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A Modeling Protocol for the OTC SIP Quality
Modeling System For Assessment of the Ozone
National Ambient Air Quality Standard
in the Ozone Transport Region

The Modeling Committee of the
Ozone Transport Commission

TABLE OF CONTENTS

1 STUDY DESIGN

- 1.1 Background
- 1.2 Objectives
- 1.3 Photochemical Modeling System
- 1.4 Deliverables
- 1.5 Schedule

2 MANAGEMENT STRUCTURE

- 2.1 OTR Oversight Committee
- 2.2 OTR Photochemical Modeling Workgroup
- 2.3 OTR Meteorological Modeling Workgroup
- 2.4 OTR Emission Inventory Development Workgroup
- 2.5 OTR Control Strategy Development Workgroup
- 2.6 OTC Modeling Committee

3 OTR MODELING DOMAIN

- 3.1 Description
- 3.2 Horizontal Grid Size
- 3.2 Number of Vertical Layers

4 OZONE EPISODES

- 4.1 EPA Episode Selection Criteria
- 4.2 Proposed Episode Selection Procedure

5 METEOROLOGICAL FIELDS

5.1 MM5 Meteorological Fields

5.2 Quality Assurance of MM5 Meteorological Fields

6 BASE CASE EMISSION INVENTORIES FOR 2002

6.1 2002 Emission Inventories for OTC States

6.2 2002 Emission Inventories for All Other OTR States

7 BASE CASE EMISSION INPUT FILES FOR 2002

7.1 Preparation of 2002 Emission Input Files for the OTR Domain

7.2 Quality Assurance of 2002 Emission Input Files for the OTR Domain

8 AIR QUALITY DATA

8.1 Initial conditions

8.2 Boundary conditions

8.3 Ambient Air Quality Data

9 DIAGNOSTIC ANALYSES

9.1 Quality Assurance Tests of Input Components

9.2 Diagnostic Tests

10 MODEL PERFORMANCE EVALUATION

10.1 Performance Criteria

10.2 Statistical Performance Measures

11 CAA EMISSION INVENTORIES FOR 2010 AND 2013

- 11.1 CAA Emission Inventories for OTC States for 2010
- 11.2 CAA Emission Inventories for all other OTR States for 2010
- 11.3 CAA Emission Inventories for OTC States for 2013
- 11.4 CAA Emission Inventories for all other OTR States for 2013

12 CAA EMISSION INPUT FILES FOR 2010 AND 2013 FOR THE OTR DOMAIN

- 12.1 2010 CAA Emission Input Files for OTR Domain
- 12.2 2013 CAA Emission Input Files for OTR Domain

13 OZONE CONTROL STRATEGY FOR THE OTR DOMAIN

- 13.1 OTC CALGRID System Screening Runs
- 13.2 OTC SIP Modeling Platform Runs
- 13.3 Analysis of Available Air Quality and Emission Databases
- 13.4 OTR Domain Ozone Control Strategy

14 OZONE CONTROL STRATEGY EMISSION INPUT FILES

- 14.1 2010 Ozone Control Strategy Emission Input Files for OTR Domain
- 14.2 2013 Ozone Control Strategy Emission Input Files for OTR Domain

15 OZONE PREDICTIONS FOR 2010 and 2013

- 15.1 Initial Conditions
- 15.2 Boundary conditions
- 15.3 CAA Ozone Predictions for 2010 and 2013
- 15.4 Ozone Control Strategy Predictions for 2010 and 2013

16 DOCUMENTATION REPORT

17 REFERENCES

APPENDIX A: Work Plan for the Development and Application of the OTC SIP Quality Modeling System For Assessment of the Ozone National Ambient Air Quality Standard in the Ozone Transport Region

APPENDIX B: Workgroups for the Development and Application of the OTC SIP Quality Modeling System For Assessment of the Ozone National Ambient Air Quality Standard in the Ozone Transport Region

APPENDIX C: MOU for the Development and Application of the OTC SIP Quality Modeling System For Assessment of the Ozone National Ambient Air Quality Standard in the Ozone Transport Region

