

Quality Assurance Project Plan (QAPP)

Project 22-003

Evaluating the Ability of Statistical and Photochemical Models to Capture the Impacts of Biomass Burning Smoke on Urban Air Quality in Texas

**Prepared for
Texas Air Quality Research Program (AQRP)
The University of Texas at Austin**

Prepared by

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Atmospheric and Environmental Research**

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Version 2.2

Atmospheric and Environmental Research has prepared this QAPP following the Environmental Protection Agency (EPA) guidelines for a Quality Assurance (QA) Category III Project: Research Model Development or Application. It is submitted to the Texas Air Quality Research Program (AQRP) as required in the Work Plan requirements.

QAPP Requirements: Project Description and Objectives, Organization and Responsibilities, Model Selection, Model Design, Model Coding, Model Calibration, Model Verification, Model Evaluation, Model Documentation, Assessment and Oversight, Reporting.

QA Requirements: Technical Systems Audits - Not Required for the Project
 Audits of Data Quality – 10% Required
 Report of Findings – Required in Final Report

Approvals Sheet

This document is a Category III Quality Assurance Project Plan for the *Evaluating the Ability of Statistical and Photochemical Models to Capture the Impacts of Biomass Burning Smoke on Urban Air Quality in Texas* project. The Principal Investigator for the project is Matthew J. Alvarado.

Electronic Approvals:

This QAPP was approved electronically on 08/24/2022 by Elena McDonald-Buller, The University of Texas at Austin.

Elena McDonald-Buller
Project Manager, Texas Air Quality Research Program

This QAPP was approved electronically on 9/8/2022 by Vincent M. Torres, The University of Texas at Austin.

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This QAPP was approved electronically on 09/12/2022 by Chola Regmi, Project Liaison, Texas Commission on Environmental Quality.

Project Liaison, Texas Commission on Environmental Quality

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1. Project Description and Objectives

In this project we will examine the impact of fires on urban air quality (AQ) in Texas using statistical modeling (Task 1). Two urban areas will be examined: Houston-Galveston-Brazoria (HGB) and El Paso. Background ozone (O_3) and fine particulate matter ($PM_{2.5}$) concentrations will be estimated using the lowest value observed at sites near the border of the area of interest, as the Texas Commission on Environmental Quality (TCEQ) has done in the past. Analyzing the impacts of fires on background and urban sites separately will allow us to examine the change in O_3 and $PM_{2.5}$ due to the mixing of smoke with urban pollution separately from the impact of smoke before it mixes with urban pollution. We will then apply the same statistical methods to both the real-world surface observations and Comprehensive Air quality Model with extensions (CAMx)-simulated surface observations to determine if the impact of fires on urban air quality as simulated in CAMx is statistically equivalent to the impacts seen in the real-world data (Task 2). We will examine any statistically significant differences to determine avenues for improving the handling of smoke and urban air chemistry in the photochemical models (Task 3).

1.1. Objectives

The objectives of this project are to:

- (1) Use generalized additive models (GAMs) driven with satellite and surface observations to examine the impact of fires on background and total O_3 and $PM_{2.5}$ in Texas urban areas.**
- (2) Examine the ability of CAMx photochemical model to simulate these fire impacts by applying similar statistical methods to the CAMx results**
- (3) Use any statistically significant differences found to prioritize different approaches to improve the ability of CAMx to simulate the impacts of domestic fires on air quality**

1.2. Description of Problem

Understanding the impact of domestic fire smoke on urban AQ requires understanding (i) the chemistry of the smoke before it reaches the city and (ii) the

changes in the urban production rate of O₃ and PM_{2.5} caused by the smoke. The relative importance of these two pathways on the air quality impacts of domestic fire smoke is not well understood and it is unclear which processes should be targeted to reduce the overall uncertainty.

In addition, three-dimensional (3D) photochemical models like CAMx can have trouble representing the near-source chemistry of the smoke plume and the impact of smoke mixing with urban pollution due to a combination of low spatial resolution near fires and incorrect representation of the chemistry of smoke-specific volatile organic compounds (VOCs; e.g., Baker et al., 2016). These limitations in physical approaches have led to the development of a variety of statistical approaches to estimate the impact of biomass burning on urban AQ (e.g., Gong et al., 2017; de Foy et al., 2021). However, little work has been done to compare the statistical and 3D photochemical approaches or to identify priorities for further development of both approaches. Thus, the United States (US) Environmental Protection Agency (EPA) and US Forest Service organized assessment of smoke research needs noted this was a key priority for future smoke chemistry research (Alvarado et al., 2022). ***A statistical analysis of the impacts of domestic fire emission on urban air quality in Texas and a statistical evaluation of the ability of the CAMx model to simulate these impacts would greatly help TCEQ air quality managers understand the impacts of domestic fires on Texas air quality and human health.***

2. Organization and Responsibilities

2.1. Key Personnel and Tasks

This section identifies the roles and responsibilities of those individuals participating in the project. The individuals responsible for maintaining and updating the Quality Assurance Project Plan (QAPP) are also identified. A project organization chart is provided in Figure 1.

