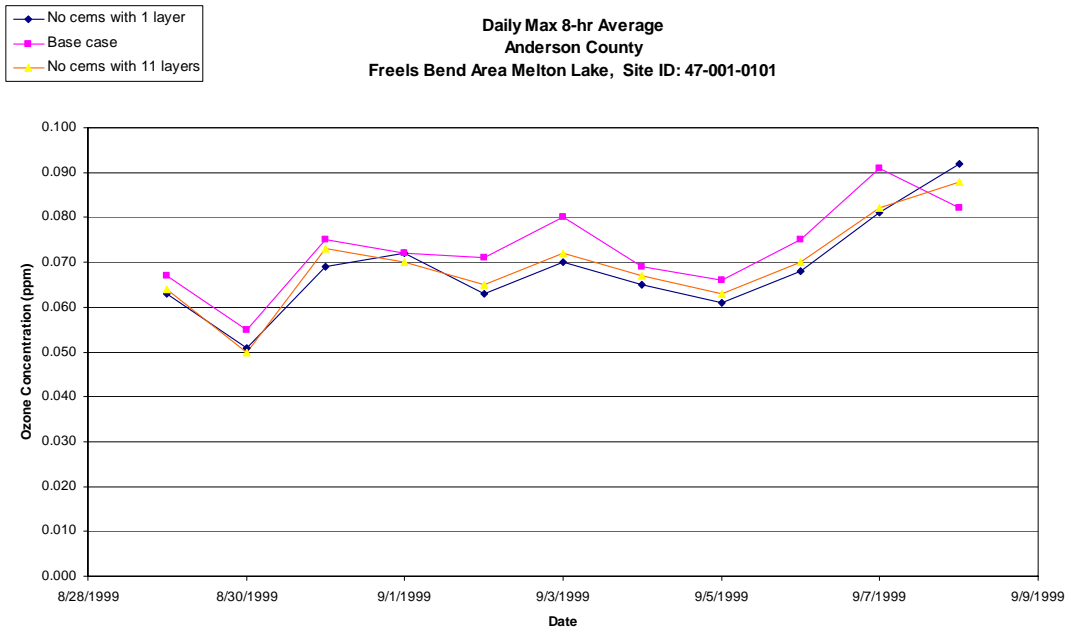


Figure 4.72 Anderson County – Comparison between – CEMS and Conventional Inventory

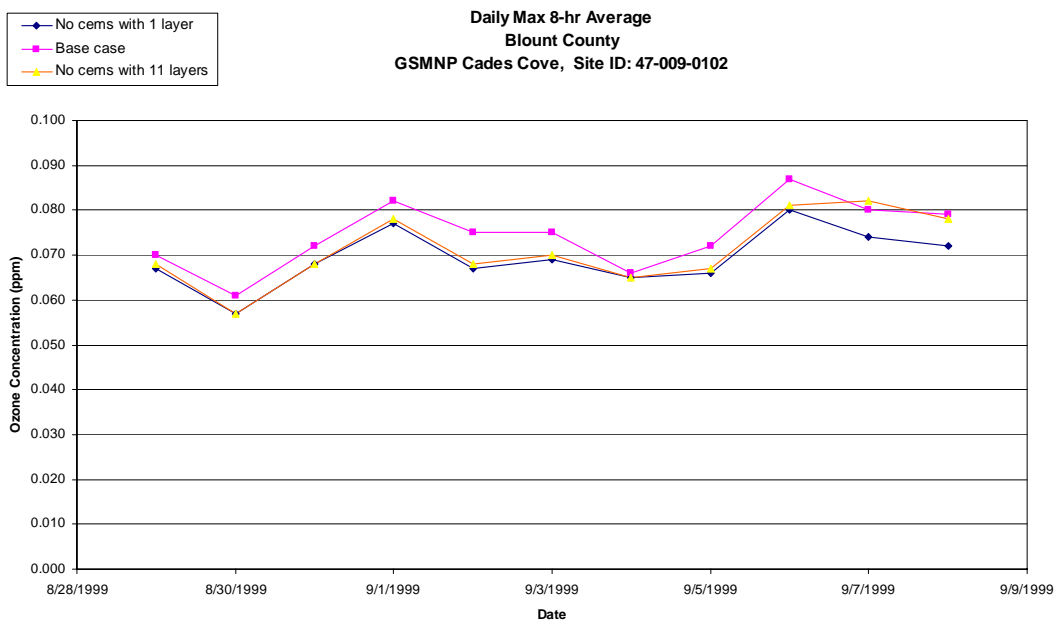


Figure 4.73 Blount County (Cades Cove) – Comparison between – CEMS and Conventional Inventory

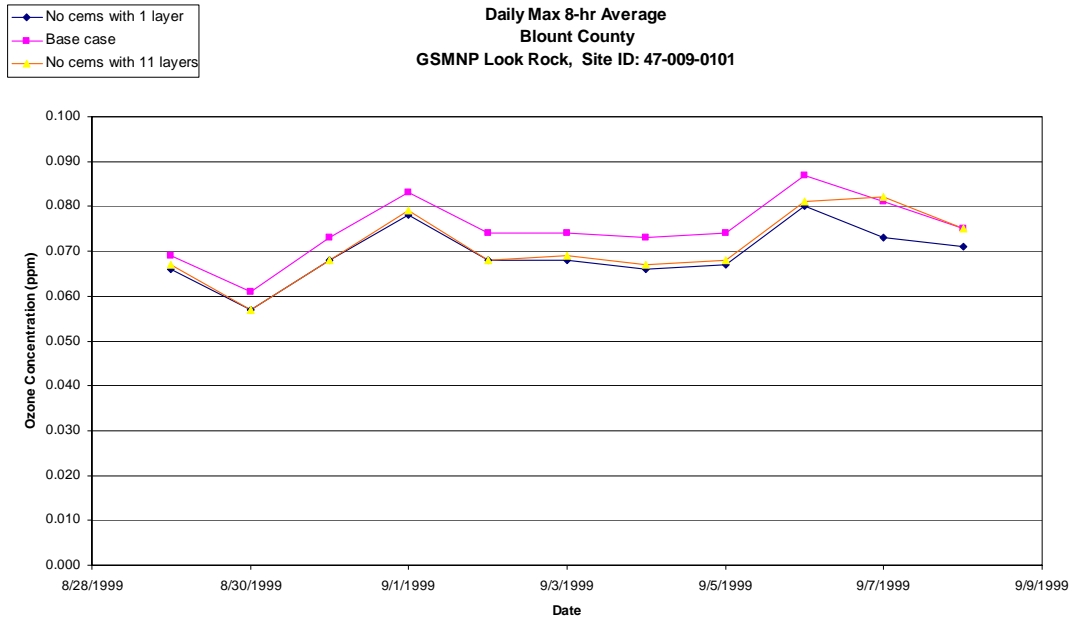


Figure 4.74 Blount County (Look Rock) – Comparison between – CEMS and Conventional Inventory

