

**Modeling Protocol for the OTC CALGRID
Screening-Level Modeling Platform for the
Evaluation of Ozone**

May 23, 2007

**New Hampshire Department of Environmental Services
Air Resources Division
29 Hazen Drive
Concord, NH 03302**

1.0 Introduction

The Ozone Transport Commission (OTC) has sponsored the development of a photochemical modeling system to assist states in the preparation of their State Implementation Plans (SIPs) for attaining the eight-hour National Ambient Air Quality Standard (NAAQS) for ozone. The Community Multiscale Air Quality Model (CMAQ) is the basis of the OTC SIP-quality modeling platform that is being used in states' eight-hour ozone attainment SIPs.

Running the CMAQ modeling platform is very resource intensive and usually requires the use of a Unix-based operating system. Therefore, the CMAQ modeling that is being done in support of the eight-hour ozone SIPs is limited to a handful of modeling centers that have the necessary expertise and computer resources. Similarly, because of the substantial effort, time, and storage space required to run the SIP-quality CMAQ platform, it is impractical to assess a large number of run scenarios.

Consequently, OTC sponsored the development of an additional grid-based photochemical modeling platform that states could use as a screening tool for running additional emissions control strategies or performing sensitivity runs. The requirements for this additional modeling platform were that it be flexible, portable, and easily accessible to agencies that wish to use it. In this manner, a larger number of run scenarios could be modeled, allowing states to screen a wider variety of potential control strategies.

The California Grid Model (CALGRID) was selected as the basis of this screening platform. CALGRID is a grid-based photochemical modeling platform that is designed to be run in a Windows environment. CALGRID has recently undergone a series of improvements and enhancements, with the most recent version being designated CALGRID Version 2.45. CALGRID Version 2.45 is being used as the screening platform for the OTC eight-hour ozone attainment SIPs. This document outlines the manner in which CALGRID will be used in these efforts.

2.0 Platform Description and Model Inputs

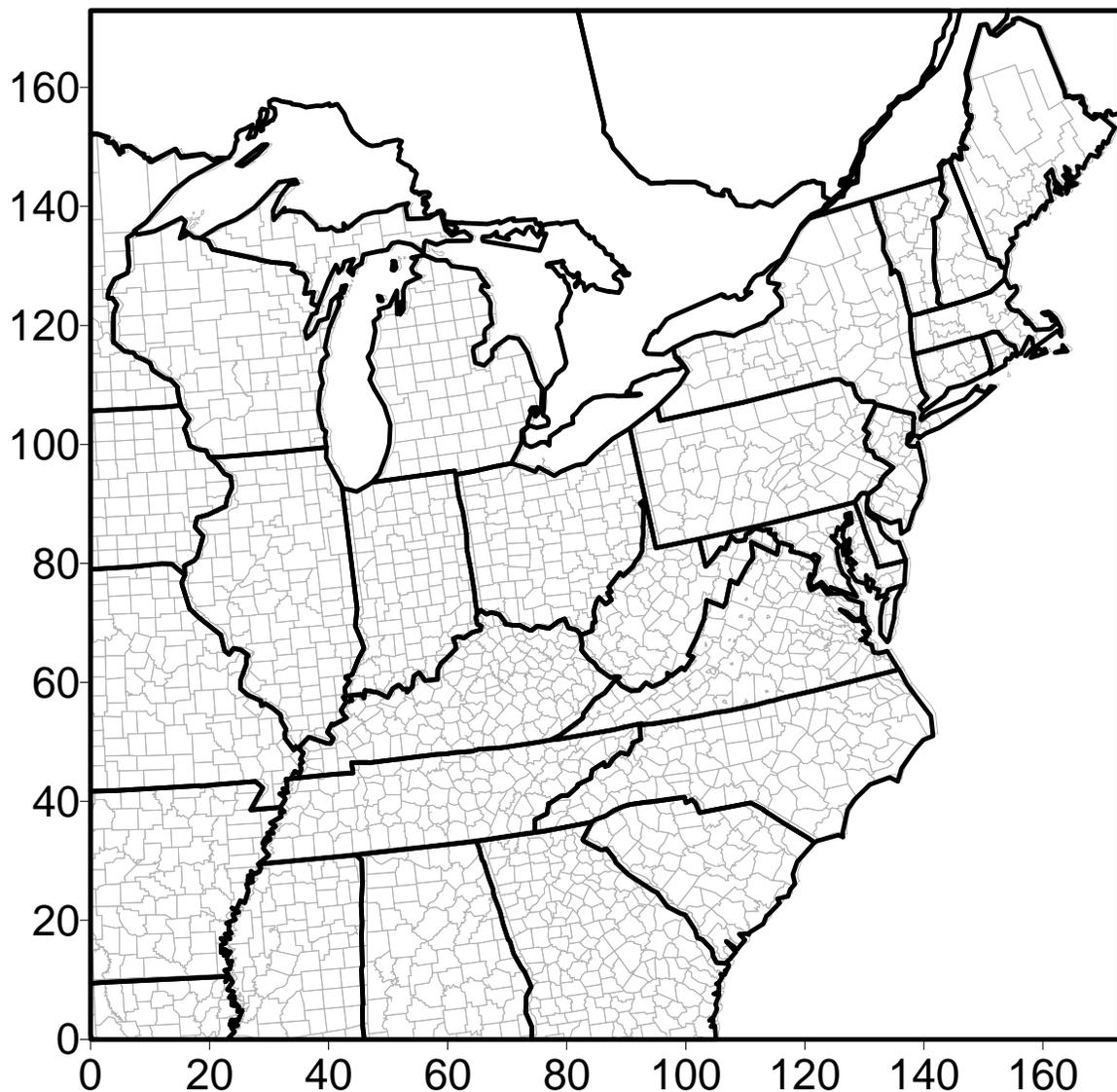
To make the CALGRID modeling platform the best possible tool to supplement the SIP-quality CMAQ platform, it was decided that CALGRID would be run on the same modeling domain using a common set of model inputs. All boundary conditions, meteorology, and emissions inputs were the same as those used for the SIP-quality CMAQ platform. Processing programs were written to convert these inputs into a format useable by the CALGRID model. The modeling domain and model inputs are described in the sections below.