1 STUDY DESIGN

1.1 Background

Moderate and serious non-attainment areas in the Ozone Transport Region (OTR) are required to attain the 8-hour ozone NAAQS by 2010 and 2013, respectively. The Ozone Transport Commission (OTC) has embarked on the task of preparing an SIP ozone modeling system for exercising photochemical grid model(s) to assess the impact of candidate ozone control strategies in moderate and serious non-attainment areas in the OTR. The OTC Directors endorsed the Modeling Protocol for the OTC SIP Quality Modeling System For Assessment of the Ozone National Ambient Air Quality Standard in the Ozone Transport Region at the November 12-13, 2003 Fall meeting of the OTC.

This modeling protocol outlines procedures to prepare and use the OTC SIP ozone modeling system to help design an ozone attainment strategy to attain the ozone 8-hour NAAQS in the OTR. Emission inventories for point, area, on-road and off-road sources of NO_x, VOC and CO will be developed for a base year of 2002. BEIS3 will be used to estimate biogenic emissions. MM5 will be used at a 12 km grid resolution and, in the photochemical grid model, 4 km grid cells will be nested in urban areas where appropriate. A model performance evaluation will be prepared for 2002. If model performance is satisfactory, emission input files reflecting candidate control strategy scenarios for 2010 and 2013 will be prepared, and 2010 and 2013 ozone levels will be simulated with the modeling system. OTC States with moderate and serious non-attainment areas will then use these modeling results to help support required ozone attainment demonstrations.

1.2 Objective

The New York Department of Environmental Conservation has agreed to be the lead agency for developing a SIP quality ozone modeling system for assessing the future year attainment of the ozone 8-hour NAAQS in the OTR. The CMAQ or CAMx model will be used to evaluate the effectiveness of control strategies in the OTR Modeling Domain. The regulatory objective will be to design an ozone control strategy that will result in attainment of the 8-hour ozone NAAQS in moderate non-attainment areas by 2010, and in serious non-attainment areas by 2013.

1.3 Photochemical modeling System

Currently there is no guideline modeling system for demonstrating ozone attainment. The OTC Modeling Committee in its prior work exercised both CMAQ and CAMx and noticed that even though these models had performed similarly in estimating ozone on an over-all basis, the level of agreement between the simulated and measured concentrations varied from good to bad

depending on the model and depending upon the simulation day. So, as part of this protocol, both models (which continue to be updated by their developers) will be applied for an episode that occurred in 2002. Based upon the performance, one of these models would be selected for further application and use to evaluate the effectiveness of proposed control strategies in the OTR. The analysis identifying the basis for the selection of the modeling system will be communicated through the OTC modeling committee.

The OTC Modeling Committee also examined two emissions processors (EMS2001 and SMOKE, both using CB4 chemistry) in its prior work and concluded that there are differences between them that could be minimized by forcing the models to use a common speciation and surrogate data base. In the current protocol, we envision the use of both of them in the initial assessment for an episode in 2002 and then, based upon the best performance, one of these emission processors would be selected for constructing emission files for the SIP quality ozone modeling system for the OTR Domain.

1.4 Deliverables

The key deliverables for the SIP quality ozone modeling system for the OTR are listed below.

- Select Ozone Episodes
- Prepare Meteorological Fields
- Prepare 2002 Emission Inventories for each OTC State
- Acquire 2002 Emission Inventories for non-OTC States in the OTR Domain
- Prepare 2002 Emission Input Files for the OTR Domain
- Complete 2002 Model Performance Evaluation for the OTR Domain
- Prepare 2010 and 2013 CAA Emission Inventories for each OTC State
- Acquire 2013 Emission Inventories for non-OTC States in the OTR Domain
- Prepare 2010 and 2013 CAA Emission Input Files for the OTR Domain
- Complete Modeling Runs for 2010 and 2013 CAA Scenarios
- Design Control Strategy for the OTR Modeling Domain.
- Prepare 2010 and 2013 Emission Input Files for OTR Control Strategy
- Complete Modeling Runs for 2010 and 2013 for Control Strategy
- Complete Evaluation Report for 2010 and 2013 Control Strategy

1.5 Schedule

The schedule for developing the SIP quality modeling system and the assessment of the ozone NAAQS in the Ozone Transport region is provided in Appendix A.