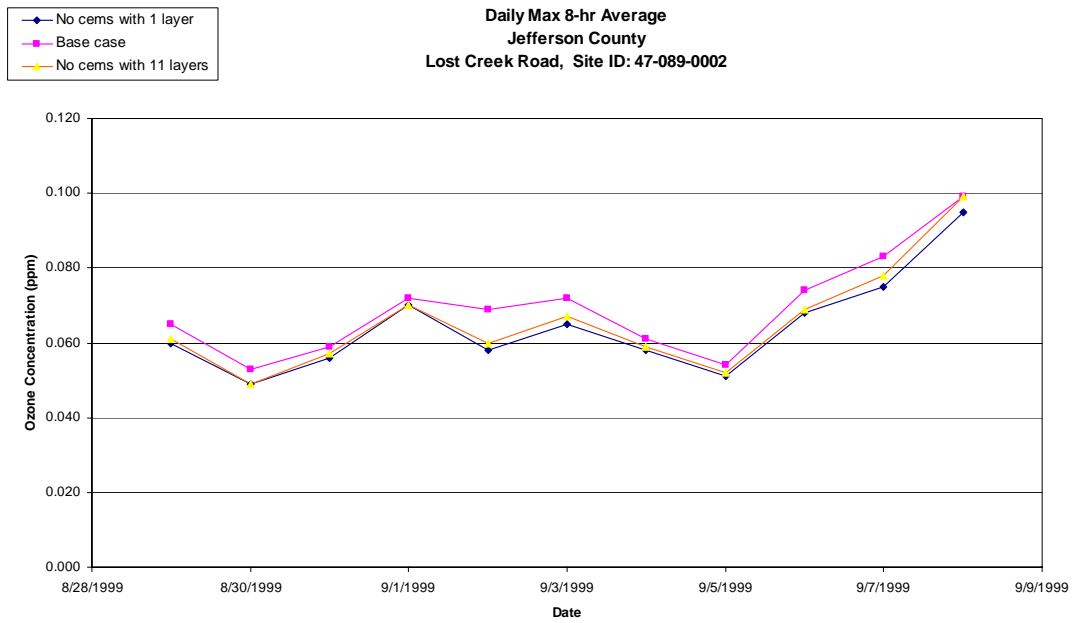


Figure 4.75 Jefferson County – Comparison between – CEMS and Conventional Inventory

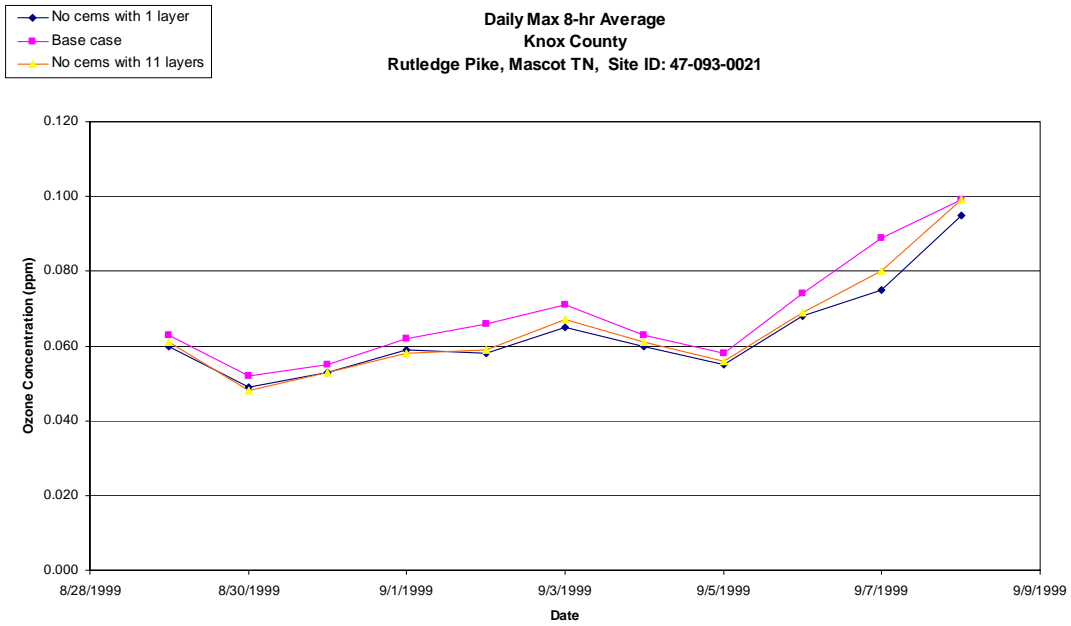


Figure 4.76 Knox County (Rutledge Pike) – Comparison between – CEMS and Conventional Inventory

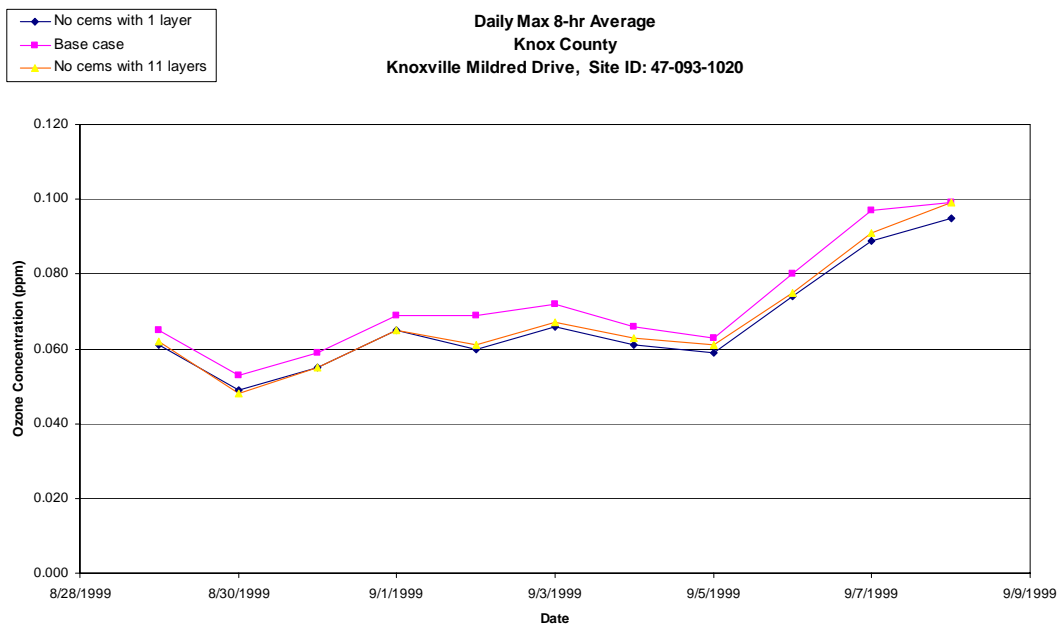


Figure 4.77 Knox County (Mildred Drive) – Comparison between – CEMS and Conventional Inventory

