Contract # 582-14-40056
PGA and Notice to Commence #FY14-01
Task 2.2

LEVEL III QUALITY ASSURANCE PROJECT PLAN (QAPP)
Photochemical Modeling for the HOTCOG Area

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1.0 PROJECT DESCRIPTION AND OBJECTIVES

ENVIRON has prepared this Level III Quality Assurance Project Plan (QAPP) for the Texas Commission on Environmental Quality (TCEQ) following EPA guidelines. The nature of the technical analysis and tasks to be conducted as part of this project are consistent with quality assurance (QA) Category III: Data Evaluation or Use for Secondary Purpose.

1.1 PURPOSE OF STUDY

The Heart of Texas Council of Government (HOTCOG) 6-county area consists of McLennan, Bosque, Hill, Falls, Limestone and Freestone Counties. The HOTCOG Air Quality Advisory Committee (AQAC) oversees ozone air quality planning for the 6-county area. The focus of the AQAC's efforts is maintaining the areas's compliance with Federal ozone air quality regulations.

The Texas Commission on Environmental Quality (TCEQ) operates a Continuous Air Monitoring Stations (CAMS) at the Waco Airport in McLennan County. Ozone data from the Waco Mazanec monitor determine whether McLennan County is in compliance with the NAAQS for ozone. Currently, the monitor has a design value of 74 ppb, which is in compliance with the NAAQS. EPA's next review of the ozone standard is scheduled to be finalized in late 2014. If EPA decides to lower the NAAQS to the 60-70 ppb range following its current review, then the McLennan County monitor will no longer comply with the NAAQS.

Development of a photochemical ozone model for the HOTCOG area is a critical step in the development of an appropriate State Implementation Plan (SIP), should this become necessary. The ozone model is a tool for understanding the formation, transport and fate of ozone in the area and is also used in developing local emission control strategies.

1.2 PROJECT OBJECTIVES

In 2012-2013, ENVIRON developed and evaluated an ozone model for the HOTCOG area for a high ozone period in June 2006 based on inputs provided by the TCEQ.

During this work, we identified model performance improvement as a necessary step toward developing a SIP-quality model free of significant systematic biases. In this project, the existing June 2006 HOTCOG area ozone model will be refined so that model performance in simulating ground-level ozone is consistent with the model's use as a SIP-quality tool. ENVIRON will also evaluate the utility of developing an ozone model for the HOTCOG area for the August - September 2006 high ozone period. Once model performance is satisfactory, AQAC will use the models to evaluate potential local emissions control strategies and other planned or anticipated emission reduction measures.

Some of the steps involved in this study may include, but are not limited to:

1. Investigating possible ozone sources transported into the HOTCOG area along with the formation of ozone within the area based on precursor emissions;

2. Investigating model sensitivity to broad changes in precursor emissions using tools such as Anthropogenic Precursor Culpability Assessment (APCA), Ozone Source Apportionment Technology (OSAT), or High-order Decoupled Direct Method (HDDM);
3. Evaluation of potential voluntary or mandatory control strategies; and
4. Integrating updated emission and meteorological modeling inputs and assessing their impact on model performance.

2.0 PROJECT ORGANIZATION AND RESPONSIBILITIES

2.1 RESPONSIBILITIES OF PROJECT PARTICIPANTS

This study will be conducted by ENVIRON International Corporation under contract to the Heart of Texas Council of Governments (HOTCOG) through HOTCOG's Rider 8 Program Grant Agreement with the TCEQ. The study will be performed under the direction of HOTCOG Air Quality Advisory Committee (AQAC). The focus of the AQAC's efforts is maintaining the areas's compliance with Federal ozone air quality regulations. The ENVIRON team working on this project and their specific responsibilities are listed below.

Table 1. The ENVIRON project team participants and their responsibilities.

Participant	Project Responsibility
Greg Yarwood	Principal Investigator, technical consultant, quality assurance review
Jeremiah Johnson	Project Manager with technical oversight of the CAMx system design, implementation and application Preparation of final project report and presentation
Sue Kemball-Cook	Technical consultant, quality assurance review
Jaegun Jung Ed Tai Justin Zagunis Thomas Pavlovic	CAMx implementation, including pre- and post-processing Model performance evaluation (MPE)

In addition, TCEQ staff will participate in the specification of CAMx simulations, review of CAMx model performance evaluation and technical documentation generated during the project. The HOTCOG Air Quality Advisory Committee will also review the technical documentation.