2 MANAGEMENT STRUCTURE

2.1 OTR Oversight Committee

OTC Air Directors will serve as the OTR Oversight Committee. The Directors will ensure that

2002, 2010 and 2013 CAA emission inventories are prepared for each OTC state in the OTR domain, and will also be responsible for obtaining emission inventories for OTR states that are not members of the OTC. The Directors will oversee the design of ozone control strategies for the OTR, and will make the final decision on any funding needed to develop the OTC SIP quality modeling system. The Directors will review all OTC SIP quality modeling system documentation before it is released to interested parties.

2.2 OTC Modeling Committee

The state members of the OTC Modeling Committee will provide policy and day to day technical guidance for the development of the OTC SIP quality modeling system. The Committee will recommend (to the OTC Air Directors) what tasks need to be funded in order to develop the OTC SIP quality modeling system in a timely fashion.

2.3 OTR Photochemical Modeling Workgroup

The OTR Photochemical Modeling Workgroup will be responsible for preparing the modeling assessment of the ozone NAAQS in the OTR. The Workgroup will be responsible for collecting and processing model input data, setting up all model input files, performing model runs, and interpreting and documenting the results of the modeling analyses for the OTR domain. The Workgroup will prepare and submit all OTC SIP quality modeling system documentation to the OTC Air Directors. Gopal Sistla, NY DEC will serve as the lead for this group.

2.4 OTR Meteorological Modeling Workgroup

The OTR Meteorological Modeling Workgroup will be responsible for preparing and assessing MM5 meteorological fields for the OTR domain. The OTR Meteorological Modeling Workgroup will work with the OTR Photochemical Modeling Workgroup to prepare all meteorological input files for the OTC SIP quality modeling system. Mike Woodman, MDE, will serve as the lead for this group.

2.5 OTR Emission Inventory Development Workgroup

The OTR Emission Inventory Development Workgroup will be responsible for obtaining or developing guidance for preparing 2002, 2010 and 2013 state emission inventories for all states in the OTR. Ray Malenfant, DE DNREC, will serve as the lead for this group.

2.6 OTR Control Strategy Development Workgroup

The OTR Control Strategy Development Workgroup will be responsible for designing an ozone control strategy for the OTR Domain that will attain the ozone NAAQS by 2010 in moderate non-attainment areas and 2013 in serious non-attainment areas. The Workgroup will work with OTR states and the OTC stationary and mobile source committees to design an effective ozone control strategy for the OTR domain. Jeff Underhill, NH DES, will serve as the lead for this group.

3 OTR MODELING DOMAIN

3.1 Description

The modeling domain selected (see Figure 1 (where?)) follows the national grid adopted by the Regional Planning Organizations (RPOs), but with focus on the eastern U.S. The areal extent of the domain was selected such that the northeastern areas of Maine are well inside the domain. Based upon the existing computer resources, the southern and western boundaries were limited to the region shown in Figure 1. At a horizontal grid resolution of 12 km, it is estimated that there are 160 grids in the east-west and 150 grids in north-south direction. Depending upon the need and available resources, a 4 km grid over the selected urban areas could also be considered in this exercise.

3.2 Horizontal Grid Size

Following EPA and as noted above, a 12 km grid resolution will be used for most of the domain, with 4 km grid cells nested in urban areas where appropriate. This is a compromise between a finer grid mesh, which would offer greater resolution but at higher computational costs. A coarser mesh may not be appropriate for urban area applications.