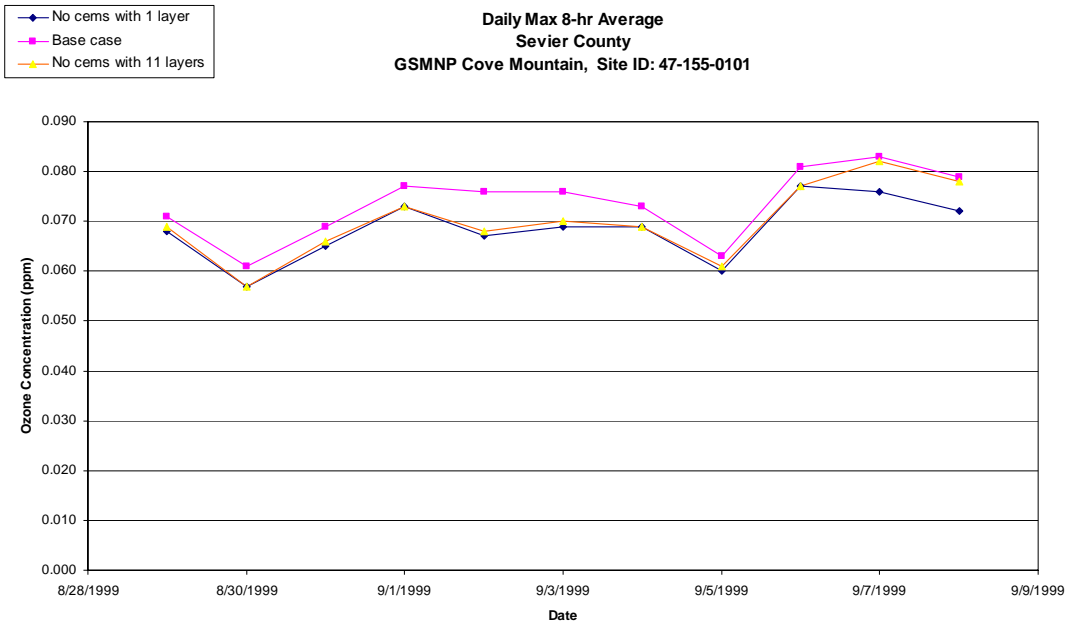


Figure 4.78 Sevier County (Cove Mountain) – Comparison between – CEMS and Conventional Inventory

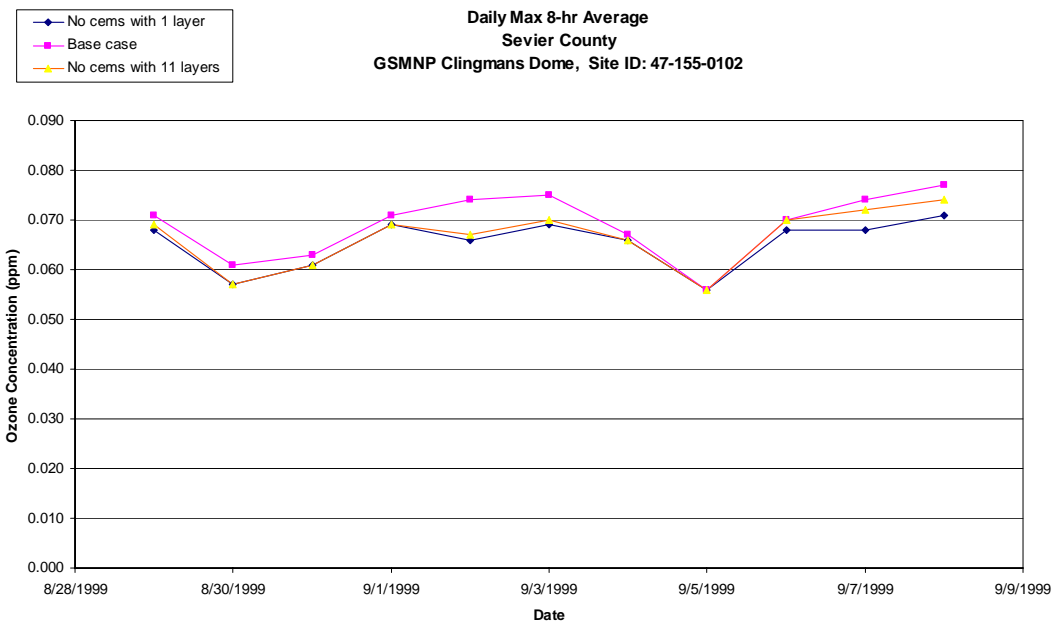


Figure 4.79 Sevier County (Clingmans Dome) – Comparison between – CEMS and Conventional Inventory

CHAPTER 5

CONCLUSIONS

The main objective of this study was to conduct a performance analysis of the CMAQ model and determine it's sensitive to ozone precursors in East Tennessee. The episode under consideration was August 29, 1999 to September 8, 1999, a period of unusually high measured ozone concentrations in the study area. The results were compared to eight monitoring stations in East Tennessee. The conclusions and the summary of results from 11 CMAQ runs for the 11 day episode are listed below:

Model Performance Results: The CMAQ model captured the general trend for the maximum 8 -hour average ozone concentrations.

- The CMAQ model captured the general trend for the maximum 8 -hour average ozone concentrations in East Tennessee.
- Based on the ppb difference between average predicted and average observed concentrations and average bias values, the model performed overall better at the Anderson, Jefferson and Knox County monitors where the model predictions were only from 3 to 9 ppb lower than the measured values.
- Based on the ppb difference between average predicted and average observed concentrations and average bias values the model performance was poor at elevated locations like the Sevier County and Blount County monitors where the model under predicted measured concentrations by 20 to 22 ppb.
- Resolving emissions in 11 vertical layers allowed the model to perform better than when only a single layer of emissions was used. With multiple layers the model predictions were 1 to 2 ppb closer to measure values.
- The ppb difference between average predicted and average observed ozone concentrations were better with CEMS data. CEMS emissions data for point sources resulted in concentration predictions that 3 to 5 ppb closer to measured concentrations

The following conclusions are based on the summary of ozone reductions for various emission reduction scenarios (Refer to Summary tables in chapter 4).

- The model is more sensitive to reductions in mobile source NO_x emissions than point source NO_x emissions. A 15% reduction in mobile NO_x emissions reduced ozone by an average of 4 ppb, while a 15% reduction in point source NO_x lowered ozone only 2 ppb.
- The model predicts that ozone in East Tennessee is sensitive to both NO_x and VOC emission reductions. A one-ton reduction in mobile source VOC emission lowered predicted ozone an average of 0.011 ppb while a one ton reduction in NO_x emissions lowered predicted ozone by 0.013 ppb. Therefore both NO_x and

VOC emission reductions may be beneficial in lowering ozone levels in East Tennessee.

- The reduction in ozone with reduction in mobile source NO_x emissions was not linear. For both Jefferson and Knox County, a 30 % reduction in mobile NO_x emissions gave only slightly lower ozone concentrations than a 15% reduction.
- For the rest of the counties (especially rural, high elevation sites), mobile source NO_x emission reductions were more effective than point source emission reductions in lowering ozone levels.
- Elevated sites yielded more reduction in ozone concentration than other ground level sites irrespective of the reduction made in ozone precursors' emissions. This indicates that the elevated sites are more sensitive to control strategies than the other sites.
- The current ozone design value for East Tennessee is 89 ppb. It will require a 4.5% reduction in maximum 8-hour ozone concentrations to achieve the NAAQS of 85 ppb. The CMAQ modeling indicates that a 20% to 30% reduction in NO_x emissions from a combination of point and mobile sources may allow the NAAQS to be achieved.