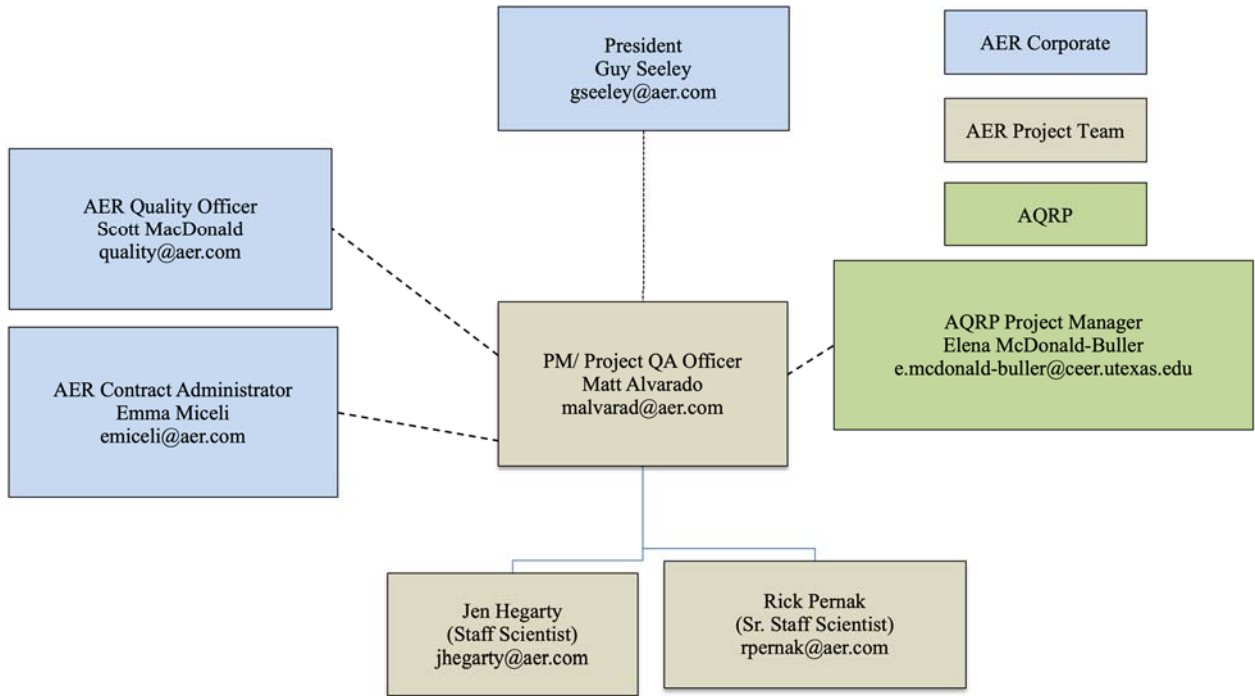


Figure 1. Atmospheric and Environmental Research (AER) organization chart for AQR Project 22-003. Persons with direct charging authority to the project are indicated in brown; persons serving in a corporate capacity are indicated in blue. AQR technical contact is shown in green. Solid blue lines indicate the reporting for this project only, while dotted lines indicate AER’s corporate hierarchy. Dashed lines are used to connect the Project Manager (PM) to AER administrative support and the TCEQ project manager.

The Atmospheric and Environmental Research (AER) persons shown in Figure 1 are divided into two main groups: those shown in the blue boxes (President, Contract Administrator, and AER Quality Officer) provide the corporate function indicated; those shown in the brown boxes have direct charging authority to the project and will carry out the technical tasks of the contract. The Project Manager (PM) Matthew Alvarado is also the Project Quality Assurance Officer and will have responsibility for maintaining and updating this QAPP via communication with the Texas Air Quality Research Program (AQR) Project Manager Elena McDonald-Buller.

The technical individuals shown in Figure 1 share responsibility for evaluating existing data obtained for this project that isn’t already covered by other TCEQ-accepted QAPPs. These evaluations, if required, will be documented, and controlled per AER’s established Quality Management System (QMS).

Below we provide a summary description of the key people, their responsibilities, and contact information:

- **Elena McDonald-Buller, AQRP Project Manager** (e.mcdonald-buller@ceer.utexas.edu, 512-471-2891) is the key AQRP contact for all technical communications, submittal of preliminary deliverables, and other tasks related to the production of deliverables prescribed in the contract.
- **Chola Regmi, TCEQ Project Liaison** (Chola.Regmi@tceq.texas.gov) is the key AQRP contact for all technical communications, submittal of preliminary deliverables, and other tasks related to the production of deliverables prescribed in the contract.
- **Matthew Alvarado, AER Project Manager and Project Quality Assurance Officer** (malvarad@aer.com, 781-761-2330) will be responsible for directing this project's day-to-day activities. He will also maintain overall responsibility for the successful completion of the project. He is also the overall AER contract manager for this TCEQ contract. He will ensure the project implementation follows all contract requirements and that project quality standards are met on all deliverables.
- **Rick Pernak, AER Senior Staff Scientist** (rpernak@aer.com) will assist Dr. Alvarado with training and evaluating the statistical modeling in Tasks 1 and 2.
- **Jennifer Hegarty, AER Staff Scientist** (jhegarty@aer.com) will assist in developing the meteorological predictors for the GAMs in Tasks 1 and 2, as well as with the interpretation of the results in Task 3.
- **Scott Macdonald, AER QA Officer** (quality@aer.com, 757-224-3237), will provide independent quality assurance to the project. He is familiar with all aspects of AER's quality control standards, procedures, and policies.
- **Emma Miceli, AER Contract Administrator** (emiceli@aer.com, 781-761-2243), will manage all non-technical aspects of the project, including generation and submission of invoices.

2.2. Schedule and Milestones

The proposed schedule and milestones for this project is shown in Table 3. If necessary, AER will propose revised milestone dates. AER will commence work upon receipt of the Notice to Proceed from the AQRP and the TCEQ.

Table 1. Projected Schedule for AQRP Project 22-003

2022	
Q3	Deliverable: Work Plan and Quality Assurance Project Plan. Due: 10 business days after notification of funding.
	Compile meteorological and fire predictors into a single dataset (Task 1).
	Gather and evaluate 2019 CAMx output from TCEQ (Task 2).
	Deliverable: Technical Report #1 – Due Sept 10, 2022
	Deliverable: Financial Status Report (FSR) #1 – Due Sept 15, 2022
Q4	Deliverable: Technical Report #2 – Due Oct 10, 2022
	Deliverable: FSR #2 – Due Oct 15, 2022
	Deliverable: First Quarterly Report Due: October 31, 2022
	Deliverable: Technical Report #3 – Due Nov 10, 2022
	Deliverable: FSR #3 – Due Nov 15, 2022
	Deliverable: Technical Report #4 – Due Dec 10, 2022
	Deliverable: FSR #4 – Due Dec 15, 2022
	Train and evaluate initial GAMs to assess the impact of smoke on background and urban air quality monitors in Texas (Task 1). Determine functional forms of fire predictors to use in Task 2 (Task 1).
2023	
Q1	Deliverable: Technical Report #5 – Due Jan 10, 2023
	Deliverable: FSR #5 – Due Jan 15, 2023
	Deliverable: Second Quarterly Report Due: January 31, 2023
	Deliverable: Technical Report #6 – Due Feb 10, 2023
	Deliverable: FSR #6 – Due Feb 15, 2023
	Deliverable: Technical Report #7 – Due Mar 10, 2023
	Deliverable: FSR #7 – Due Mar 15, 2023
	Apply GAMs to CAMx model output and evaluate differences from Task 1 (Task 2). Investigate causes of the differences (Task 2).
	Deliverable 2: Software and input/output files for the GAM models from Task 1, along with a brief technical memo on the models and evaluation. Due: March 31, 2023
	Q2
Deliverable: FSR #8 – Due Apr 15, 2023	
Deliverable: Third Quarterly Report Due: April 30, 2023	
Deliverable: Technical Report #9 – Due May 10, 2023	

	Deliverable: FSR #9 – Due May 15, 2023
	Deliverable: Technical Report #10 – Due Jun 10, 2023
	Deliverable: FSR #10 – Due Jun 15, 2023
	Identify conditions under which CAMx mis-estimates fire impacts (Task 3).
	Deliverable: Software and input/output files for the GAM models from Task 2, along with a brief technical memo on the models and evaluation. Due: June 30, 2023
Q3	Deliverable: Technical Report #11 – Due Jul 10, 2023
	Deliverable: FSR #11 – Due Jul 15, 2023
	Deliverable: Fourth Quarterly Report Due: July 31, 2023
	Deliverable: Technical Report #12 – Due Aug 10, 2023
	Deliverable: FSR #12 – Due Aug 15, 2023
	Write final report and draft presentation to AQRP Workshop.
	Deliverable: Presentation at AQRP Workshop Due: Approximately 1 month before end of project.
	Deliverable: Training for TCEQ staff on GAMs and the software from this study. Due: Approximately 1 month before end of project.
	Deliverable: Draft Final Report Due: August 15, 2023
	Deliverable: Final Report Due: August 31, 2023
	Deliverable: FSR #13 – Due Sep 15, 2023
	Deliverable: Final FSR – Due Oct 15, 2023

3. Model Selection

This section applies to the selection of pre-existing models for model application. In this project, the Hybrid Single-Particle Lagrangian Integrated Trajectory model (HYSPLIT) and the Stochastic Time-Inverted Lagrangian Transport (STILT) model fall into this category.

3.1. Requirements Design

Camalier et al. (2007) found that the distance and direction of the endpoint of a 24-hour back-trajectory from an urban area (starting at noon local solar time at a height of 300m) were important meteorological predictors for urban O₃ in eastern US cities. They used the Lagrangian Particle Dispersion Model (LPDM) HYSPLIT for calculating these back trajectories.