3.3 Number of Vertical Layers

Similar to the horizontal grid spacing which is fixed by the default set forth in the design of the meteorological model, in this case 12 km, the definition of the vertical structure could also be adopted one-to-one of the meteorological model. However, based upon prior experience, the vertical extent of the model was set around a height of 6 to 8 km. Also, as the number of levels in the vertical increases, so does the computational time as well as the storage requirements for the data. On the other hand, limiting the vertical resolution to a few layers would inherently discard the detailed information provided by the meteorological model. Thus a compromise solution would be to maintain the high resolution with a one-to-one design of the vertical layers up to approximately 1 or 2 km yielding around 7 to 10 levels, followed by a collapse of the MM5 upper layers to around 6 to 8 km to form another 6 to 8 levels. Thus, under this scenario there would be a total of 13 to 18 layers in the vertical with 7 to 10 levels below 2 km and the remaining between 2 and 8 km. It should be noted that the mid-point of layer 1 in this analysis is around 10 m.

4 OZONE EPISODES

4.1 Episode Selection Criteria

Since it would be impractical to model every violation day, EPA has recommended targeting a select group of episode days for ozone attainment demonstrations. Such episode days should be (1) meteorologically representative of typical high ozone exceedance days in the domain,

and (2) so severe that any control strategies predicted to attain the ozone NAAQS for that episode day would also result in attainment for all other exceedance days.

4.2 Proposed Episode Selection Procedure

While the above suggested approach is perhaps feasible for isolated urban areas, such an approach may not be meaningful given the areal extent of concern and the modeling domain. Also, selection of episodes from different years would require the generation of the meteorological fields and emissions database, which would be an extremely difficult proposition given the modeling domain. A major portion of the ozone season of 2002 will be simulated with the OTC SIP modeling system. The 2002 ozone season had significant number of high exceedance days (the spatial distribution of the daily 1-hr and 8-hr maxima over the eastern U. S. can be examined at the site ftp://www.dec.state.ny.us/dar/air_research/htdocs/index.html). It is anticipated that the total number of days examined under this approach would far exceed the recommended two or three episodes, and would also provide for better assessment of the simulated pollutant fields. EPA has also recommended using 2002 as the base year for the SIP emission inventory.

5 METEOROLOGICAL FIELDS

5.1 MM5 Meteorological Fields

The MM5 setup has been described by Zhang (2000) for generating meteorological fields that are to be based on modified Blackadar scheme for the boundary layer. Since there are a variety of options that can be exercised in the application of MM5, initial testing will be performed for a high ozone event of 2002 with the most commonly used default options as well as with modified boundary layer schemes. It is anticipated that these MM5 simulations will be able to define the set of options which will be used to develop the remainder of the simulation period. Details of these experiments and results will be posted on the web site as well as will be presented at the appropriate venues.

5.2 Quality Assurance of Meteorological Fields

As a part of this effort, the simulated meteorological fields will be compared to data collected under CASTNET. Prior experience has shown that this approach provides for an independent assessment of the simulated meteorological conditions. Also, data from any other special measurements will be sought and compared. This analysis should provide a degree of confidence in the simulated meteorological fields and their use in photochemical grid modeling. This work will be coordinated through the meteorological model work group.

6 BASE CASE EMISSION INVENTORIES FOR 2002

6.1 2002 Base Case Emission Inventories for OTC states

Each state in the OTR Domain will prepare a 2002 base year Emission Inventory that include VOC, NO_x, and CO for a typical ozone summer day. States are to follow EPA guidance documents for this base year inventory which is due to EPA by June 1, 2004. Note this inventory may also be qualified as the consolidated emissions regulatory report (CERR).

All emission categories will be estimated for each county and state and the seasonal factors will facilitate spatial and temporal adjustments for modeling. Point and area source data will be submitted by individual states to EPA for uploading to EPA's National Emission Inventory (NEI) database using the required EPA format. MOBILE6.2 input files and VMT data will be submitted to NEI so that EPA can generate on-road mobile emissions for each state by county in a format that can be easily gridded and speciated. Similarly, off-road input files will be sent to EPA for running the latest NONROAD model. Biogenic emissions will be estimated with EPA's BEIS-3 emissions model.

It is anticipated that these inventories developed by the states will follow the EPA prescribed approach and should be formatted in a consistent manner. While this protocol is to deal with the 8-hr ozone issues, the inventory would also contain the necessary information for exercising the particulate option of the photochemical model. This would be of help in those cases where the one-atmosphere option is to be exercised in the assessment. Biogenic emissions will be estimated with EPA's BEIS-3 emissions model

6.1 2002 Base Case Emission Inventories for All Other States in the OTR

A 2002 base year emission inventory that include VOC, NO_x, and CO for a typical ozone summer day will be obtained for all non-OTC states in the OTR. It is anticipated that these inventories will be developed following EPA guidance, and will be formatted in a consistent manner.