2.1 Modeling Domain

The OTC CMAQ/CALGRID modeling domain was set up on a Lambert Conic Conformal projection and covers the eastern United States and parts of Canada. The

southwest corner of the domain was set at 264 km, -888 km and the northeast corner was set to 2328 km, 1176 km. A 12-km grid cell resolution was used with 172 grid cells in the east-west direction and 172 grid cells in the north-south direction. For the vertical grid definition, 22 layers were used in the CMAQ simulations. For CALGRID, the processing programs that were used to reformat the boundary conditions, meteorology, and emissions mapped the 22 layers used for CMAQ to a total of nine vertical layers for the CALGRID modeling. The OTC CMAQ/CALGRID modeling domain is shown in Figure 1.

Figure 1: Map of the OTC CMAQ/CALGRID Modeling Domain



2.2 Boundary Conditions

For the OTC CMAQ modeling, boundary conditions were derived from GEOS-Chem (Goddard Earth Observing System) global atmospheric simulations by running CMAQ

on the 36-km continental grid. For the CALGRID platform, initial conditions, side boundary conditions, and top layer concentrations were derived from the CMAQ boundary conditions files by means of a processing program. This program mapped the 22 vertical layers used in the CMAQ simulations to the nine layers used with CALGRID. It produced the necessary side boundary file and top layer concentration file for each modeled episode day. It also produced an initial conditions file for each episode day processed; these files could be retained so that the user could begin a CALGRID simulation on any desired episode day.

2.3 Meteorology

The meteorological modeling that was done in support of the OTC CMAQ SIP-quality modeling platform was performed by the University of Maryland (UMD) in conjunction with staff at the New York State Department of Environmental Conservation (NYSDEC). UMD used the Penn State/National Center for Atmospheric Research 5th Generation Mesoscale Model (MM5) Version 3.6 to generate year 2002 meteorological inputs. The details of this work are described in NYSDEC's Technical Support Document TSD-1a, *Meteorological Modeling Using Penn State/NCAR 5th Generation Mesoscale Model (MM5), February 1, 2006*. For the CALGRID modeling platform, a processing program was used to interpolate the MM5 outputs to the CALGRID modeling grid and map them to CALGRID's vertical layer structure. QA/QC plots were generated during the processing to ensure the accuracy of the interpolated data. Figures 2 through 4 show example QA/QC plots from the re-formatting of the meteorological data.