The STILT model is an enhanced version of the HYSPLIT model (Draxler and Hess, 1998) aimed at mass conservation, a critical consideration for inversion work. STILT computes the “footprint” (adjoint of the transport field) by following an ensemble of tracer particles backwards in time from the location of each measurement (“receptor”). The footprint (units: ppm/μmol m⁻² s⁻¹) quantifies the concentration enhancement at the receptor at each point in time due to unit surface flux at each upwind location. Here we will generate daily STILT footprints for each urban area driven with 12 km North American Mesoscale (NAM) meteorological data. These footprints will be initialized at local noon at a height of 300 m and will go at least 72 hours back in time.

3.2. Required Model Capabilities

We need LPDMs capable of calculating 72-hour back trajectories to determine the upwind influence of smoke. Given the impact of the sea/land breeze from the Gulf of Mexico on many of our urban areas of interest, the LPDM should be run with reasonably high horizontal resolution (12-km) meteorological fields, and these fields must be available for our entire study period in a format that can be used by the LPDM.

3.3. Selected Model

Based on the above requirements, we have selected the HYSPLIT and STILT models driven with 12-km NAM meteorology for this project.

3.4. Model Setup Requirements

HYSPLIT will be configured to run simple 24-hour back-trajectories from each urban area of interest. STILT will be configured to run daily 72-hour ensemble back-trajectory analyses from each urban area of interest. The required meteorological inputs will be taken from the NAM-12 fields processed for HYSPLIT by the National Oceanic and Atmospheric Administration (NOAA) Air Resources Laboratory (ARL).

4. Model Design

There are two “models” that will be developed in this project:

- The GAMs to be developed for Tasks 1 and 2,
- The computer software used to determine the background concentration of O₃ and PM_{2.5}.

Related models and/or the codes needed to develop them have been developed at AER under previous work (e.g., Alvarado et al., 2015). Below, we discuss each of these models in turn, describing the conceptual model framework, the proposed model development plan, and the required data sources for each.

4.1. GAMs for O₃ and PM_{2.5}

4.1.1. *Conceptual Model*

The formation and loss of pollutants such as O₃ and PM_{2.5} are strongly influenced by meteorology and biomass burning. For example, rising temperatures can increase the rate of secondary chemical formation of O₃ and PM_{2.5}, and several PM_{2.5} species (e.g., NH₄NO₃, semi-volatile organic aerosol) will evaporate to the gas phase as temperatures increase. Other meteorological controls include the wind speed and direction (which affects how much air a given amount of pollutant emissions mixes into and what emission sources are upwind of the urban area of interest), boundary layer height (which also affects pollutant mixing), relative humidity and cloud cover (which affect chemical reaction rates), precipitation (which increases the deposition of PM_{2.5}), etc. Most of these effects can be qualitatively evaluated by considering simple Eulerian

photochemical box models for the urban area of interest, such as those described in Section 23.2.1 of Seinfeld and Pandis (1998).

In this project we will train GAMs to determine the impact of smoke on background and urban core maximum daily 8-hour average (MDA8) O₃ and daily average PM_{2.5}. Examining background and total urban O₃ and PM_{2.5} separately will allow us to examine the impact of long-range transport of fire smoke separately from the impacts that result when the smoke mixes with urban pollution.

4.1.2. Model Algorithm Development

AER will derive GAMs for O₃ and PM_{2.5}. For O₃, only data during the O₃ season (March to October) will be analyzed, but PM_{2.5} data for the entire year will be analyzed. The parameters of the GAMs will be determined using the GAM modeling function in the R software environment following the approach of Camalier et al. (2007) and Alvarado et al. (2015). A log link function will be used, and a natural spline will be used to allow for a non-linear response between each meteorological parameter and the pollutant concentration.

Once these “baseline” GAMs have been developed, AER will explore whether the addition or substitution of other meteorological variables can significantly increase the amount of variability explained by the model. The most physically meaningful and statistically important variables will be selected using standard, non-automated methods, such as “backward one variable deletion” based on the F statistic (Venables and Ripley, 2002). Model residuals will be analyzed as well to determine the importance of different meteorological variables. Highly correlated variables will be excluded from the process, and only variables that are significant at the alpha=0.01 level will be retained. The predictive power of the models will be measured by the R² statistic. All predictor variables and relationships will be reviewed to ensure that in our expert judgment there are plausible causal relationships between the predictor variables and PM_{2.5} and O₃, rather than chance correlations.