7 BASE CASE EMISSION INPUT FILES FOR 2002

7.1 Preparation of 2002 Emission Input Files for the OTR Domain

Emissions data will be processed using EMS95/EMS2000, and SMOKE. The surrogate data files for the OTR grid have been previously developed by NY DEC and will be used in this study. For those pollutants that depend upon ambient temperature, MM5 layer-1 gridded temperature fields will be used.

7.2 Quality Assurance of 2002 Emission Input Files for the OTR Domain

The processing of the emissions data will be accompanied with several quality checks before the data are exercised in the simulations. Prior experiences have shown that considerable time and resources are often invested in developing the gridded emissions data. While there are many avenues to improve or correct the data, based upon consensus of the OTC

Photochemical Modeling Workgroup, a definite closure of the emissions processing will be adhered to and any further changes or corrections will be archived and incorporated at a later date. In performing this work close attention will be paid to the emissions within the OTR and, if necessary, corrections will be incorporated on the advice of the OTC Photochemical Modeling Workgroup

Hourly plume heights will be calculated and emissions from sources with plume heights below the top of the first layer will be assigned to the appropriate 5 by 5 kilometer surface grid cell. Emissions from sources with plume heights above the top of the first layer will be assigned to the appropriate grid cell in the second layer.

Biogenic emissions will be prepared for each episode day using BEIS-3. The temperature data from MM5 layer-1 will be used along with cloud cover information obtained from MM5.

8 AIR QUALITY DATA

7.1 Initial conditions

Prior experiences have shown that a 3-day ramp-up period is sufficient to establish pollutant levels that are encountered in the beginning of the ozone episode. The initial conditions at the startup would be for "clean" conditions.

7.2 Boundary conditions

In prior studies attempts have been made to include any information that is available from ozonesonde and from monitors that are near the western and northern boundaries of the modeling domain. For this study, similar attempts will be made to obtain pollutant data at the boundaries. In the absence of reliable boundary condition data, "clean " conditions will be assumed for boundary conditions.

7.3 Ambient Air Quality Data

Ambient air quality data will be extracted from the EPA AQS archive for ozone, CO, NO_x, and total and speciated hydrocarbons reported as part of the PAMS network. Also, data from CASTNET will be obtained. Since the OTR modeling domain extends over two time zones, while the model simulations are reflective of a single time zone, EST, there will be a need to "correct" the clock and assemble the ambient air quality database. Any special measurements that are relevant to this study during the summer of 2002 will also be acquired, including upper air measurements.

9 DIAGNOSTIC ANALYSES

9.1 Quality Assurance Tests of Input Components

Before proceeding with modeling, all air quality, emissions, and meteorological data will be reviewed to ensure completeness, accuracy, and consistency. Any errors, missing data or inconsistencies, will be addressed using appropriate methods that are consistent with standard practices.

9.2 Diagnostic Tests

Attempts will be made to do diagnostic testing, to ensure that the simulated ozone patterns are in agreement with the measurements over the entire simulation period. While it is unrealistic to expect day-to-day agreement between the measured and predicted data, close attention will be paid to the changes in pattern of the measured ozone levels and the ability of the model to capture such changes.

10 MODEL PERFORMANCE EVALUATION

10.1 Performance Criteria

This is an area that will likely require substantial dialog among member states. While there are many statistical tests that can be applied, it is important to define a priori some of the conditions of the analysis and the targets of evaluation. Also, it is quite critical to define the areal extent for which the assessment needs to be done to address the performance of the model. A "strawman" outlining the procedures will be developed for the model performance evaluation. The strawman could have 3 or 4 levels of tests covering all or portions of the domain using daily maximum, daily average, daytime average, 8-hour maxima, and other combinations of ozone concentrations to assess the model performance. Similarly, the statistical tests are to be applied to the precursor data as well, recognizing that all tests applied to the ozone data may or may not be valid. Thus, it is suggested that the statistical tests be geared appropriately based on the quality and quantity of the database.