Figure 2: QA/QC Plot of Humidity Data

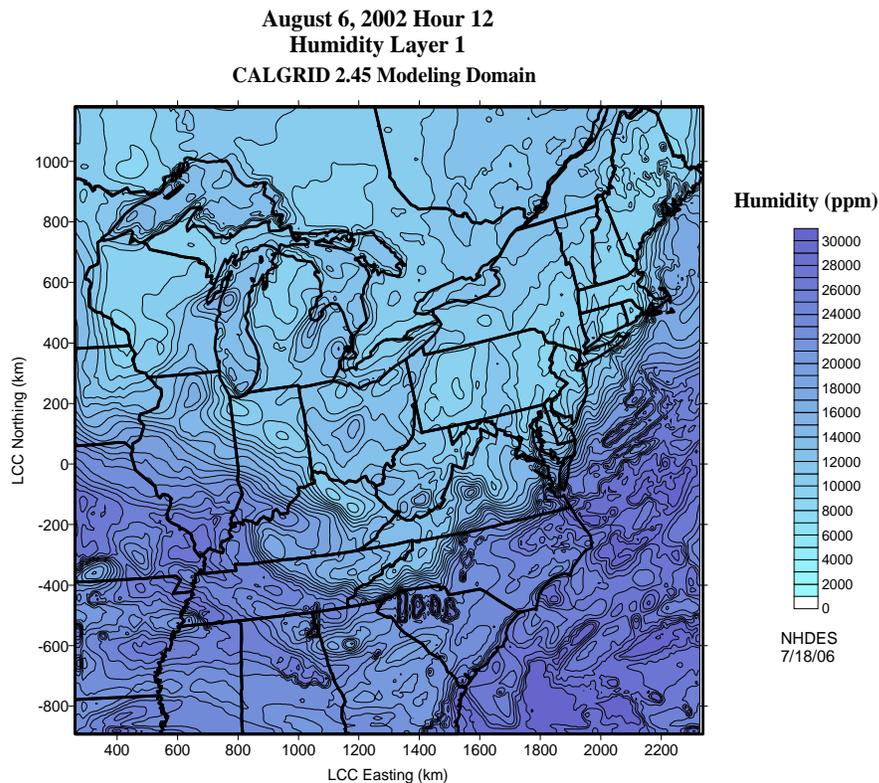


Figure 3: QA/QC Plot of Temperature Data

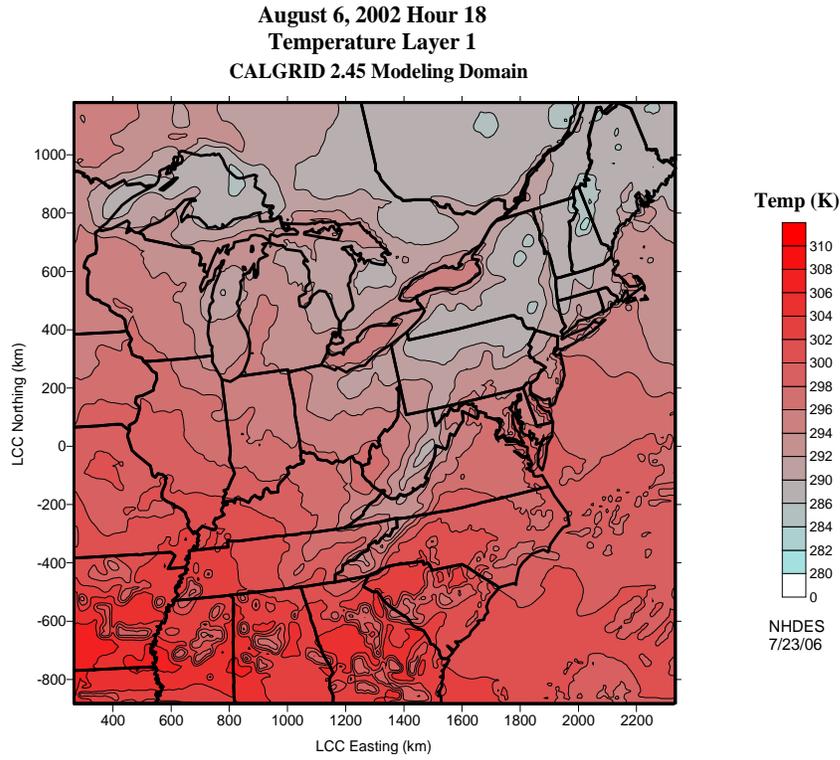
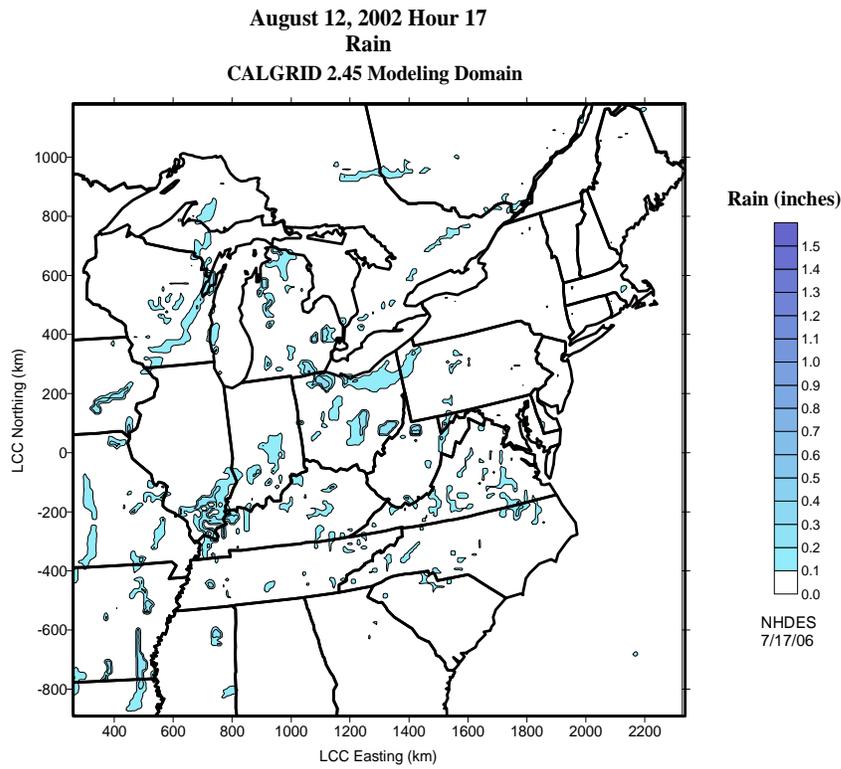