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APPENDIX

APPENDIX

A-1 Observed Maximum 8-hr Average Ozone Concentrations at Monitor Site

Date	Anderson	Blount - Cades Cove	Blount - Look Rock	Jefferson	Knox-0021	Knox-1020	Sevier-0101	Sevier-0102
8/29/1999	0.063	0.076	0.079	0.068	0.072	0.071	0.083	0.084
8/30/1999	0.064	0.077	0.078	0.066	0.066	0.065	0.082	0.079
8/31/1999	0.070	0.077	0.09	0.064	0.069	0.07	0.088	0.08
9/1/1999	0.083	0.089	0.105	0.079	0.079	0.074	0.097	0.086
9/2/1999	0.066	0.084	0.102	0.038	0.09	0.087	0.104	0.084
9/3/1999	0.086	0.071	0.101	0.074	0.077	0.087	0.098	0.086
9/4/1999	0.097	0.086	0.107	0.093	0.094	0.097	0.101	0.096
9/5/1999	0.065	0.066	0.09	0.048	0.054	0.06	0.08	0.083
9/6/1999	0.054	0.056	0.071	0.046	0.053	0.056	0.083	0.086
9/7/1999	0.076	0.093	0.096	0.069	0.073	0.084	0.097	0.102
9/8/1999	0.084	0.084	0.098	0.074	0.086	0.09	0.095	0.09

A-2 Vertical Resolution of the Modeling Domain

CMAQ Layer*	Range of Sigma Pressures [‡]	Approximate Elevation above ground surface (m) [†]
1	1.000 to 0.983	0 to 130
2	0.983 to 0.965	130 to 269
3	0.965 to 0.932	269 to 530
4	0.932 to 0.882	530 to 937
5	0.882 to 0.833	937 to 1,353
6	0.833 to 0.751	1,353 to 2,090
7	0.751 to 0.675	2,090 to 2,828
8	0.675 to 0.600	2,828 to 3,613
9	0.600 to 0.450	3,613 to 5,423
10	0.450 to 0.250	5,423 to 8,569
11	0.250 to 0.000	8,569 to 16,262

* Layer 1 is the lowest layer (from the ground level)

‡ Sigma Pressure $\sigma_p = (P_z - P_t)/(P_s - P_t)$

Where,

P_z = Pressure at elevation 'z' in millibars

P_t = Pressure at the top in millibars (100 mb)

P_s = Pressure at the land surface in millibars (1000 mb)

† Elevations are approximate, since they are back calculated from sigma pressure values.

A-3 Default Time and Space Invariant Initial Conditions in the CMAQ Model Used for the 36 km Domain

Species	Units	Sigma Pressure Levels*					
		1.0 to 0.98	0.98 to 0.93	0.93 to 0.84	0.84 to 0.60	0.60 to 0.30	0.30 to 0.0
SO2	ppm	3.000E-04	2.000E-04	1.000E-04	1.000E-04	2.000E-05	1.000E-05
SULF	ppm	1.000E-30	1.000E-30	1.000E-30	1.000E-30	1.000E-30	1.000E-30
NO2	ppm	1.670E-04	1.670E-04	8.400E-05	0.000E+00	0.000E+00	0.000E+00
NO	ppm	8.300E-05	8.300E-05	4.200E-05	0.000E+00	0.000E+00	0.000E+00
O3	ppm	3.500E-02	3.500E-02	4.000E-02	5.000E-02	6.000E-02	7.000E-02
HNO3	ppm	5.000E-05	5.000E-05	5.000E-05	5.000E-05	7.000E-05	1.000E-04
H2O2	ppm	1.000E-03	1.000E-03	1.500E-03	1.000E-03	8.000E-04	2.000E-04
ALD	ppm	3.000E-05	3.500E-05	3.000E-05	2.000E-05	2.000E-05	1.000E-05
HCHO	ppm	2.500E-04	2.500E-04	2.500E-04	2.000E-04	1.000E-04	5.000E-05
OP1	ppm	2.500E-07	2.500E-07	2.500E-07	2.000E-07	1.000E-07	5.000E-08
OP2	ppm	3.000E-08	3.500E-08	3.000E-08	2.000E-08	2.000E-08	1.000E-08
PAA	ppm	3.000E-05	3.000E-05	3.000E-05	2.500E-05	2.000E-05	1.500E-05
ORA1	ppm	1.000E-06	1.000E-06	5.000E-07	5.000E-07	5.000E-07	0.000E+00
ORA2	ppm	1.000E-06	1.000E-06	5.000E-07	5.000E-07	5.000E-07	0.000E+00
NH3	ppm	1.000E-04	1.000E-04	3.000E-05	2.000E-05	2.000E-05	1.000E-05
N2O5	ppm	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
NO3	ppm	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
PAN	ppm	2.000E-05	2.000E-05	1.000E-05	1.000E-05	1.000E-05	0.000E+00
HC3	ppm	4.000E-05	4.000E-05	3.200E-05	1.200E-05	4.000E-06	0.000E+00
HC5	ppm	4.000E-05	4.000E-05	3.200E-05	1.200E-05	4.000E-06	0.000E+00
HC8	ppm	2.000E-05	2.000E-05	1.600E-05	6.000E-06	2.000E-06	0.000E+00
ETH	ppm	1.000E-04	1.000E-04	1.000E-04	7.500E-05	1.000E-05	5.000E-06
CO	ppm	8.000E-02	8.000E-02	8.000E-02	7.000E-02	6.500E-02	5.000E-02
OL2	ppm	5.000E-06	3.000E-06	2.000E-06	1.000E-06	1.000E-06	0.000E+00
OLT	ppm	2.000E-07	2.000E-07	1.000E-07	0.000E+00	0.000E+00	0.000E+00
OLI	ppm	1.000E-07	1.000E-07	0.000E+00	0.000E+00	0.000E+00	0.000E+00
TOL	ppm	1.000E-06	1.000E-06	1.000E-06	1.000E-06	0.000E+00	0.000E+00
XYL	ppm	2.000E-07	2.000E-07	1.000E-07	0.000E+00	0.000E+00	0.000E+00
ACO3	ppm	1.000E-09	1.000E-09	1.000E-09	1.000E-09	1.000E-09	1.000E-09
TPAN	ppm	1.000E-08	1.000E-08	1.000E-08	1.000E-08	1.000E-08	1.000E-08
HONO	ppm	1.000E-09	1.000E-09	1.000E-09	1.000E-09	1.000E-09	1.000E-09
HNO4	ppm	2.000E-09	2.000E-09	2.000E-09	2.000E-09	2.000E-09	2.000E-09
KET	ppm	5.000E-04	5.000E-04	5.000E-04	3.330E-04	3.330E-04	1.670E-04
GLY	ppm	2.500E-07	2.500E-07	2.500E-07	2.000E-07	1.000E-07	5.000E-08
MGLY	ppm	2.500E-07	2.500E-07	2.500E-07	2.000E-07	1.000E-07	5.000E-08
DCB	ppm	2.500E-07	2.500E-07	2.500E-07	2.000E-07	1.000E-07	5.000E-08
ONIT	ppm	2.000E-05	2.000E-05	1.600E-05	6.000E-06	2.000E-06	0.000E+00
CSL	ppm	1.000E-09	1.000E-09	1.000E-09	1.000E-09	1.000E-09	1.000E-09

