APPENDIX D

PHOTOCHEMICAL MODELING PROTOCOL

Federal Clean Air Act Section 179B Demonstration State Implementation Plan Revision for the 2015 Eight-Hour Ozone National Ambient Air Quality Standards

Project Number 2019-106-SIP-NR
Proposal
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CHAPTER 1: INTRODUCTION

The Texas Commission on Environmental Quality (TCEQ) is conducting modeling in support of the Federal Clean Air Act Section 179B Demonstration State Implementation Plan Revision for the 2015 Eight-Hour Ozone National Ambient Air Quality Standards, hereafter referred to as the 179B SIP revision. The United States Environmental Protection Agency’s (EPA) 2018 Modeling Guidance for Demonstrating Air Quality Goals for Ozone, PM$_{2.5}$, and Regional Haze, hereafter referred to as 2018 modeling guidance, recommends that the following topics be core elements of any modeling protocol:

- Overview of the air quality issue being considered including historical background;
- List of the planned participants in the analysis and their expected roles;
- Schedule for completion of key steps in the analysis and final documentation;
- Description of the conceptual model for the area;
- Description of periods to be modeled, how they comport with the conceptual model, and why they are sufficient;
- Models to be used in the demonstration and why they are appropriate;
- Description of model inputs and their expected sources (e.g., emissions, meteorology, etc.);
- Description of the domain to be modeled (expanse and resolution);
- Process for evaluating base year model performance (meteorology, emissions, and air quality) and demonstrating that the model is an appropriate tool for the intended use;
- Description of the future years to be modeled and how projection inputs will be prepared;
- Description of the attainment test procedures and (if known) planned weight of evidence;
- Expected diagnostic or supplemental analyses needed to develop weight of evidence analyses; and
- Commitment to specific deliverables fully documenting the completed analysis.

Much of the requested information has already been compiled into a document entitled Appendix 1: Technical Description: 2012 TCEQ Modeling Platform (referred to hereafter as the TD), available as part of Appendix E of the proposed Dallas-Fort Worth (DFW) and Houston-Galveston-Brazoria (HGB) Serious Classification Attainment Demonstration State Implementation Plan (SIP) revisions for the 2008 eight-hour ozone National Ambient Air Quality Standard (NAAQS). This protocol will address most of the above items through references to the TD. The latest version of the TD was completed in the spring of 2016 and the modeling platform has undergone several updates since the TD’s completion; significant changes to the modeling platform will be noted in this Appendix. One significant change is that the modeling and data analysis for the 179B SIP revision will follow the 2018 modeling guidance, and not the 2014 draft guidance noted in the TD.
CHAPTER 2: BACKGROUND

The Texas Commission on Environmental Quality (TCEQ) is conducting photochemical grid modeling in support of the Federal Clean Air Act (FCAA) Section (§) 179B demonstration SIP revision for the 2015 eight-hour ozone National Ambient Air Quality Standard (179B SIP revision). The demonstration includes a modeling analysis of the impacts of international anthropogenic emissions on the ability of Bexar County to attain the 2015 eight-hour ozone NAAQS by 2020. This modeling followed the EPA's modeling guidance where applicable.

The modeling guidance recommends several qualitative methods that acknowledge the limitations and uncertainties of photochemical models when used to project ozone concentrations into future years. First, the modeling guidance recommends using model results in a relative sense and applying the model response to the observed ozone data. Second, the modeling guidance recommends using available air quality, meteorology, and emissions data to develop a conceptual model for eight-hour ozone formation and to use that analysis in episode selection. Third, the modeling guidance recommends using other analyses, i.e., weight of evidence (WoE), to supplement and corroborate the model results.

CHAPTER 3: PARTICIPATING ORGANIZATIONS

The TCEQ plans to conduct all photochemical modeling used in this SIP revision on its own Linux computing clusters. TCEQ's Air Modeling and Data Analysis (AMDA) section has the responsibility for planning and conducting the SIP modeling. AMDA is part of the Air Quality Division of TCEQ's Office of Air. The Office of Air organization chart is shown in Figure 3-1: TCEQ Office of Air Organization Chart.
Figure 3-1: TCEQ Office of Air Organization Chart
The responsible TCEQ technical oversight groups are provided in Section 2.3: Technical and Policy Organizations of the TD.
CHAPTER 4: SCHEDULE

The schedule of activities for completing modeling activities for the 179B demonstration SIP revision is shown below in Table 4-1: *Schedule of Modeling Activities.*