Figure 4: QA/QC Plot of Rainfall Data



2.4 Emissions

The Regional Planning Organizations (RPOs) and their contractors were responsible for preparing modeling emissions inventories for use in the OTC CMAQ SIP-quality modeling. The RPOs prepared a set of accurate, up-to-date, and quality assured emissions inventories for the 2002 Base Case and three future years, 2009, 2012, and 2018. For the future years, emissions inventories were prepared for two emissions control scenarios: one reflecting those emissions controls that are in place or likely to be in place by 2009, and another that reflects additional control strategies that may be needed to demonstrate attainment with the eight-hour ozone standard. The first scenario is referred to as “On The Books/On The Way” (OTB/OTW), and the second is referred to as “Beyond On The Way” (BOTW). These inventories were broken down into the following general emissions source categories: biogenic, point, area, non-road mobile, and on-road mobile.

Using these inventories, NYSDEC and the other modeling centers, the Virginia Department of Environmental Quality (VADEQ) and Northeast States for Coordinated Air Use Management (NESCAUM), generated the necessary emissions inputs for CMAQ using the Sparse Matrix Operator Kernel Emissions (SMOKE) model. For the CALGRID modeling effort, the pre-merged SMOKE emissions files were obtained from the modeling centers and re-formatted for input into EMSPROC, the emissions pre-processor for the CALGRID modeling system. The pre-merged SMOKE files that were obtained from the modeling centers were broken down into the biogenic, point, area, non-road, and on-road categories mentioned earlier. These files by component were then converted for use with EMSPROC, thus giving users of the CALGRID modeling system the flexibility to analyze a wide variety of emissions control strategies. QA/QC plots were generated during the re-formatting of the emissions data to ensure that an accurate modeling inventory was generated for the CALGRID platform. Example emissions QA/QC plots are shown in Figures 5 through 8.