Species	Units	Sigma Pressure Levels*					
		1.0 to 0.98	0.98 to 0.93	0.93 to 0.84	0.84 to 0.60	0.60 to 0.30	0.30 to 0.0
ISO	ppm	1.500E-04	1.500E-04	0.000E+00	0.000E+00	0.000E+00	0.000E+00
HO	ppm	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
HO2	ppm	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
MACR	ppm	1.500E-05	1.500E-05	0.000E+00	0.000E+00	0.000E+00	0.000E+00
MVK	ppm	3.000E-05	3.000E-05	0.000E+00	0.000E+00	0.000E+00	0.000E+00
ASO4I	µg/m ³	4.810E-03	4.810E-03	3.207E-03	3.207E-03	6.413E-04	3.207E-04
ASO4J	µg/m ³	5.964E-01	5.964E-01	3.976E-01	3.976E-01	7.952E-02	3.976E-02
NUMATKN	#/m ³	1.437E+09	1.437E+09	9.583E+08	9.583E+08	1.917E+08	9.583E+07
NUMACC	#/m ³	2.123E+08	2.123E+08	1.416E+08	1.416E+08	2.831E+07	1.416E+07
ASOIL	µg/m ³	1.890E-05	1.890E-05	1.890E-05	1.890E-05	1.890E-05	1.890E-05
NUMCOR	#/m ³	1.000E+00	1.000E+00	1.000E+00	1.000E+00	1.000E+00	1.000E+00
SRFATKN	m ² /m ³	7.931E-07	7.931E-07	5.287E-07	5.287E-07	1.057E-07	5.287E-08
SRFACC	m ² /m ³	8.544E-06	8.544E-06	5.696E-06	5.696E-06	1.139E-06	5.696E-07
AORGBI	µg/m ³	1.000E-05	1.000E-05	6.670E-06	6.670E-06	1.330E-06	6.670E-07
AORGBJ	µg/m ³	9.900E-04	9.900E-04	6.600E-04	6.600E-04	1.320E-04	6.600E-05
AORGAI	µg/m ³	1.000E-05	1.000E-05	6.670E-06	6.670E-06	1.330E-06	6.670E-07
AORGAJ	µg/m ³	9.900E-04	9.900E-04	6.600E-04	6.600E-04	1.320E-04	6.600E-05

* Sigma Pressure as defined in Appendix A-2.

Initial conditions for other levels are automatically interpolated by the ICON. Any needed species conversion to CB4 species is done by the ICON processor (Byun and Ching, 1999).

A-4 Default Time and Space Invariant Boundary Conditions in the CMAQ Model Used for the 36 km Domain

North

Species	Units	Sigma Pressure Levels*					
		1.0 to 0.98	0.98 to 0.93	0.93 to 0.84	0.84 to 0.60	0.60 to 0.30	0.30 to 0.0
SO2	ppm	3.000E-04	2.000E-04	1.000E-04	1.000E-04	2.000E-05	1.000E-05
SULF	ppm	1.000E-30	1.000E-30	1.000E-30	1.000E-30	1.000E-30	1.000E-30
NO2	ppm	1.670E-04	1.670E-04	8.400E-05	0.000E+00	0.000E+00	0.000E+00
NO	ppm	8.300E-05	8.300E-05	4.200E-05	0.000E+00	0.000E+00	0.000E+00
O3	ppm	3.500E-02	3.500E-02	4.000E-02	5.000E-02	6.000E-02	7.000E-02
HNO3	ppm	5.000E-05	5.000E-05	5.000E-05	5.000E-05	7.000E-05	1.000E-04
H2O2	ppm	1.000E-03	1.000E-03	1.500E-03	1.000E-03	8.000E-04	2.000E-04
ALD	ppm	3.000E-05	3.500E-05	3.000E-05	2.000E-05	2.000E-05	1.000E-05
HCHO	ppm	2.500E-04	2.500E-04	2.500E-04	2.000E-04	1.000E-04	5.000E-05
OP1	ppm	2.500E-07	2.500E-07	2.500E-07	2.000E-07	1.000E-07	5.000E-08
OP2	ppm	3.000E-08	3.500E-08	3.000E-08	2.000E-08	2.000E-08	1.000E-08
PAA	ppm	3.000E-05	3.000E-05	3.000E-05	2.500E-05	2.000E-05	1.500E-05
ORA1	ppm	1.000E-06	1.000E-06	5.000E-07	5.000E-07	5.000E-07	0.000E+00
ORA2	ppm	1.000E-06	1.000E-06	5.000E-07	5.000E-07	5.000E-07	0.000E+00
NH3	ppm	1.000E-04	1.000E-04	3.000E-05	2.000E-05	2.000E-05	1.000E-05
N2O5	ppm	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
NO3	ppm	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
PAN	ppm	1.000E-04	1.000E-04	5.000E-05	5.000E-05	1.500E-05	0.000E+00
HC3	ppm	4.000E-05	4.000E-05	3.200E-05	1.200E-05	4.000E-06	0.000E+00
HC5	ppm	4.000E-05	4.000E-05	3.200E-05	1.200E-05	4.000E-06	0.000E+00
HC8	ppm	2.000E-05	2.000E-05	1.600E-05	6.000E-06	2.000E-06	0.000E+00
ETH	ppm	1.000E-04	1.000E-04	8.000E-05	3.000E-05	1.000E-05	0.000E+00
CO	ppm	8.000E-02	8.000E-02	8.000E-02	7.000E-02	6.500E-02	5.000E-02
OL2	ppm	5.000E-06	3.000E-06	2.000E-06	1.000E-06	1.000E-06	0.000E+00
OLT	ppm	2.000E-07	2.000E-07	1.000E-07	0.000E+00	0.000E+00	0.000E+00
OLI	ppm	1.000E-07	1.000E-07	0.000E+00	0.000E+00	0.000E+00	0.000E+00
TOL	ppm	1.000E-06	1.000E-06	1.000E-06	1.000E-06	0.000E+00	0.000E+00
XYL	ppm	2.000E-07	2.000E-07	1.000E-07	0.000E+00	0.000E+00	0.000E+00
ACO3	ppm	1.000E-09	1.000E-09	1.000E-09	1.000E-09	1.000E-09	1.000E-09
TPAN	ppm	1.000E-08	1.000E-08	1.000E-08	1.000E-08	1.000E-08	1.000E-08
HONO	ppm	1.000E-09	1.000E-09	1.000E-09	1.000E-09	1.000E-09	1.000E-09
HNO4	ppm	2.000E-09	2.000E-09	2.000E-09	2.000E-09	2.000E-09	2.000E-09
KET	ppm	5.000E-04	5.000E-04	5.000E-04	3.330E-04	3.330E-04	1.670E-04
GLY	ppm	2.500E-07	2.500E-07	2.500E-07	2.000E-07	1.000E-07	5.000E-08
MGLY	ppm	2.500E-07	2.500E-07	2.500E-07	2.000E-07	1.000E-07	5.000E-08
DCB	ppm	2.500E-07	2.500E-07	2.500E-07	2.000E-07	1.000E-07	5.000E-08
ONIT	ppm	2.000E-05	2.000E-05	1.600E-05	6.000E-06	2.000E-06	0.000E+00