4.1.3. Required Data Sources

Ambient Air Quality Data

Maximum daily 8-hour average (MDA8) O₃ mixing ratios and daily average PM_{2.5} concentrations will be calculated for each HGB and El Paso site from the surface air quality data in the Texas Air Monitoring Information System (TAMIS). Sites in each urban area will be separated into background (for sites on the outskirts of the city) and urban (for sites near the city core). For each urban area, the minimum value of MDA8 O₃ and daily average PM_{2.5} from background sites upwind of the urban core will be selected as the background estimate for that day. As the concentrations of O₃ and PM_{2.5} can vary within the urban core, all sites in the urban core will be included in the urban GAM model. The impacts of the fire and meteorological predictors will be assumed to be the same for all sites, with an additional site-specific random intercept used to account for the mean differences between sites (i.e., a Generalized Additive Mixed Effects Model, or GAMM, where the only random effect is in the intercept, so that the intercept varies between sites, but all other effects are the same between sites).

Meteorological Predictors

The meteorological predictors to be used in this study (Table 2) are based on our previous GAM studies of the ability of meteorological predictors to estimate the concentrations of O₃ and PM_{2.5} at urban and background monitoring sites in Texas. Our team has shown that these meteorological predictors, plus the previous day’s MDA8 O₃ or daily average PM_{2.5}, can explain approximately 70% of the variability in background and urban O₃, and about 30-40% of the variability in background and urban PM_{2.5} (e.g., Alvarado et al., 2015b; McVey et al., 2018; Pernak et al., 2019; Brown-Steiner et al., 2021).

Table 2. Meteorological parameters used in the GAMs.

1) Afternoon mean temperature (°C, <i>afternoon_mean_T</i> , 1-4 PM CST)
2) Diurnal temperature change (°C, <i>diurnal_T</i>)
3) Daily average wind speed (m/s, <i>daily_ws</i>)
4) Daily average wind direction (degrees clockwise from North, <i>daily_wd</i>)
5) Daily average water vapor density (g/m ³ , <i>SWVP</i>)

6) Morning surface temperature difference (1200 Universal Coordinated Time, UTC) (temperature at 925 or 700 mb–temperature at surface at 1200 UTC) (°C, T_{dif_925mb} or T_{dif_700mb})
7) Transport direction (degrees clockwise from North, $HYSPLIT_Bearing$)
8) Transport distance (m, $HYSPLIT_dist$)

Variables 1-5 in Table 1 were calculated from the surface meteorological data in the TAMIS. Variable 6, which reflects the vertical stability of the atmosphere each day, was calculated from upper atmosphere data in the Integrated Global Radiosonde Archive (IGRA Version 2). Given El Paso’s higher elevation, an upper atmosphere level of 700 mbar was used for this city as opposed to the 925 mbar value used for all other urban areas. Variables 7 and 8 were calculated from 24-hour NOAA HYSPLIT back-trajectories driven with 12 km horizontal resolution NAM data. As in Camalier et al. (2007), these back-trajectories are calculated assuming an initial height of 300 m above ground level (AGL) and are started at noon local solar time. The endpoints of the back-trajectories were used to calculate the 24-hour transport direction and distance for each urban area for the 2007-2016 period.

Fire and Smoke Predictors

The NOAA Hazard Mapping System (HMS) Fire and Smoke product will be our primary source of fire predictors, as we have shown that days where the HMS product indicates smoke over Houston tend to be associated with enhancements in CO, O₃, and NO_x (Figure 2). This gives us confidence in the ability of our statistical modeling to be able to identify a statistically significant impact of fires on air quality in HGB and El Paso. To make the HMS, satellite analysts compare automated fire detections to the infrared satellite images used to produce them to ensure each fire exists (Ruminski et al., 2006; Schroeder et al., 2008; Brey et al., 2018). Small fires are more difficult to detect and are underreported (*e.g.*, Hu et al., 2016). False fire detections are removed, and fires that were not automatically detected are added manually.

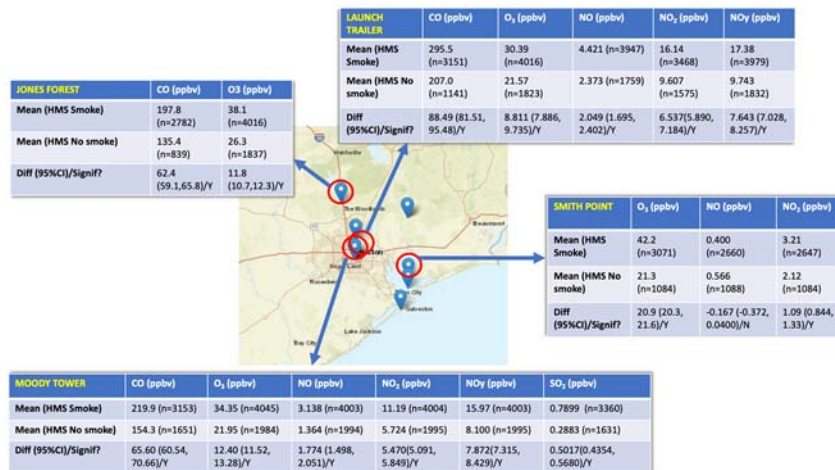


Figure 2. Map of selected surface air quality monitoring sites in HGB. Tables show concentrations of species measured at each circled site, divided into HMS-smoke and HMS-no smoke categories.