2.2 PROJECT SCHEDULE

The project is divided into four major tasks: (1) Evaluation of CAMx model inputs; (2) CAMx simulations; (3) Evaluation of CAMx simulations; and (4) Documentation of all analyses and recommendations for future work in a final report. The table below shows the overall schedule for completion of this project including interim milestones.

Table 2. Summary of project schedule and milestones.

Work Element	Completion Date
QAPP submitted to the TCEQ for review and approval	June 1, 2014
Evaluate CAMx model inputs	September 30, 2014
Perform CAMx simulations	March 31, 2015
Evaluate CAMx simulations	May 30, 2015

Work Element	Completion Date
Draft Final Report submitted to TCEQ for comments	July 15, 2015
Final Report acceptable to the TCEQ	August 15, 2015

3.0 SCIENTIFIC APPROACH

3.1 DATA NEEDED TO MEET PROJECT OBJECTIVES

There are three main data sets that are required to accomplish the project objectives. These are:

1. Photochemical modeling input data; and
2. Ambient data from TCEQ Continuous Air Monitoring Stations (CAMS) in the HOTCOG area and surrounding Texas areas
3. Ambient data from EPA's CASTNET monitoring sites may be used to evaluate model performance outside of Texas in order to assess the model's simulation of transport of background ozone into Texas.

The minimum requirements for the data are that they provide information that is representative for the modeling domain and the temporal extent of the simulation period. The data should derive from sources and procedures that have been peer-reviewed and the methods used in applying the data should be consistent with best current scientific practices. The ambient data will be used for evaluation of the photochemical model's performance in simulating monitored ground level ozone and precursors in the HOTCOG area and in other Texas areas. Ambient data will also be used to evaluate the utility of the August-September 2006 period as a modeling episode for the HOTCOG area.

3.2 DATA SOURCES

3.2.1 Photochemical Modeling Input Data

CAMx model input data for the June 2006 and August – September 2006 modeling episodes will be downloaded from TCEQ's Rider 8 website: http://www.tceq.texas.gov/airquality/airmod/rider8/rider8Modeling. This data has been quality-assured by the TCEQ. ENVIRON will evaluate and/or refine model inputs in order to improve model performance.

3.2.2 Observational Data

Ambient data for the TCEQ's CAMS sites in the HOTCOG and surrounding areas are available from the TCEQ's website http://www.tceq.state.tx.us/cgi-bin/compliance/monops/site_info.pl. This data has been quality-assured by the TCEQ. Quality assured data from CASTNET monitoring sites will be downloaded from the EPA's website http://epa.gov/castnet/javaweb/index.html.

4.0 QUALITY METRICS

In this section, we specify the quality requirements for the data used in this study and describe the procedures for determining the quality of the secondary data.

4.1 PHOTOCHEMICAL MODELING INPUT DATA

CAMx input data will be downloaded from TCEQ's Rider 8 Modeling website. This data has been quality-controlled by the TCEQ. Any new or revised model inputs will be independently reviewed and quality-assured. During the course of this project, ENVIRON may perform meteorological modeling using the Weather Research and Forecast (WRF; Skamarock et al., 2008) model. Any WRF meteorological model outputs that may be generated during this project will be analyzed using visualization and model performance software to ensure the meteorological model is configured correctly. The wind speed, wind direction and temperature fields will be independently reviewed by someone who did not conduct the WRF modeling so that more than 10% of the WRF data will be audited.

4.2 OBSERVATIONAL DATA

CAMS monitoring site data will be downloaded electronically from the TCEQ website. This data is already quality-controlled by the TCEQ. CASTNET monitoring site data will be downloaded from the EPA website. This data has been quality-assured by the EPA.

4.2 CAMX OUTPUT DATA

ENVIRON will analyze CAMx model output using visualization and model performance software to ensure that the model and its inputs are configured correctly. When performing sensitivity simulations, we will ensure that the CAMx runfiles are identical except for the configuration option or input file(s) relevant to the sensitivity being tested. The ozone and select ozone precursor concentration fields will be independently reviewed by someone who did not conduct the CAMx modeling so that more than 10% of the CAMx output data will be audited.

5.0 DATA ANALYSIS, INTERPRETATION AND MANAGEMENT

5.1 ANALYSIS OF WRF MODEL OUTPUT

If WRF meteorological modeling is performed during this study, ENVIRON will use its meteorological-statistical program METSTAT to statistically assess how well the WRF output matches observations. METSTAT extracts the WRF grid cell's values that correspond to each observation site, and performs paired-in-time statistics. We will calculate bias and error statistics for wind speed, direction, temperature, and humidity (Table 3). Each statistical metric will be compared to performance benchmarks to evaluate how well the model performed.