Figure 5: QA/QC Plot of Surface Source CO Emissions

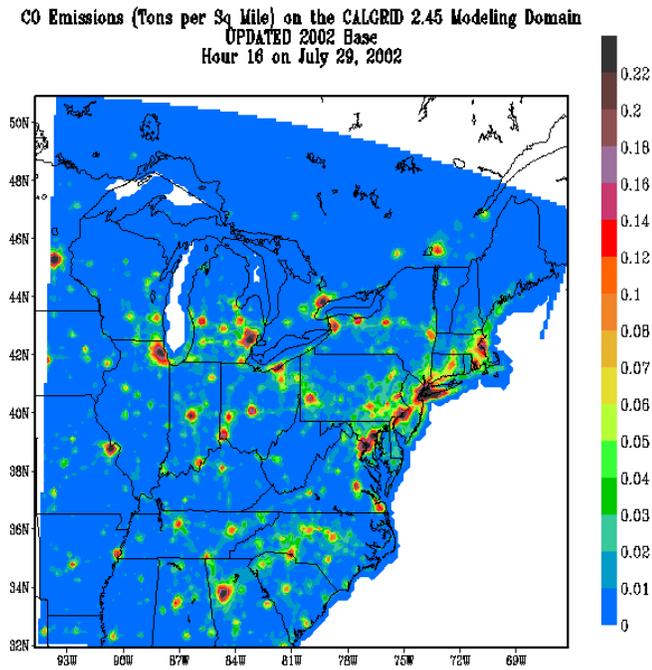


Figure 6: QA/QC Plot of Surface Source VOC Emissions

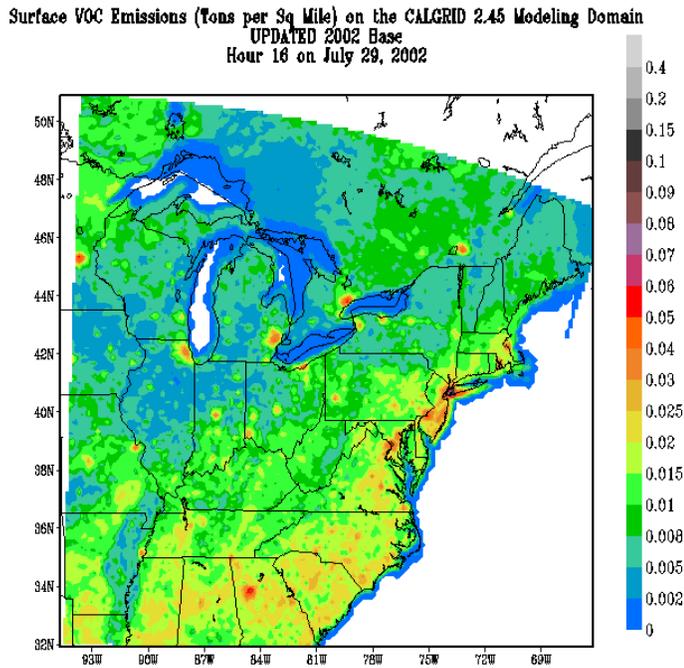


Figure 7: QA/QC Plot of Point Source NOx Emissions

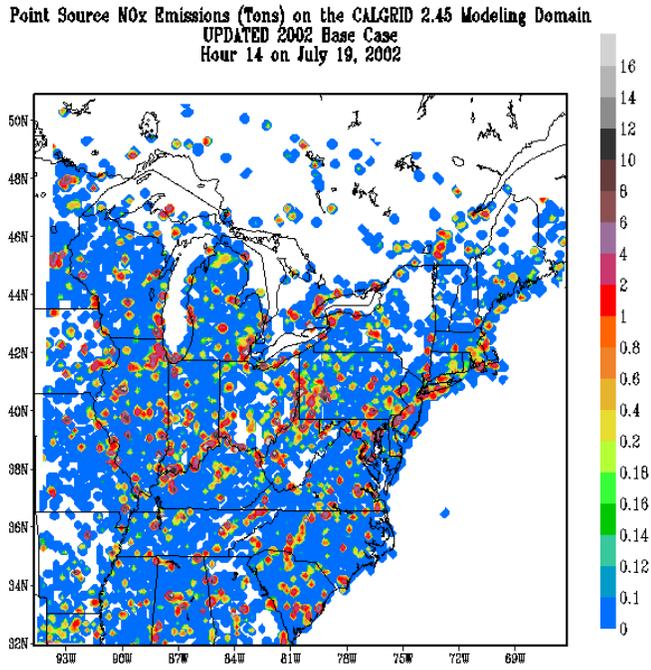
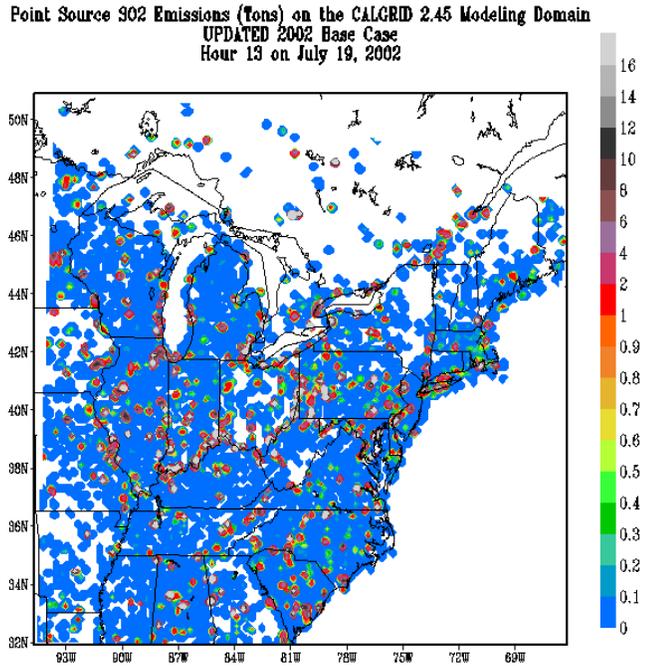


Figure 8: QA/QC Plot of Point Source SO2 Emissions



3.0 CALGRID Model Outputs

A variety of post-processing programs have been developed to assist users of the CALGRID modeling platform in visualizing and tabulating model results. These post-processors are designed to take the hourly concentration output generated by the CALGRID model and produce statistical results for desired averaging periods and geographic areas. CALGRID can also generate output suitable for plotting with standard graphical packages such as the Center for Ocean-Land-Atmosphere Studies' Grid Analysis and Display System (GrADS) or Golden Software's SURFER.

As with the CMAQ SIP-quality modeling platform, it was decided that the CALGRID screening results should be used in a relative manner. Ratios of model-predicted base case and future scenario concentrations would be applied to current monitored ozone design values to generate estimated future design values (DVs) for the future-year scenario of interest. It is these DVs that are used in the determination of attainment.

4.0 Episode Selection

For the CMAQ SIP-quality modeling analysis, the five-month ozone season of 2002 was selected for modeling because it met EPA's episode selection criteria of containing episode days that are meteorologically representative of typical high ozone exceedance days and that are severe enough that any control strategy that is predicted to reach attainment on those days would reach attainment on other less severe days.

Similarly, the CALGRID screening platform was run for the summer period from May 15 to September 15, 2002 for the 2002 Base Case and 2009 OTB/OTW and BOTW scenarios. However, running the full summer episode, even with the CALGRID screening platform, is very time-consuming and resource intensive. In order to increase production and maximize the number of scenarios that can be evaluated with the CALGRID screening platform, it was decided that shorter modeling episodes would be selected that adequately reproduced the results obtained by running the full summer episode. An extensive analysis was undertaken to run a number of shorter summer episodes and compare the resulting predicted DVs with those obtained for the full summer episode. The 2002 Base Case and 2009 OTB/OTW scenarios were used in this evaluation. It was found that the combined DVs calculated from the July 6 to July 23, 2002 and July 30 to August 16, 2002 modeling episodes best represented those from the full summer episode (note that July 6th and July 30th are considered to be model warm-up days).