As part of the model assessment, qualitative analysis will also be performed by comparing predicted and measured pollutant fields to establish if the spatial patterns are captured by the modeling system. This is a critical step, since the measured concentrations may fall into a neighboring grid cell (but not at the measured location itself) and may be found to be in good agreement.

Another area that is quite important is the predictive ability of the model with respect to height. Recognizing that the pollutants trapped above the mixed layer during the overnight hours would mix down during the daytime, comparison will be made between measurements and model predictions. Also, as noted in the work plan, special attention will be paid to elevated monitoring stations, such as the television tower near Durham, North Carolina; and the Sears Tower in Chicago, Illinois, and any other special monitors.

10.2 Statistical Performance Measures

The recommended EPA procedures will be used to calculate the recommended performance measures. At a minimum, the following three statistical performance measures will be used to assess CAMx model performance for each episode.

- Unpaired highest-prediction accuracy

This measure quantifies the difference between the highest observed eight hour value in the domain and the highest predicted value in the domain. The acceptable performance range is plus or minus 15-20 percent.

- Normalized bias

This measure indicates the degree to which simulated eight hour values are over or under-predicted. The acceptable performance range is plus or minus 5-15 percent.

- Gross error of all pairs above 40 ppb

This measure indicates the average discrepancy between predicted and observed values and provides an overall assessment of model performance. The acceptable performance range is 30-35 percent.

11 CAA EMISSION INVENTORIES FOR 2010 AND 2013

11.1 CAA Emission Inventories for OTC States for 2010

Each OTC state in the OTR Domain will prepare a 2010 CAA emission inventory that is consistent with the regulations and rules adopted or expected to be in-place. The inventory will be developed consistent with EPA guidance. The states will develop the information on growth factors and controls used in the development of the inventory. Each state will submit a report on the development of these future year inventories.

Since the electric energy generation and use are highly inter-connected, coupled with the existing rules on trading and banking of pollutants, it is expected that an inventory consistent with this information would be developed for all electric energy generation units using models such as IPM.

Recognizing that any prediction of future emissions are subject to changes, the OTC Modeling Committee would develop a decision framework on obtaining these emissions to be consistent with the OTC SIP quality modeling system schedule (Appendix A).

11.2 CAA Emission Inventories for all other OTR States for 2010

A 2010 CAA emission inventory that includes VOC, NO_x, and CO for a typical ozone summer day will be obtained for all non-OTC states in the OTR. It is anticipated that these inventories will be developed following EPA guidance, and will be formatted in a consistent manner

11.3 CAA Emission Inventories for OTC States for 2013

Each OTC state in the OTR Domain will prepare a 2013 CAA emission inventory that is consistent with the regulations and rules adopted or expected to be in-place. The inventory will be developed consistent with EPA guidance. The states will develop the information on growth factors and controls used in the development of the inventory. Each state will submit a report on the development of these future year inventories.

Since the electric energy generation and use are highly inter-connected, coupled with the existing rules on trading and banking of pollutants, it is expected that an inventory consistent with this information will be developed for all electric energy generation units using models such as IPM.

11.4 CAA Emission Inventories for All Other states for 2013

A 2013 CAA emission inventory that includes VOC, NO_x, and CO for a typical ozone summer day will be obtained for all non-OTC states in the OTR. It is anticipated that these inventories will be developed following EPA guidance, and will be formatted in a consistent manner

12 CAA EMISSION INPUT FILES FOR 2010 AND 2013 FOR THE OTR DOMAIN

12.1 CAA Emission Input Files for OTR Domain for 2010

2010 CAA emissions data will be processed using EMS2001 and/or SMOKE. For those pollutants that depend upon ambient temperature, MM5 layer-1 gridded temperature fields will be used to estimate hourly emission rates. The biogenic emission input files prepared for the base 2002 will be used as a surrogate for 2010 biogenic emissions. The processing of the emissions data will be accompanied with the quality assurance checks previously described in section 7.2 Quality Assurance of 2002 Emission Input Files for the OTR Domain.