Table 3. Definition of performance metrics for meteorological and photochemical modeling.

Metric	Definition[1]
Mean Bias (MB)	$\frac{1}{N}\sum_{i=1}^{N}(P_i - O_i)$
Mean Error (ME)	$\frac{1}{N}\sum_{i=1}^{N}\lvert P_i - O_i\rvert$
Mean Normalized Bias (MNB) (-100% to +∞)	$\frac{1}{N}\sum_{i=1}^{N}\left(\frac{P_i - O_i}{O_i}\right)$
Mean Normalized Error (MNE) (0% to +∞)	$\frac{1}{N}\sum_{i=1}^{N}\left\lvert\frac{P_i - O_i}{O_i}\right\rvert$
Normalized Mean Bias (NMB) (-100% to +∞)	$\frac{\sum_{i=1}^{N}(P_i - O_i)}{\sum_{i=1}^{N} O_i}$
Normalized Mean Error (NME) (0% to +∞)	$\frac{\sum_{i=1}^{N}\lvert P_i - O_i\rvert}{\sum_{i=1}^{N} O_i}$
Fractional Bias (FB) (-200% to +200%)	$\frac{2}{N}\sum_{i=1}^{N}\left(\frac{P_i - O_i}{P_i + O_i}\right)$
Fractional Error (FE) (0% to +200%)	$\frac{2}{N}\sum_{i=1}^{N}\left\lvert\frac{P_i - O_i}{P_i + O_i}\right\rvert$
Coefficient of Determination (r^2) (0 to 1)	$\left(\frac{\sum_{i=1}^{N}(P_i - \overline{P})(O_i - \overline{O})}{\sqrt{\sum_{i=1}^{N}(P_i - \overline{P})^2 \sum_{i=1}^{N}(O_i - \overline{O})^2}}\right)^2$

[1] P_i and O_i are prediction and observation at the *i*-th site, respectively; $\overline{P}$ and $\overline{O}$ are mean prediction and observation, respectively.

Emery et al. (2001) derived and proposed a set of daily performance benchmarks for typical meteorological model performance. These standards were based upon the evaluation of about 30 meteorological simulations (using a variety of regional meteorological models) since 1993 in support of air quality applications as reported by Tesche et al. (2001) and other studies. The purpose of these benchmarks was not to give a passing or failing grade to any one particular meteorological model application, but rather to put its results into the proper context of other models and meteorological data sets. Since 2001, the benchmarks have been promoted by the EPA-sponsored National Ad Hoc Meteorological Modeling Group and have been consistently relied upon to evaluate Pennsylvania State University / National Center for Atmospheric Research (MM5) and WRF model performance in many regulatory modeling projects throughout Texas and the U.S. As part of the Western Regional Air Partnership (WRAP) meteorological modeling of the western United States, including complex conditions in the Rocky Mountain Region and in Alaska, Kemball-Cook et al., (2005) proposed model performance benchmarks for complex conditions. McNally (2009) performed a reassessment of these benchmarks using WRF runs, and suggested a revision to the humidity benchmark. The determination to use simple or complex benchmarks will be made on a site-by-site basis depending on the presence of significant terrain or local circulations (e.g. Houston sea breeze).

The benchmarks for each variable are shown in Table 4. Being outside one or more of these ranges does not mean the meteorological data fields for a particular parameter are unacceptable. However, such a result indicates that caution should be exercised in the use of such variables, and in interpreting subsequent air quality modeling based on those meteorological fields. If wind, temperature and humidity bias and error statistics are reasonably near their respective benchmarks, WRF model performance will be considered acceptable.

Table 4. WRF Performance Benchmarks.