**Table 4-1: Schedule of Modeling Activities**

<table>
<thead>
<tr>
<th>Modeling Activity</th>
<th>Time Frame</th>
</tr>
</thead>
<tbody>
<tr>
<td>- Develop base case emissions</td>
<td>March 2019 – June 2019</td>
</tr>
<tr>
<td>- Evaluate meteorological modeling</td>
<td></td>
</tr>
<tr>
<td>- Conduct emissions modeling and processing</td>
<td></td>
</tr>
<tr>
<td>- Conduct base case photochemical modeling</td>
<td></td>
</tr>
<tr>
<td>- Conduct model performance evaluations</td>
<td></td>
</tr>
<tr>
<td>- Develop future base emissions with applicable growth and current controls</td>
<td>July 2019 – October 2019</td>
</tr>
<tr>
<td>- Conduct future base modeling and source apportionment</td>
<td></td>
</tr>
<tr>
<td>- Calculate future design values at all regulatory monitors in Bexar County</td>
<td></td>
</tr>
<tr>
<td>- Estimate international anthropogenic emissions contribution to the future design values at all regulatory monitors in Bexar County</td>
<td></td>
</tr>
<tr>
<td>- Evaluate source apportionment results</td>
<td></td>
</tr>
</tbody>
</table>
CHAPTER 5: CONCEPTUAL MODEL

Bexar County is a new non attainment area for the 2015 ozone NAAQS, and the TCEQ has developed a Conceptual Model of ozone formation in Bexar County that will be made available as part of the 179B SIP revision. The conceptual model will characterize ozone trends, precursors, formation, and transport into the broader San Antonio metropolitan area that includes the Bexar County non attainment area and will provide a comprehensive picture of not only where and when ozone forms, but also how and why ozone forms in the area.
CHAPTER 6: EPISODE SELECTION

The May through September 2012 time period will be used for the ozone modeling episode as it has been comprehensively developed and assessed through multiple SIP revisions for Texas. More details on the episode selection process for the 2012 modeling period are discussed in Section 4: Episode Selection of the TD. Suitability of the May through September 2012 episode for ozone modeling for Bexar County will be evaluated as part of the technical analysis undertaken for the 179B SIP revision.
CHAPTER 7: MODELS USED

The TCEQ plans to use the models detailed in Table 7-1: *Planned Models for 179B SIP Revision Modeling* in developing the 179B SIP Revision. Section 5: *Model Selection* of the TD provides additional details about these models.

Table 7-1: Planned Models for 179B SIP Revision Modeling

<table>
<thead>
<tr>
<th>Type</th>
<th>Model</th>
<th>Version</th>
</tr>
</thead>
<tbody>
<tr>
<td>Photochemical</td>
<td>Comprehensive Air Quality Model with extensions (CAMx)</td>
<td>6.5</td>
</tr>
<tr>
<td>Meteorological</td>
<td>Weather Research and Forecasting (WRF) model</td>
<td>3.7.1</td>
</tr>
<tr>
<td>Emissions Processing</td>
<td>Emissions Processing System (EPS3)</td>
<td>3.22 or later</td>
</tr>
<tr>
<td>Biogenic</td>
<td>Biogenic Emission Inventory System (BEIS)</td>
<td>3.61</td>
</tr>
<tr>
<td>Initial and Boundary Conditions</td>
<td>The global atmospheric chemistry model driven by assimilated meteorological observations from the Goddard Earth Observing System (GEOS-Chem)</td>
<td>12.2.0</td>
</tr>
</tbody>
</table>
CHAPTER 8: MODEL INPUTS AND SOURCES

Modeling input and output for the WRF model are described in detail in Section 7.1: *Meteorological Model Input and Output* of the TD. Some configuration changes have occurred since the time the TD was written, so Table 6 in the TD will be replaced by Table 8-1: *2012 Base Case WRF Setup*.

**Table 8-1: 2012 Base Case WRF Setup**

<table>
<thead>
<tr>
<th>Grid</th>
<th>Nudging Type</th>
<th>PBL</th>
<th>Cumulus</th>
<th>Radiation</th>
<th>Land-Surface</th>
<th>Microphysics</th>
</tr>
</thead>
<tbody>
<tr>
<td>36 km, 12 km</td>
<td>3-D Analysis</td>
<td>YSU</td>
<td>Kain-Fritsch</td>
<td>RRTM / Dudhia</td>
<td>Pleim-Xiu</td>
<td>WSM5</td>
</tr>
<tr>
<td>4 km</td>
<td>3-D Analysis Surface Analysis; Observational radar profiler</td>
<td>YSU</td>
<td>Multi-scale Kain-Fritsch</td>
<td>RRTM / Dudhia</td>
<td>Pleim-Xiu</td>
<td>WSM6</td>
</tr>
</tbody>
</table>

km = kilometer; PBL = Planetary Boundary Layer; YSU = Yonsei University; RRTM = Rapid Radiative Transfer Model; WSMx = WRF Single-Moment x-Class Microphysics Scheme

Data input, output, and processing with EPS3 is described in Section 7.2: *Emissions Processing System Input and Output* of the TD. Several updates were made to emissions inputs since the TD was written, including new Canadian, Mexican, on-road, and biogenic emission estimates. Details of these updates are available in the recently proposed DFW and HGB Serious Classification Attainment Demonstration SIP revisions for the 2008 eight-hour ozone NAAQS.