After identifying fire locations, HMS analysts use imagery from multiple NOAA and NASA satellites to identify the geographic extent of smoke plumes (Rolph et al., 2009; Ruminski et al., 2006). Due to the frequent interference by cloud cover, the number and extent of smoke plumes reported in the HMS represents a conservative estimate.

In addition to the HMS, we will use the Fire Inventory from the National Center for Atmospheric Research (FINN, Wiedinmyer et al., 2011) to obtain high resolution (~1 km²) estimates of total NO_x, VOC, and PM_{2.5} emissions from fires. These emissions will be convolved with daily estimates of upwind influences on HGB and El Paso measurements (i.e., upwind surface “footprints” calculated from meteorological models; see Section 1.2.2) to determine the daily transport of O₃ precursors and primary PM_{2.5} to each city.

We will test several fire and smoke predictors based on the HMS and FINN data, including:

- a. A binary predictor for the presence of smoke according to the NOAA HMS (Figure 1)
- b. The total HMS fire counts in surrounding regions binned by distance from the city (e.g., every 500 km out to 2000 km from the city) and direction (e.g., NE,

SE, NW, or SW quadrant). The exact criteria for each distance and wind direction bin will be determined during model training.

- c. The FINN NO_x, VOC, and PM_{2.5} emissions multiplied by the daily surface “footprints” (Section 1.2.2). The footprints will be separated into domestic and international surface influences to isolate the impacts of domestic fire emissions, and into fresh and aged smoke to examine how smoke age affects the impacts.

CAMx

CAMx is a widely used 3D Eulerian chemical transport model that simulates regional air quality over spatial scales ranging from neighborhoods to continents. Meteorological inputs are supplied to CAMx from separate weather prediction models (e.g., Weather Research and Forecasting Model, WRF) while emission inputs are supplied from external pre-processing systems (e.g., Sparse Matrix Operator Kernel Emissions, SMOKE). Here we will use TCEQ CAMx air quality simulations from 2019 (at 4 km resolution over Houston and El Paso, mapped to TAMIS monitoring sites) as predictands for extended versions of our GAM models to assess the ability of CAMx to simulate the air quality impacts of fires (Task 2, Section 1.3.2). Using this pre-existing TCEQ generated output will allow us to evaluate the CAMx model while keeping the cost and complexity of the project modest.

HYSPLIT/STILT Inputs

In addition, the HYSPLIT and STILT modeling for this task will require NAM-12 km meteorological data, as discussed in Section 3.4 above. These data sets in HYSPLIT-ready format are available from the HYSPLIT website (<http://ready.arl.noaa.gov/HYSPLIT.php>).

4.2. Software to Determine Background Values of O₃ and PM_{2.5}

4.2.1. Conceptual Model

As noted above, daily surface concentrations of O₃ and PM_{2.5} in urban areas can be considered as the sum of O₃ and PM_{2.5} produced within the urban area (either through primary emissions of PM_{2.5} or through secondary chemical production of O₃ and PM_{2.5}) and a “regional background” that is transported into the urban area by the large-

scale circulation. Accurate estimates of this regional background are critical to determining the potential for further reductions in O₃ and PM_{2.5} concentrations in urban areas through control of local emissions of SO₂, primary PM_{2.5}, and the precursors of O₃, and PM_{2.5}.

In this project we will be applying the TCEQ method to estimate this background using the lowest values of MDA8 O₃ and daily average PM_{2.5} observed at defined “background” sites near the border of the areas of interest (Berlin et al., 2013). AER will also assess the spatial and temporal variations in this background level with respect to meteorology.

4.2.2. Software Development

AER will update our software that identifies the daily regional background estimates of O₃ and PM_{2.5} using the TCEQ method. In applying the TCEQ method to estimate regional background O₃, AER will:

- a) Work with TCEQ to identify “background” monitor sites near the edge of each urban area and in areas near the Texas border. These background sites will be chosen to be at a significant distance from major pollutant emission sources.
- b) For each day of the O₃ season (March through October), calculate the MDA8 O₃ values at each background monitor site.
- c) Use the lowest MDA8 value observed at the selected background sites as the preliminary estimate of the regional background O₃.
- d) Perform a least-squares linear regression with area-wide peak MDA8 O₃ as the dependent variable and the estimated background O₃ as the independent variable for each area and each month of the O₃ season.
- e) Flag days at which the residual values from the least-squares linear regression are greater than 2 standard deviations for further analysis.
- f) For the days flagged in step (e) above, examine the raw O₃ data (at the highest available time resolution, ~5 min.) and other available data (e.g., satellite O₃ observations) to determine if the preliminary estimate of regional background O₃ is too low due to conditions that affect only some monitor sites rather than the urban area as a

whole, such as is the case in Houston when the Gulf breeze is weak. If so, AER will select a more representative site for that day's background estimate.