Species	Units	Sigma Pressure Levels*					
		1.0 to 0.98	0.98 to 0.93	0.93 to 0.84	0.84 to 0.60	0.60 to 0.30	0.30 to 0.0
ISO	ppm	1.500E-04	1.500E-04	0.000E+00	0.000E+00	0.000E+00	0.000E+00
HO	ppm	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
HO2	ppm	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
MACR	ppm	1.500E-05	1.500E-05	0.000E+00	0.000E+00	0.000E+00	0.000E+00
MVK	ppm	3.000E-05	3.000E-05	0.000E+00	0.000E+00	0.000E+00	0.000E+00
ASO4I	µg/m ³	4.810E-03	4.810E-03	3.207E-03	3.207E-03	6.413E-04	3.207E-04
ASO4J	µg/m ³	5.964E-01	5.964E-01	3.976E-01	3.976E-01	7.952E-02	3.976E-02
NUMATKN	#/m ³	1.437E+09	1.437E+09	9.583E+08	9.583E+08	1.917E+08	9.583E+07
NUMACC	#/m ³	2.123E+08	2.123E+08	1.416E+08	1.416E+08	2.831E+07	1.416E+07
ASOIL	µg/m ³	1.890E-05	1.890E-05	1.890E-05	1.890E-05	1.890E-05	1.890E-05
NUMCOR	#/m ³	1.000E+00	1.000E+00	1.000E+00	1.000E+00	1.000E+00	1.000E+00
SRFATKN	m ² /m ³	7.931E-07	7.931E-07	5.287E-07	5.287E-07	1.057E-07	5.287E-08
SRFACC	m ² /m ³	8.544E-06	8.544E-06	5.696E-06	5.696E-06	1.139E-06	5.696E-07
AORGBI	µg/m ³	1.000E-05	1.000E-05	6.670E-06	6.670E-06	1.330E-06	6.670E-07
AORGBJ	µg/m ³	9.900E-04	9.900E-04	6.600E-04	6.600E-04	1.320E-04	6.600E-05
AORGAI	µg/m ³	1.000E-05	1.000E-05	6.670E-06	6.670E-06	1.330E-06	6.670E-07
AORGAI	µg/m ³	9.900E-04	9.900E-04	6.600E-04	6.600E-04	1.320E-04	6.600E-05

* Sigma Pressure as defined in appendix A-2.

Boundary conditions for other levels are automatically interpolated by the BCON. Any needed species conversion to CB4 species is done by the BCON processor (Byun and Ching, 1999).

A-4 Continued

East

Species	Units	Sigma Pressure Levels*					
		1.0 to 0.98	0.98 to 0.93	0.93 to 0.84	0.84 to 0.60	0.60 to 0.30	0.30 to 0.0
SO2	ppm	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
SULF	ppm	1.000E-30	1.000E-30	1.000E-30	1.000E-30	1.000E-30	1.000E-30
NO2	ppm	1.000E-05	1.000E-05	0.000E+00	0.000E+00	0.000E+00	0.000E+00
NO	ppm	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
O3	ppm	3.000E-02	3.500E-02	4.000E-02	5.000E-02	6.000E-02	7.000E-02
HNO3	ppm	5.000E-05	5.000E-05	5.000E-05	5.000E-05	5.000E-05	1.500E-04
H2O2	ppm	2.000E-03	2.000E-03	2.000E-03	2.000E-03	1.500E-03	1.500E-03
ALD	ppm	4.000E-05	4.000E-05	4.000E-05	4.000E-05	4.000E-05	4.000E-05
HCHO	ppm	2.500E-04	2.500E-04	2.500E-04	2.000E-04	1.500E-04	1.000E-04
OP1	ppm	2.500E-07	2.500E-07	2.500E-07	2.000E-07	1.500E-07	1.000E-07
OP2	ppm	4.000E-08	4.000E-08	4.000E-08	4.000E-08	4.000E-08	4.000E-08
PAA	ppm	5.000E-05	5.000E-05	5.000E-05	5.000E-05	5.000E-05	5.000E-05
ORA1	ppm	1.500E-06	5.000E-07	5.000E-07	5.000E-07	5.000E-07	5.000E-07
ORA2	ppm	1.500E-06	5.000E-07	5.000E-07	5.000E-07	5.000E-07	5.000E-07
NH3	ppm	5.000E-05	5.000E-05	5.000E-05	2.000E-05	2.000E-05	2.000E-05
N2O5	ppm	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
NO3	ppm	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
PAN	ppm	1.500E-05	1.500E-05	1.500E-05	1.500E-05	1.500E-05	1.500E-05
HC3	ppm	1.200E-05	1.200E-05	1.200E-05	8.000E-06	4.000E-06	4.000E-06
HC5	ppm	1.200E-05	1.200E-05	1.200E-05	8.000E-06	4.000E-06	4.000E-06
HC8	ppm	6.000E-06	6.000E-06	6.000E-06	4.000E-06	2.000E-06	2.000E-06
ETH	ppm	1.000E-04	1.000E-04	1.000E-04	6.700E-05	3.300E-05	3.300E-05
CO	ppm	8.000E-02	8.000E-02	8.000E-02	7.500E-02	7.000E-02	6.500E-02
OL2	ppm	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
OLT	ppm	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
OLI	ppm	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
TOL	ppm	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
XYL	ppm	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
ACO3	ppm	1.000E-09	1.000E-09	1.000E-09	1.000E-09	1.000E-09	1.000E-09
TPAN	ppm	1.000E-08	1.000E-08	1.000E-08	1.000E-08	1.000E-08	1.000E-08
HONO	ppm	1.000E-09	1.000E-09	1.000E-09	1.000E-09	1.000E-09	1.000E-09
HNO4	ppm	2.000E-09	2.000E-09	2.000E-09	2.000E-09	2.000E-09	2.000E-09
KET	ppm	5.000E-04	5.000E-04	5.000E-04	5.000E-04	5.000E-04	5.000E-04
GLY	ppm	2.500E-07	2.500E-07	2.500E-07	2.000E-07	1.500E-07	1.000E-07
MGLY	ppm	2.500E-07	2.500E-07	2.500E-07	2.000E-07	1.500E-07	1.000E-07
DCB	ppm	2.500E-07	2.500E-07	2.500E-07	2.000E-07	1.500E-07	1.000E-07
ONIT	ppm	6.000E-06	6.000E-06	6.000E-06	4.000E-06	2.000E-06	2.000E-06

Species	Units	Sigma Pressure Levels*					
		1.0 to 0.98	0.98 to 0.93	0.93 to 0.84	0.84 to 0.60	0.60 to 0.30	0.30 to 0.0
ISO	ppm	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
HO	ppm	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
HO2	ppm	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
MACR	ppm	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
MVK	ppm	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
ASO4I	µg/m ³	6.413E-03	6.413E-03	6.413E-03	6.413E-03	6.413E-04	3.207E-04
ASO4J	µg/m ³	7.952E-01	7.952E-01	7.952E-01	7.952E-01	7.952E-02	3.976E-02
NUMATKN	#/m ³	1.917E+09	1.917E+09	1.917E+09	1.917E+09	1.917E+08	9.583E+07
NUMACC	#/m ³	2.831E+08	2.831E+08	2.831E+08	2.831E+08	2.831E+07	1.416E+07
ASOIL	µg/m ³	1.890E-05	1.890E-05	1.890E-05	1.890E-05	1.890E-05	1.890E-05
NUMCOR	#/m ³	1.000E+00	1.000E+00	1.000E+00	1.000E+00	1.000E+00	1.000E+00
SRFATKN	m ² /m ³	1.057E-06	1.057E-06	1.057E-06	1.057E-06	1.057E-07	5.287E-08
SRFACC	m ² /m ³	1.139E-05	1.139E-05	1.139E-05	1.139E-05	1.139E-06	5.696E-07
AORGBI	µg/m ³	1.330E-05	1.330E-05	1.330E-05	1.330E-05	1.330E-06	6.670E-07
AORGBJ	µg/m ³	1.320E-03	1.320E-03	1.320E-03	1.320E-03	1.320E-04	6.600E-05
AORGAI	µg/m ³	1.330E-05	1.330E-05	1.330E-05	1.330E-05	1.330E-06	6.670E-07
AORGAI	µg/m ³	1.320E-03	1.320E-03	1.320E-03	1.320E-03	1.320E-04	6.600E-05

* Sigma Pressure as defined in appendix A-2.