Data inputs to and output from the CAMx model, including initial and boundary conditions from the GEOS-Chem global model, are described in Section 7.3: *CAMx Model Input and Output* of the TD. Updates to initial and boundary conditions development were made since the TD was written, including use of a newer version of GEOS-Chem and newer global emissions inventories. These updates will be discussed in the final 179B SIP revision documentation.
The CAMx modeling domain definition is provided in Section 6.1: CAMx Modeling Domains of the TD. One notable modification since the TD was written is the addition of one vertical layer on top of the older structure to assure that the tropopause is always below the model top boundary. Details of this update is available in the recently proposed DFW and HGB Serious Classification Attainment Demonstration SIP revisions for the 2008 eight-hour ozone NAAQS.

The WRF modeling domain, described in Section 6.3: WRF Modeling Domains of the TD, also has been modified slightly by splitting the lowest layer into two, allowing the model to better resolve near-surface effects. These two layers are recombined into one before the WRF meteorology is input into CAMx.
CHAPTER 10: MODEL PERFORMANCE EVALUATION

Procedures for evaluating performance of the WRF simulations are described in Section 7.1.3: Meteorological Model Output of the TD. Example model performance evaluation (MPE) plots for the version of WRF current at the time the TD was written are provided in Attachment 1 of the TD. MPE is also part of the Quality Assurance/Quality Control (QA/QC) procedures employed at the TCEQ, described in Section 2: Meteorological Modeling QA/QC of the QA/QC Plan.

Performance evaluation of emissions models is inherently difficult except for highly-controlled experimental settings. Evaluation of emissions using ambient concentrations usually requires a model to account for atmospheric dispersion, advection, and chemistry, so it is best to evaluate the combined emissions-photochemical modeling setup together. Emissions model outputs can, however, be visualized using graphical routines so that they can be compared with knowledge of the sources’ spatiotemporal characteristics. Both Section 7.2: Emissions Processing System Input and Output of the TD and Section 1.1: Elevated Source Emissions of the QA/QC Plan describe in detail how the TCEQ evaluates emissions model outputs.

MPE of the CAMx modeling is described in detail in Section 9: Model Performance Evaluation of the TD. As discussed in the TD, the TCEQ uses the Geo-Referenced Interactive Model Results Evaluation and Analysis Program (GRIMREAPr) for MPE. GRIMREAPr is a set of analysis tools developed by the TCEQ to evaluate model results and assess model performance in a geographical frame of reference. In addition to the standard time-series, scatter plots, model performance statistics, etc., that are produced for each model run, GRIMREAPr provides an interactive visualization environment to view static or animated concentration data for every chemical species output by CAMx. The view can be zoomed in or out using the cursor controls and can display differences between model runs and bias at monitoring sites; it also displays time series of observed and modeled concentrations on command. GRIMREAPr also provides the capability to overlay the model run with satellite cloud imagery, radar imagery, and Hybrid Single Particle Lagrangian Integrated Trajectory (HYPLIT) back or forward trajectories at user-selected sites. GRIMREAPr is a powerful tool for analyzing model output and identifying possible errors or deficiencies in the model formulation. A more detailed description of GRIMREAPr with examples was presented at the 14th Annual Community Modeling and Analysis System Annual Conference.

In addition, the TCEQ will conduct MPE of the global modeling for the 2012 base year using two sets of observational datasets, the World Data Centre for Reactive Gases (WDCRG) and the World Ozone and Ultraviolet Radiation Data Centre (WOUDC). Details of the data used in MPE of global modeling are provided in Table 10-1: Datasets for the MPE of 2012 GEOS-Chem Modeling.

Table 10-1: Datasets for the MPE of 2012 GEOS-Chem Modeling

<table>
<thead>
<tr>
<th>Network</th>
<th>Species</th>
<th>Coverage</th>
<th>Resolution</th>
<th>Performance Tools</th>
</tr>
</thead>
<tbody>
<tr>
<td>WDCRG</td>
<td>Ozone, NO₂, SO₂</td>
<td>Surface, many global sites</td>
<td>Typically hourly, sometimes daily</td>
<td>Scatterplots, performance statistics maps</td>
</tr>
<tr>
<td>CASTNET</td>
<td>Ozone</td>
<td>3-D, United States</td>
<td>Typically hourly</td>
<td>Statistics and plots</td>
</tr>
</tbody>
</table>
CHAPTER 11: FUTURE YEAR MODELING

The future year of 2020 will be modeled based on the attainment date for the Bexar County marginal nonattainment area, September 24, 2021. Similar to the descriptions in Section 7.2: Emissions Processing System Input and Output of the TD for creating 2017 emission inventories, anthropogenic emissions source categories for 2020 will be created by applying growth and control factors to base year emissions.