AER will perform similar work to apply the TCEQ method to estimate daily regional background estimates of PM_{2.5}, with the following exceptions: the daily average PM_{2.5} values will be used for analysis, and daily background estimates will be made for every day between 2007-2016, rather than just during the O₃ season.

Once the regional background estimates are derived, AER will use our previously developed software (Alvarado et al., 2015) to use these estimates to explore the spatial and temporal patterns in the regional background levels, such as seasonal patterns and inter-annual variability.

4.2.3. Required Data Sources

The required data sources are the same as described above in Section 4.1.3.

5. Model Coding

5.1. GAMs for O₃ and PM_{2.5}

The GAMs will be derived using the R software language, and R scripts used in deriving and applying the generated models will be supplied to TCEQ.

5.2. Software to Determine Background Values of O₃ and PM_{2.5}

All software developed in this part of the project will be in R, Python, or Microsoft Excel®, depending on which is most useful for each part of the task, and will be supplied to TCEQ along with the draft and final reports.

6. Model Calibration

Model calibration, defined as “adjusting model parameters within physically defensible ranges until the resulting predictions give the best possible or desired degree of fit to the observed data,” only directly applies to the development of the GAMs. As noted in Section 4.1.2 above, the parameters of the GAMs will be determined using the GAM modeling function in the R software environment. A log link function will be used,

and a natural spline will be used to allow for a non-linear response between each meteorological parameter and the O₃ and PM_{2.5} concentration.

Different combinations of predictor variables will be evaluated as part of the development. The most physically meaningful and statistically important variables will be selected using standard, non-automated methods, such as “backward one variable deletion” based on the F statistic (Venables and Ripley, 2002). Model residuals will be analyzed as well to determine the importance of different meteorological variables. Highly correlated variables will be excluded from the process, and only variables that are significant at the alpha = 0.01 level will be retained. The predictive power of the models will be measured by the R² statistic. All predictor variables and relationships will be reviewed to ensure that in our expert judgment the models represent plausible causal relationships between the predictor variables and O₃ and PM_{2.5}, rather than chance correlations.

7. Model Verification

Model verification, defined as “comparing the predictions of a calibrated model with data that were not used in the model development and calibration,” again only directly applies to the development of the GAMs for Objective A. One of the dangers of using GAMs to perform the meteorological adjustment of pollutant trends is the possibility of “over-fitting,” where some of the variability that is due to changes in air quality policy is accounted for in the GAM by the meteorological variables. AER will explore the potential errors from over-fitting using techniques such as cross validation. In cross validation, some of the data (the testing set) is removed before building the GAM. The remaining data (the training set) is used to derive the GAM parameters. The testing set will be used to test the performance of the GAM in predicting “unseen” data.

8. Model Evaluation

Model evaluation applies to the application of the STILT and HYSPLIT models to calculate back-trajectories described in Section 3, as well as the two model development

tasks described in Section 4. The evaluation of these components is discussed in turn below.

8.1 Evaluation techniques

8.1.1. HYSPLIT and STILT Back-Trajectories

AER has extensive experience with the running and evaluation of LPDMs, including HYSPLIT and STILT (e.g., Hegarty et al., 2013; Alvarado et al., 2015). AER personnel will use their expert judgment to evaluate the STILT and HYSPLIT back-trajectories produced in this project by assessing them for realism and fidelity with the NAM-12 meteorological fields used in their generation. The settings of each model will be reviewed to ensure that they are correct prior to the production of the back-trajectories. Selected back-trajectories will be inspected to see if the final calculated transport directions and distances are consistent with the synoptic-scale meteorological conditions for that day, and the annual statistics of the final calculated transport directions and distances will be compared with annual wind roses for the region. This will satisfy the requirement to audit 10% of the data for quality.

8.1.2. GAMs for O₃ and PM_{2.5}

The predictive power of the GAMs will be evaluated as described in Section 6, while the performance of the models in predicting 'unseen' data will be assessed in the cross-validation exercise described in Section 7. In addition, AER personnel will use their expert judgment to evaluate the performance of the GAMs. The causal nature of the relationships captured by the GAMs will be evaluated against our conceptual understanding of the impacts of meteorology on O₃ and PM_{2.5} chemistry and transport. Any identified significant meteorological predictors without such conceptual causal relationships will be identified, and separate GAMs that do not include the questionable predictors will be produced. The residuals of the GAM will be examined, and any days with extreme residuals will be flagged for further analysis. The adjusted trends in O₃ and PM_{2.5} produced by the models will also be assessed for their realism and connection with known policy and economic drivers of these trends. These last two steps will satisfy the requirement to audit 10% of the data for quality.

8.1.3. Software to Determine Background Values of O₃ and PM_{2.5}

First, several of the background values determined by the software will be inspected by hand to ensure the model is selecting the correct monitors as background. As discussed in Section 4.2.2, values that are more than 2 standard deviations from the least-squares regression line will be flagged for further analysis. This will satisfy the requirement to audit 10% of the data for quality.