Boundary conditions for other levels are automatically interpolated by the BCON. Any needed species conversion to CB4 species is done by the BCON processor (Byun and Ching, 1999).

A-4 Continued

South

Species	Units	Sigma Pressure Levels*					
		1.0 to 0.98	0.98 to 0.93	0.93 to 0.84	0.84 to 0.60	0.60 to 0.30	0.30 to 0.0
SO2	ppm	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
SULF	ppm	1.000E-30	1.000E-30	1.000E-30	1.000E-30	1.000E-30	1.000E-30
NO2	ppm	1.000E-05	1.000E-05	0.000E+00	0.000E+00	0.000E+00	0.000E+00
NO	ppm	1.000E-05	1.000E-05	0.000E+00	0.000E+00	0.000E+00	0.000E+00
O3	ppm	3.000E-02	3.500E-02	4.000E-02	5.000E-02	6.000E-02	7.000E-02
HNO3	ppm	5.000E-05	5.000E-05	5.000E-05	5.000E-05	5.000E-05	1.500E-04
H2O2	ppm	2.000E-03	2.000E-03	2.000E-03	2.000E-03	1.500E-03	1.000E-03
ALD	ppm	4.000E-05	4.000E-05	4.000E-05	4.000E-05	4.000E-05	5.000E-06
HCHO	ppm	2.500E-04	2.500E-04	2.500E-04	2.000E-04	1.500E-04	1.000E-04
OP1	ppm	2.500E-07	2.500E-07	2.500E-07	2.000E-07	1.500E-07	1.000E-07
OP2	ppm	4.000E-08	4.000E-08	4.000E-08	4.000E-08	4.000E-08	5.000E-09
PAA	ppm	1.000E-04	1.000E-04	1.000E-04	1.000E-04	5.000E-05	5.000E-05
ORA1	ppm	1.500E-06	5.000E-07	5.000E-07	5.000E-07	5.000E-07	5.000E-07
ORA2	ppm	1.500E-06	5.000E-07	5.000E-07	5.000E-07	5.000E-07	5.000E-07
NH3	ppm	5.000E-05	5.000E-05	5.000E-05	3.000E-05	2.000E-05	2.000E-05
N2O5	ppm	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
NO3	ppm	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
PAN	ppm	1.500E-05	1.500E-05	1.500E-05	1.500E-05	1.500E-05	1.500E-05
HC3	ppm	1.200E-05	1.200E-05	1.200E-05	4.000E-06	4.000E-06	4.000E-06
HC5	ppm	1.200E-05	1.200E-05	1.200E-05	4.000E-06	4.000E-06	4.000E-06
HC8	ppm	6.000E-06	6.000E-06	6.000E-06	2.000E-06	2.000E-06	2.000E-06
ETH	ppm	1.000E-04	1.000E-04	1.000E-04	6.700E-05	6.700E-05	6.700E-05
CO	ppm	7.000E-02	7.000E-02	7.000E-02	7.000E-02	6.500E-02	5.500E-02
OL2	ppm	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
OLT	ppm	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
OLI	ppm	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
TOL	ppm	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
XYL	ppm	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
ACO3	ppm	1.000E-09	1.000E-09	1.000E-09	1.000E-09	1.000E-09	1.000E-09
TPAN	ppm	1.000E-08	1.000E-08	1.000E-08	1.000E-08	1.000E-08	1.000E-08
HONO	ppm	1.000E-09	1.000E-09	1.000E-09	1.000E-09	1.000E-09	1.000E-09
HNO4	ppm	2.000E-09	2.000E-09	2.000E-09	2.000E-09	2.000E-09	2.000E-09
KET	ppm	5.000E-04	5.000E-04	5.000E-04	5.000E-04	5.000E-04	5.000E-05
GLY	ppm	2.500E-07	2.500E-07	2.500E-07	2.000E-07	1.500E-07	1.000E-07
MGLY	ppm	2.500E-07	2.500E-07	2.500E-07	2.000E-07	1.500E-07	1.000E-07
DCB	ppm	2.500E-07	2.500E-07	2.500E-07	2.000E-07	1.500E-07	1.000E-07
ONIT	ppm	6.000E-06	6.000E-06	6.000E-06	2.000E-06	2.000E-06	2.000E-06
CSL	ppm	1.000E-09	1.000E-09	1.000E-09	1.000E-09	1.000E-09	1.000E-09

Species	Units	Sigma Pressure Levels*					
		1.0 to 0.98	0.98 to 0.93	0.93 to 0.84	0.84 to 0.60	0.60 to 0.30	0.30 to 0.0
HO	ppm	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
HO2	ppm	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
MACR	ppm	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
MVK	ppm	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
ASO4I	µg/m ³	6.413E-03	6.413E-03	6.413E-03	3.207E-03	6.413E-04	3.207E-04
ASO4J	µg/m ³	7.952E-01	7.952E-01	7.952E-01	3.976E-01	7.952E-02	3.976E-02
NUMATKN	#/m ³	1.917E+09	1.917E+09	1.917E+09	9.583E+08	1.917E+08	9.583E+07
NUMACC	#/m ³	2.831E+08	2.831E+08	2.831E+08	1.416E+08	2.831E+07	1.416E+07
ASOIL	µg/m ³	1.890E-05	1.890E-05	1.890E-05	1.890E-05	1.890E-05	1.890E-05
NUMCOR	#/m ³	1.000E+00	1.000E+00	1.000E+00	1.000E+00	1.000E+00	1.000E+00
SRFATKN	m ² /m ³	1.057E-06	1.057E-06	1.057E-06	5.287E-07	1.057E-07	5.287E-08
SRFACC	m ² /m ³	1.139E-05	1.139E-05	1.139E-05	5.696E-06	1.139E-06	5.696E-07
AORGBI	µg/m ³	1.330E-05	1.330E-05	1.330E-05	6.670E-06	1.330E-06	6.670E-07
AORGBJ	µg/m ³	1.320E-03	1.320E-03	1.320E-03	6.600E-04	1.320E-04	6.600E-05
AORGAI	µg/m ³	1.330E-05	1.330E-05	1.330E-05	6.670E-06	1.330E-06	6.670E-07
AORGAJ	µg/m ³	1.320E-03	1.320E-03	1.320E-03	6.600E-04	1.320E-04	6.600E-05

* Sigma Pressure as defined in appendix A-2.

Boundary conditions for other levels are automatically interpolated by the BCON. Any needed species conversion to CB4 species is done by the BCON processor (Byun and Ching, 1999).