Since biogenic emissions are dependent upon the meteorological conditions on a given day, the same episode-specific emissions used in the base case modeling will be used in the 2020 future year modeling. Since future year wildfires cannot be predicted, the wildfire emissions inventory developed for the base case modeling will also be used in the 2020 future year modeling. The 2020 boundary conditions from GEOS-Chem will be used.
The TCEQ plans to use a combination of global (GEOS-Chem) and regional (CAMx) models to determine international anthropogenic emissions contribution to future design values at regulatory monitors in the Bexar County nonattainment area. The TCEQ plans to estimate the international anthropogenic contribution as the difference between a reference future year design value \( (DV^\text{Ref}_F) \) and a “zero-out the rest of the world” (ZROW) future year design value \( (DV^\text{ZROW}_F) \). Equation 12-1: *International Anthropogenic Contribution Calculation* below shows the methodology used to determine the international anthropogenic contribution.

\[
\text{International Anthropogenic Contribution} = DV^\text{Ref}_F - DV^\text{ZROW}_F
\]

where: \(DV^\text{Ref}_F = DV_B \times RRF_{\text{Ref}}\) and \(DV^\text{ZROW}_F = DV_B \times RRF_{\text{ZROW}}\)

**Equation 12-1: International Anthropogenic Contribution Calculation**

In Equation 12-1, \(DV_B\) is the base design value and RRFs are Relative Response Factors used to calculate future year design value at a monitor per 2018 modeling guidance. A RRF, as shown in Equation 12-2: \(RRF\), is calculated from a pair of base/future year runs as the ratio of the average future year modeled MDA8 ozone concentrations and the average base year modeled MDA8 ozone concentrations on the top 10 modeled MDA8 base year days.

\[
RRF = \frac{\text{Average of modeled MDA8 on the top ten base year days in a future year simulation}}{\text{Average of modeled MDA8 on the top ten base year days in a base year simulation}}
\]

**Equation 12-2: RRF Calculation**

For \(RRF_{\text{Ref}}\) the base and future year modeled MDA8 ozone concentrations were from the Reference case 2012 base year and 2020 future year simulations. For \(RRF_{\text{ZROW}}\) the future year modeled MDA8 ozone concentrations were from the ZROW case 2020 simulation while the base year modeled MDA8 concentration remains the same as the Reference case 2012 simulation. In accordance with the 2018 modeling guidance, the maximum concentration of the three-by-three grid cell array surrounding each monitor on the top 10 base year days was used to calculate the RRFs for each monitor in both the Reference and ZROW cases. The \(DV_B\) is the average of the regulatory design values for the three consecutive years containing the 2012 base year.

In addition to the international anthropogenic contribution to the future year design value estimation, ancillary evidence may also be used to corroborate or contradict the model predictions and to demonstrate that but for emissions emanating from outside the United States, the Bexar County nonattainment area would attain the 2015 eight-hour ozone standard. Analyses such examination of trends in monitored design values, back trajectories, and source apportionment modeling; and literature review of academic and white papers would be utilized to support the demonstration. If time permits, additional modeling, including a ZROW of the base year that keeps the boundary conditions constant between the base and future year may be conducted.
CHAPTER 13: DOCUMENTATION

The modeling guidance recommends including the following elements of documentation as part of SIP revision:

- Executive summary that provides an overview of the analysis and the key conclusions;
- Reference to the modeling protocol noting any major deviations from the original plans;
- List of the institutional participants in the attainment demonstration and their roles;
- Description of air quality in the area and how that shaped the analysis;
- Justification for the model, episodes, domain, and grid(s) used in the analysis;
- Description of the development of the emissions inputs used in the base year modeling, including tabular summaries by state/county, as appropriate;
- Description of the development of meteorological inputs used in the base year modeling;
- Description of all other base year modeling inputs;
- Evaluation of base year model performance (meteorology, emissions, and air quality), including a description of the observational database used in the evaluation and any diagnostic or sensitivity tests used to improve the model;
- Description of the strategy used to estimate international anthropogenic emissions contribution to future year design values;
- Description of any supplemental analyses designed to bolster the results; and
- Detailed summary of the entire analysis that leads to the conclusion that but for emissions emanating outside of the United States, the Bexar County nonattainment area would attain the 2015 ozone NAAQS.

The TCEQ will include the above-listed elements in the submitted 179B SIP revision.