5.0 CALGRID Model Performance Evaluation

A qualitative and quantitative assessment was made of the CALGRID screening platform's ability to reproduce observed ozone concentrations. To assess its performance, the CALGRID screening platform was run for the 2002 Base Case for the July 30 to August 16, 2002 modeling episode. Predicted maximum eight-hour ozone concentrations at monitor locations were compared against observations for 2002. Figure

9 shows the relative bias between maximum eight-hour ozone observations and predicted CALGRID eight-hour ozone concentrations for the 2002 Base Case for the episode from July 30 through August 12. Figures 10 through 13 show plots of predicted 2002 Base Case ozone concentrations against 2002 observations for selected episode days. Although the CALGRID model has a tendency to over-predict, especially in the urban core areas of northern Virginia, Maryland, southeastern Pennsylvania, New York City and Boston, it does a reasonable job of reproducing the pattern of the 2002 maximum ozone observations.

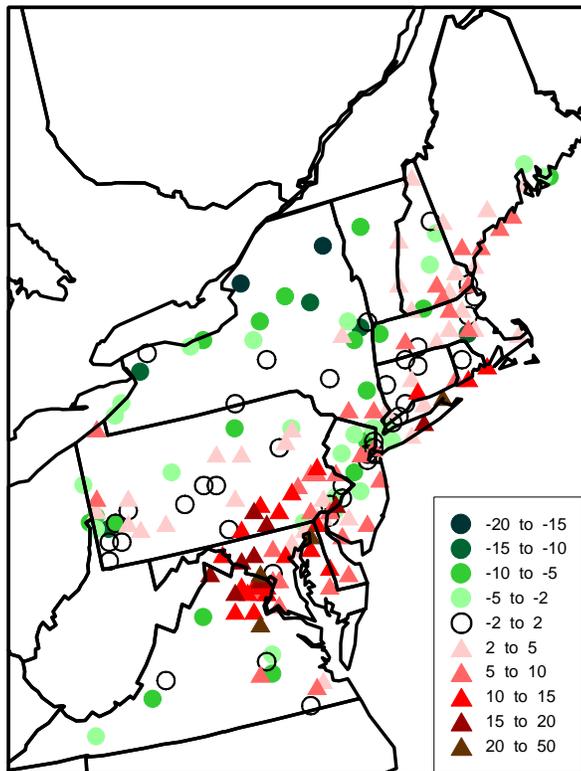
Figure 9: Relative Bias Between Maximum 8-hour Ozone Concentrations Predicted with CALGRID and Observations

Relative Bias (CALGRID minus Observed)

Based on Model Data for
July 30 - August 12, 2002
2002 Base Case Emissions
versus Observed Data