A-4 Continued

West

Species	Units	Sigma Pressure Levels*					
		1.0 to 0.98	0.98 to 0.93	0.93 to 0.84	0.84 to 0.60	0.60 to 0.30	0.30 to 0.0
SO2	ppm	3.000E-04	2.000E-04	2.000E-04	1.000E-04	0.000E+00	0.000E+00
SULF	ppm	1.000E-30	1.000E-30	1.000E-30	1.000E-30	1.000E-30	1.000E-30
NO2	ppm	1.670E-04	1.670E-04	1.670E-04	8.400E-05	0.000E+00	0.000E+00
NO	ppm	8.300E-05	8.300E-05	8.300E-05	4.200E-05	0.000E+00	0.000E+00
O3	ppm	3.500E-02	4.000E-02	4.500E-02	5.000E-02	6.000E-02	7.000E-02
HNO3	ppm	5.000E-04	5.000E-04	5.000E-04	5.000E-04	2.000E-04	1.000E-04
H2O2	ppm	2.000E-03	2.000E-03	2.000E-03	2.000E-03	8.000E-04	2.000E-04
ALD	ppm	4.000E-05	4.000E-05	4.000E-05	4.000E-05	4.000E-05	5.000E-06
HCHO	ppm	4.000E-04	4.000E-04	4.000E-04	4.000E-04	1.000E-04	5.000E-05
OP1	ppm	4.000E-07	4.000E-07	4.000E-07	4.000E-07	1.000E-07	5.000E-08
OP2	ppm	4.000E-08	4.000E-08	4.000E-08	4.000E-08	4.000E-08	5.000E-09
PAA	ppm	2.500E-05	2.500E-05	2.500E-05	2.500E-05	2.000E-05	1.000E-05
ORA1	ppm	2.500E-06	2.500E-06	2.500E-06	2.500E-06	5.000E-07	5.000E-07
ORA2	ppm	2.500E-06	2.500E-06	2.500E-06	2.500E-06	5.000E-07	5.000E-07
NH3	ppm	3.000E-04	3.000E-04	3.000E-04	2.000E-04	1.000E-04	5.000E-05
N2O5	ppm	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
NO3	ppm	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
PAN	ppm	1.500E-04	1.500E-04	1.500E-04	7.500E-05	1.500E-05	1.500E-05
HC3	ppm	8.000E-05	8.000E-05	8.000E-05	6.000E-05	8.000E-06	4.000E-06
HC5	ppm	8.000E-05	8.000E-05	8.000E-05	6.000E-05	8.000E-06	4.000E-06
HC8	ppm	4.000E-05	4.000E-05	4.000E-05	3.000E-05	4.000E-06	2.000E-06
ETH	ppm	1.000E-04	1.000E-04	1.000E-04	7.500E-05	1.000E-05	5.000E-06
CO	ppm	8.000E-02	8.000E-02	8.000E-02	8.000E-02	6.500E-02	5.000E-02
OL2	ppm	1.000E-05	1.000E-05	5.000E-06	5.000E-06	1.000E-06	0.000E+00
OLT	ppm	2.000E-06	1.000E-06	5.000E-07	3.000E-07	0.000E+00	0.000E+00
OLI	ppm	1.000E-06	2.000E-07	1.000E-07	0.000E+00	0.000E+00	0.000E+00
TOL	ppm	1.000E-05	5.000E-06	5.000E-06	3.000E-06	0.000E+00	0.000E+00
XYL	ppm	3.000E-06	2.000E-06	4.000E-07	4.000E-07	0.000E+00	0.000E+00
ACO3	ppm	1.000E-09	1.000E-09	1.000E-09	1.000E-09	1.000E-09	1.000E-09
TPAN	ppm	1.000E-08	1.000E-08	1.000E-08	1.000E-08	1.000E-08	1.000E-08
HONO	ppm	1.000E-09	1.000E-09	1.000E-09	1.000E-09	1.000E-09	1.000E-09
HNO4	ppm	2.000E-09	2.000E-09	2.000E-09	2.000E-09	2.000E-09	2.000E-09
KET	ppm	5.000E-04	5.000E-04	5.000E-04	5.000E-04	5.000E-04	5.000E-05
GLY	ppm	4.000E-07	4.000E-07	4.000E-07	4.000E-07	1.000E-07	5.000E-08
MGLY	ppm	4.000E-07	4.000E-07	4.000E-07	4.000E-07	1.000E-07	5.000E-08
DCB	ppm	4.000E-07	4.000E-07	4.000E-07	4.000E-07	1.000E-07	5.000E-08
ONIT	ppm	4.000E-05	4.000E-05	4.000E-05	3.000E-05	4.000E-06	2.000E-06
CSL	ppm	1.000E-09	1.000E-09	1.000E-09	1.000E-09	1.000E-09	1.000E-09
ISO	ppm	1.500E-04	3.000E-05	1.500E-05	0.000E+00	0.000E+00	0.000E+00
HO	ppm	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00

		Sigma Pressure Levels*					
Species	Units	1.0 to 0.98	0.98 to 0.93	0.93 to 0.84	0.84 to 0.60	0.60 to 0.30	0.30 to 0.0
MVK	ppm	3.000E-05	6.000E-06	3.000E-06	0.000E+00	0.000E+00	0.000E+00
ASO4I	µg/m ³	9.620E-03	6.413E-03	6.413E-03	3.207E-03	6.413E-04	3.207E-04
ASO4J	µg/m ³	1.193E+00	7.952E-01	7.952E-01	3.976E-01	7.952E-02	3.976E-02
NUMATKN	#/m ³	2.875E+09	1.917E+09	1.917E+09	9.583E+08	1.917E+08	9.583E+07
NUMACC	#/m ³	4.247E+08	2.831E+08	2.831E+08	1.416E+08	2.831E+07	1.416E+07
ASOIL	µg/m ³	1.890E-05	1.890E-05	1.890E-05	1.890E-05	1.890E-05	1.890E-05
NUMCOR	#/m ³	1.000E+00	1.000E+00	1.000E+00	1.000E+00	1.000E+00	1.000E+00
SRFATKN	m ² /m ³	1.586E-06	1.057E-06	1.057E-06	5.287E-07	1.057E-07	5.287E-08
SRFACC	m ² /m ³	1.709E-05	1.139E-05	1.139E-05	5.696E-06	1.139E-06	5.696E-07
AORGBI	µg/m ³	2.000E-05	1.330E-05	1.330E-05	6.670E-06	1.330E-06	6.670E-07
AORGBJ	µg/m ³	1.980E-03	1.320E-03	1.320E-03	6.600E-04	1.320E-04	6.600E-05
AORGAI	µg/m ³	2.000E-05	1.330E-05	1.330E-05	6.670E-06	1.330E-06	6.670E-07
AORGAJ	µg/m ³	1.980E-03	1.320E-03	1.320E-03	6.600E-04	1.320E-04	6.600E-05

* Sigma Pressure as defined in appendix A-2.

Boundary conditions for other levels are automatically interpolated by the BCON. Any needed species conversion to CB4 species is done by the BCON processor (Byun and Ching, 1999).

VITA

Karthikeyan (Surya) Ramaswamy was born in Tuticorin, India on 9th September, 1979. He enrolled in the Mechanical Engineering program at University of Madras, Chennai (Madras), India in 1997. He graduated from the University of Madras with a bachelor's degree in Mechanical Engineering in June 2001. He then worked for LEA Consultant as a CAD Engineer for 6 months. After that, he came to the United States to pursue his higher studies in 2002. In fall 2002, he enrolled in the graduate program in the Department of Civil and Environmental Engineering at the University of Tennessee, Knoxville and accepted a graduate teaching assistantship and graduate research assistantship from the department. During the years at the University of Tennessee, he was involved in photochemical modeling of ozone using the U.S. EPA's Models-3 system. He worked on many air dispersion modeling and estimated emissions from various mobile sources using MOBILE6. He received his M.S degree in Environmental Engineering, with a concentration in Air Quality from the University of Tennessee, Knoxville in May 2005.