12.2 CAA Emission Input Files for OTR Domain for 2013

2013 CAA emissions data will be processed using EMS2001 and/or SMOKE. For those pollutants that depend upon ambient temperature, MM5 layer-1 gridded temperature fields will be used to estimate hourly emission rates. The biogenic emission input files prepared for the base 2002 will be used as a surrogate for 2013 biogenic emissions. The processing of the emissions data will be accompanied with the quality assurance checks previously described in Section 7.2 Quality Assurance of 2002 Emission Input Files for the OTR Domain.

13 OTR DOMAIN OZONE CONTROL STRATEGY

13.1 OTC CALGRID System Screening Runs

A series of CALGRID screening runs will be performed to investigate the level of emissions reductions needed both within and outside of the OTR. This will help to identify potential emission reductions scenarios that can be used to lower ozone levels in the OTR.

13.2 OTC SIP Modeling Platform Runs

OTC SIP modeling platform CAA runs for 2010 and 2013 will be reviewed to help determine the level of emissions reductions needed to attain the ozone NAAQS. VOC and NOX sensitivity runs will also be performed to help identify potential emission reductions scenarios that can be used to lower ozone levels in the OTR.

13.3 Analysis of Available Air Quality and Emission Databases

A review of air quality and emission databases (for example, EPA Clear Skies and Transport Rule emission files) will be performed to help identify potential source sectors of ozone precursors. Analysis of available EPA modeling results will also be performed to help identify potential source sectors of ozone precursors in, and upwind, of the OTR domain.

13.4 Ozone Control Strategy for the OTR Domain

The OTR Control Strategy Development Team will review CALGRID results, other available databases, and EPA databases, to help identify potential control programs. The Team will work with OTR states and the OTC stationary, area and mobile source committees to design ozone control strategies for the OTR Domain with the goal of meeting regulatory target dates.

14 OZONE CONTROL STRATEGY EMISSION INPUT FILES

14.1 Ozone Control Strategy Emission Input Files for the OTR Domain for 2010

Emissions files for the selected ozone control strategy for the OTR Domain for 2010 will be prepared in a consistent manner as per schedule. If necessary, additional IPM simulations may be performed to obtain EGU emission estimates.

14.2 Ozone Control Strategy Emission Input Files for the OTR Domain for 2013

Emissions files for the selected ozone control strategy for the OTR Domain for 2013 will be prepared in a consistent manner as per schedule. If necessary, additional IPM simulations may be performed to obtain EGU emission estimates.

15 OZONE PREDICTIONS FOR ATTAINMENT IN 2010 and 2013

15.1 Initial Conditions

The initial conditions at the startup will be for “clean” conditions. The OTR Modeling Team will use the 2002 initial condition files as a surrogate for initial conditions in 2010.

15.2 Boundary conditions

EPA will be consulted for guidance in estimating boundary conditions for 2010 and 2013 or under default would utilize those adapted for the Base 2002 base year simulation.

15.3 CAA Ozone Predictions for 2010 and 2013

The model will be run with the CAA emission files developed for 2010 and 2013. Tile plots, difference plots and model statistics will be prepared to help characterize the extent of any remaining non-attainment areas predicted in the OTR in 2010 and 2013.

15.4 Ozone Control Strategy Ozone Predictions for 2010 and 2013

The model will be run with OTR control strategy emission files prepared for 2010 and 2013. Tile plots, difference plots and model statistics will be prepared to help characterize the extent of any remaining non-attainment areas predicted in the OTR for the year 2010 and 2013.

16 DOCUMENTATION

A report titled “Assessment of the Ozone National Ambient Air Quality Standards in the Ozone Transport Region will be prepared by the OTR Modeling Team. The report would cover model performance evaluation, and an evaluation of the OTR control strategy runs for 2010 and 2013. This technical document will be made available to all interested parties and will be used by the member States in their SIP submission documentation as needed.

17 REFERENCES

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OTC Modeling Protocol ver 11/27/2007

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