Parameter	Emery et al. (2001)	Kemball-Cook et al. (2005)	McNally (2009)
Conditions	Simple	Complex	Complex
Temperature Bias	≤ ±0.5 K	≤ ±2.0 K	≤ ±1.0 K
Temperature Error	≤ 2.0 K	≤ 3.5 K	≤ 3.0 K
Temperature IOA	≥ 0.8	(not addressed)	(not addressed)
Humidity Bias	≤ ±1.0 g/kg	≤ ±0.8 g/kg	≤ ±1.0 g/kg
Humidity Error	≤ 2.0 g/kg	≤ 2.0 g/kg	≤ 2.0 g/kg
Humidity IOA	≥ 0.6	(not addressed)	(not addressed)
Wind Speed Bias	≤ ±0.5 m/s	≤ ±1.5 m/s	(not addressed)
Wind Speed RMSE	≤ 2.0 m/s	≤ 2.5 m/s	(not addressed)
Wind Speed IOA	≥ 0.6	(not addressed)	(not addressed)
Wind Dir. Bias	≤ ±10 degrees	(not addressed)	(not addressed)
Wind Dir. Error	≤ 30 degrees	≤ 55 degrees	(not addressed)

5.2 ANALYSIS OF CAMX MODEL OUTPUT

ENVIRON will evaluate CAMx model performance in simulating observed near-surface ozone and precursors using both graphical and statistical methods. Graphical methods will include spatial maps and time-series comparing model predictions to observations at the Waco Mazanec monitoring site. Graphics may be developed using a mix of several plotting applications, including GIS, PAVE, Surfer, and NCAR/NCL. Statistical methods will include computation of metrics for bias and error between predictions and observations for the species listed above. Standard statistical metrics as described in EPA air quality modeling guidance (EPA, 2007) will be calculated. These include normalized mean and fractional bias (NMB and FB), and normalized mean and fractional absolute error (NME and FE) (Table 3). Use of mean normalized bias (MNB) and error (MNE) is not encouraged due to the propensity for misinterpretation and lack of symmetry around zero (they tend to be skewed by low observed concentrations with the bias skewed towards large positive numbers). Linear regression analysis (e.g., coefficient of determination, r^2) will be used to examine the model's ability to capture observed variability.

ENVIRON will evaluate changes in model performance resulting from updates made to meteorological and emissions inputs, and prepare a presentation detailing the results of the model performance evaluation. External evaluation and review of the model performance evaluations will be performed by the HOTCOG Air Quality Advisory Committee and TCEQ staff.

5.3 EVALUATION OF AUGUST – SEPTEMBER 2006 OZONE EPISODE

ENVIRON will consider ozone modeling for the August – September 2006 high ozone episode. In order to utilize this episode for modeling, it has to meet EPA requirements:

- Select a mix of episodes that reflect a variety of meteorological conditions that frequently correspond with observed 8-hour daily maximum ozone concentrations greater than the NAAQS at different monitoring sites within the area under study;
- Select periods during which observed 8-hour daily maximum ozone concentrations are close to the 8-hour ozone design value (*i.e*., three-year average of fourth highest 8-hour ozone concentration) at each key monitor;
- Select periods for which extensive air quality/meteorological databases exist; and
- Model a sufficient number of days so that the model attainment test can be applied at all of the ozone monitoring sites that are in violation of the NAAQS

ENVIRON will make a decision regarding the inclusion of the August – September 2006 episode after review and evaluation from the HOTCOG Air Quality Advisory Committee and TCEQ staff.

5.4 DATA STORAGE REQUIREMENTS

Data generated for this project, including model inputs, final model outputs and various air quality observational data and statistical performance calculations, will be securely archived during the project on portable hard drives and stored for a period of at least three years following the completion of the project. All data obtained for this project will be stored in electronic format. Our teams' experience has been that 100+ GB hard drives provide an accessible and portable system for storing data files of the size routinely encountered in the type of modeling activities for this effort.

6.0 REPORTING

6.1 PROJECT DELIVERABLES

The schedule for all deliverables is presented in Section 2, Table 2.

6.2 FINAL PROJECT DELIVERABLES

Draft and Final Reports will be delivered to the TCEQ Project Manager electronically (i.e., via file transfer protocol (FTP) or e-mail) in Microsoft Word format no later than the deliverable due date shown in Table 2. All electronic deliverables will meet State of Texas Accessibility requirements in 1 TAC 213. The Reports will detail the methods and results and will include the following components:

1. An executive summary or abstract
2. A brief introduction discussing the background and objectives, including relationships to other studies if applicable

3. A discussion of the pertinent accomplishments, shortfalls, and limitations of the work completed under each Workplan task.
4. Recommendations, if any, for what should be considered next as a new study.

The Final Report will provide a comprehensive overview of activities undertaken and data collected and analyzed during the work. The Final Report will highlight major activities and key findings, describe problems encountered and associated corrective actions, and detail relevant statistics including data, parameter, or model completeness, accuracy, and precision.

7.0 REFERENCES

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