Green Circles are where
CALGRID Underpredicts

Red Triangles are where
CALGRID Overpredicts



NHDES 11/21/06

Figure 10: Comparison of Maximum 8-hour Ozone Concentrations for August 11, 2002

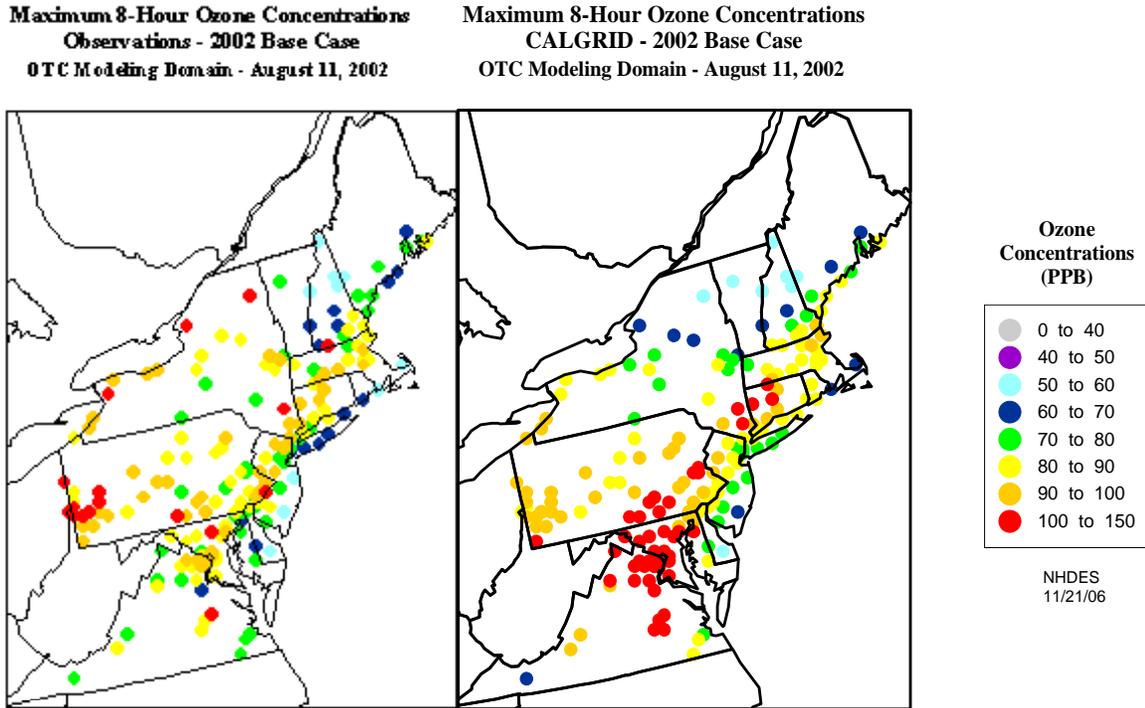


Figure 11: Comparison of Maximum 8-hour Ozone Concentrations for August 12, 2002

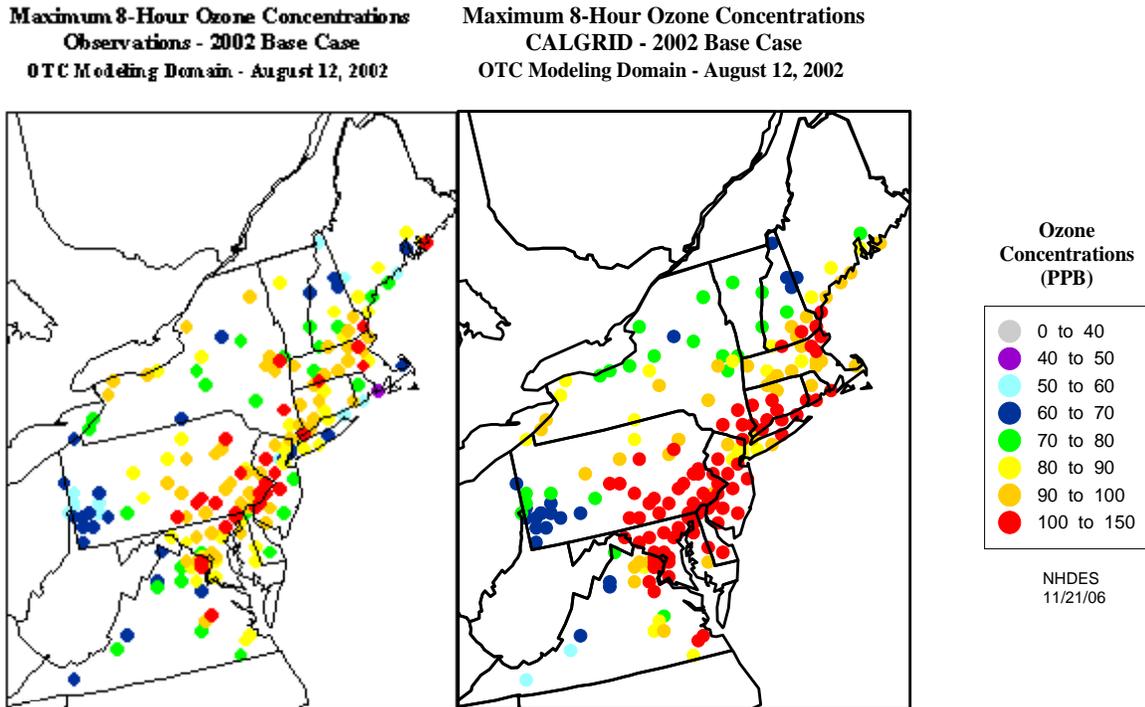


Figure 12: Comparison of Maximum 8-hour Ozone Concentrations for August 13, 2002

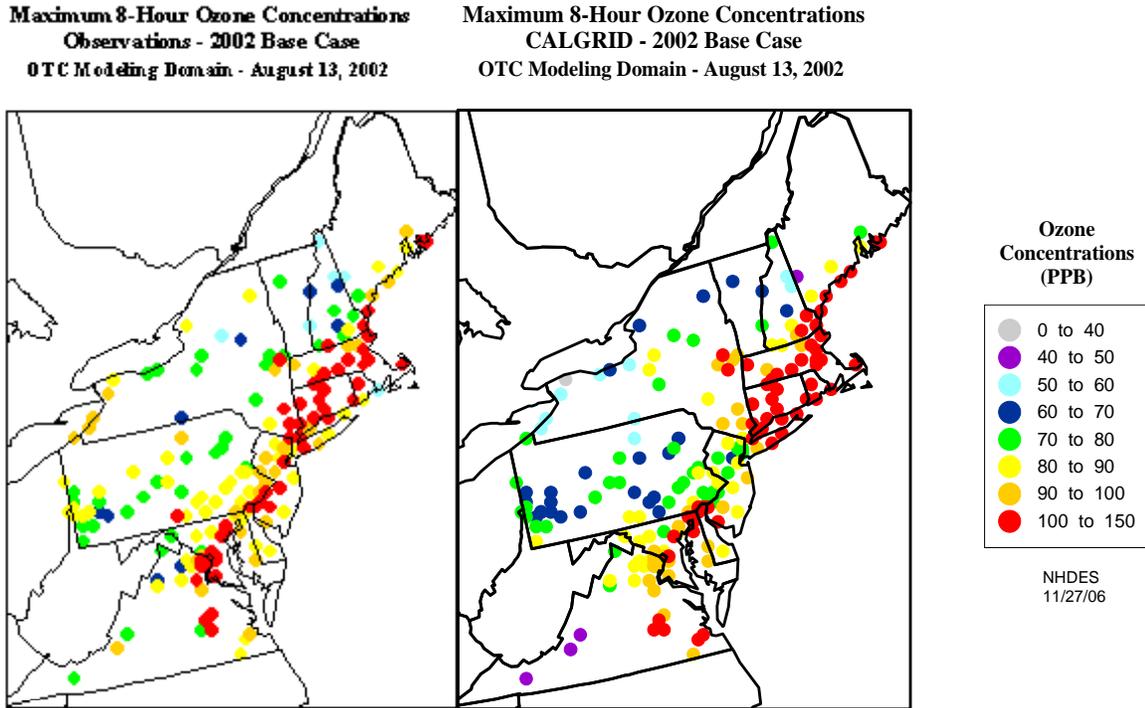
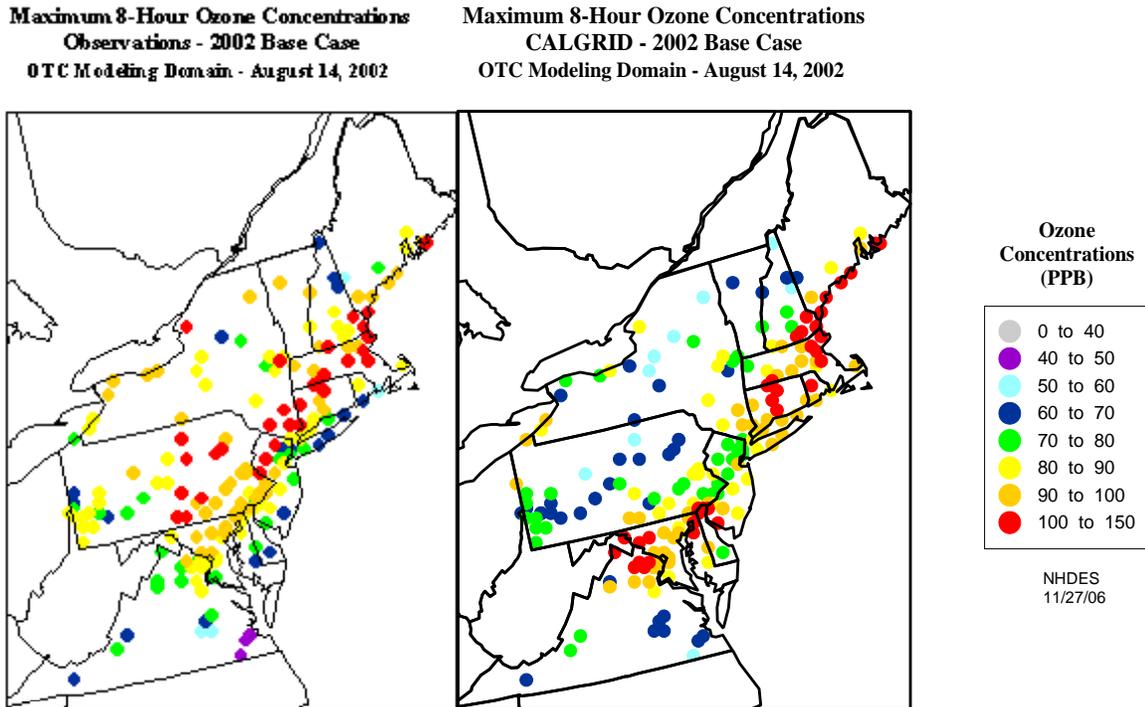


Figure 13: Comparison of Maximum 8-hour Ozone Concentrations for August 14, 2002



6.0 CALGRID Model Runs

The OTC CALGRID modeling platform will be run for the 2002 Base Case, 2009 OTB/OTB, and 2009 BOTW. These simulations will be run for the full summer (May 15 to September 15, 2002) episode as well as for the shorter summer modeling episodes described earlier. A variety of control scenarios and sensitivity runs will be performed for the shorter episodes as requested by the OTC Modeling Committee or individual state agencies. The results of these runs may be used to evaluate, at a screening level, any additional emissions reductions that may be required, thus relieving the technical burden on the CMAQ modeling centers. CALGRID screening results may also be used in individual states' weight-of-evidence (WOE) analyses. If states request it, the CALGRID modeling platform will be delivered so that they may run additional modeling scenarios at their discretion.