Second, AER personnel will use their expert judgment to determine if the derived background values, and their spatial and temporal variation, are a) consistent with our conceptual models of O₃ and PM_{2.5} emissions, chemistry, and transport and b) consistent with previous studies in the scientific literature (e.g., Berlin et al., 2013). The uncertainties in these background estimates and the conditions under which they are expected to be valid will be determined.

8.2. Peer Review and Reconciliation with User Requirements

The information collected from the exercises described in Sections 7 and 8.1 will be used to make a final, overall assessment of the model data usability that will be included in the final report.

9. Model Documentation

As part of Task 6 a Final Report will be provided to TCEQ. This report will include:

- The final model description, hardware, and software requirements, including programming language, model portability, memory requirements, required hardware/software for application, and data standards for information storage and retrieval
- The equations on which the model is based
- The underlying assumptions used in the model development
- Flow charts of model inputs, processing, and outputs
- Descriptions of the software routines
- Data base description

- A copy of the source code
- Explanation of error messages
- Parameter values and sources
- Restrictions on model application, including assumptions, parameter values and sources, boundary and initial conditions, validation/calibration of the model, output and interpretation of model runs.
- Limiting conditions on model applications, with details on where the model is or is not suited
- Actual input data (type and format) used
- Overview of the immediate (non-manipulated or post-processed) results of the model runs (model application only)
- Output of model runs and interpretation
- User's guide (electronic or paper)
- Instructions for preparing data files (model development only)
- Example problems complete with input and output
- A report of the model calibration, validation, and evaluation (model development only).

AER will also attach R scripts and other computer codes used to generate and/or analyze the GAMs.

For all other objectives, AER will produce a final report that includes thorough documentation of our findings and recommendations for future work. All scripts and methods used in the project will be documented in the final report in a similar manner to that described for the GAMs above.

10. Assessment and Oversight

Assessments will be conducted to determine whether the QAPP is being implemented as approved, to increase confidence in the information obtained, and to determine whether the information is suitable for its intended purpose.

10.1. Assessments and Response Actions

The AER QA Officer for the Work Order will be the PM Dr. Alvarado. He will direct the conduct of both internal and external assessments during the project in accordance with AER's QMS. Internal assessments consist of periodic Project Reviews and code reviews. These activities are required under our ISO 9001 procedures and are described briefly below. The PM will also serve as Configuration Manager for the project.

The Project Review provides a status update of project schedule and budget, the status of any deliverables, and any reasons for modification, if necessary. Any issues of note relating to deliverables, milestones, or scope changes are reviewed. Staffing changes and Other Direct Costs are also reviewed. The review concludes with an accounting of any additional concerns. Since this project will use existing data in addition to the planned model development and application, the project data will also be assessed to determine suitability for its intended use, and to document whether project specifications were met.

Code reviews will be performed periodically, including prior to every deliverable or internal release, at the end of the project, and at specific intervals to be determined at the beginning of the project. These reviews will be performed by a different AER employee than the one who carried out the original work. During the review, model source code, settings, input, and output will be reviewed, and any errors will be noted and rectified. These code reviews fulfill the 10% audits of data quality stipulated by the TCEQ contract and Work Order for Category III QAPPs.

All technical personnel listed in Section 2 will share responsibility for identifying and resolving problems encountered during the routine performance of their duties. These issues will be shared with the PM during regular internal project meetings and resolved under the direction of the PM. Problematic issues will be reported to upper management through procedures described in Section 10.2 below.

10.2. Reports to Management

An Executive Session Review (ESR) by the AER executive leadership is another periodic requirement of the AER QMS. The ESR is similar in scope and frequency as the Project Review described in Section 10.1 but includes a review of scientific and technical issues and any management and infrastructure support required. Any serious issues in project performance or quality of deliverables will be reported during the ESR.

11. Reporting

11.1. Deliverables

The deliverables for the project are listed in Table 1. The PM Dr. Alvarado is responsible for evaluating the quality of all deliverables prior to delivery.

11.2. Data Retention

All project data will be stored on AER on-site storage or on AER's Amazon Web Services (AWS) virtual private cloud for at least three years after the end of the project. On-site data is backed up to tape on a weekly basis while AWS data is backed up automatically via mirroring on multiple AWS storage facilities. On-site tape backups are retained after the three-year period for an additional seven years.

11.3. Final Report

AER will deliver a Draft Final Report and Final Report to the AQRP Project Manager electronically (i.e., via file transfer protocol (FTP) or e-mail) in Microsoft Word and PDF formats. The Final Report will include the following components:

1. An executive summary or abstract.
2. A brief introduction that discusses the background and objectives. Include relationships to other studies if applicable.
3. A discussion of the pertinent accomplishments, shortfalls, and limitations of the activities completed under each 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 any data collected and analyzed, including a report on the results of the Audits of Data Quality. The Final Report will highlight major activities and key findings, provide pertinent analysis, describe encountered problems, and associated corrective actions, and/or detail relevant statistics, including data, parameter, or model completeness, accuracy, and precision.

12. References

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