Quality Assurance Project Plan

Project 17 – 024

Improving the Modeling of Wildfire Impacts on Ozone and Particulate Matter for Texas Air Quality Planning

Prepared for

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

Prepared by

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Atmospheric and Environmental Research (AER)

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Atmospheric and Environmental Research (AER) has prepared this QAPP following EPA guidelines for a Quality Assurance (QA) Category III Project: Research Model Development. 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; Reporting; and References.

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 "Improving the Modeling of Wildfire Impacts on Ozone and Particulate Matter for Texas Air Quality Planning" project. The Principal Investigator for the project is Matthew J. Alvarado of AER.

Electronic Approvals:

This QAPP was approved electronically on 09/15/2016 by Elena McDonald-Buller, The University of Texas at Austin.

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This QAPP was approved electronically on 09/26/2016 by Matthew J. Alvarado, Atmospheric and Environmental Research (AER).

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Introduction

This document is the Quality Assurance Project Plan (QAPP) for Texas Air Quality Research Program (AQRP) Project 16-024. It adopts a graded approach to QA to ensure the quality-related activities of the project are commensurate with its scope and resources. This QAPP specifies or references policies, procedures, specifications, standards, and documentation that will lead to data of adequate quality to meet project objectives and minimize data loss. The general outline of this document follows the National Risk Management Research Laboratory (NRMRL) QAPP Requirements for Research Model Development and Application Projects.

Atmospheric and Environmental Research, Inc. has received the ISO 9001:2008 certification from National Quality Assurance (NQA). This means AER has established, documented, and maintains a Quality Management System (QMS) that meets the requirements of ISO 9001. The QMS documentation consists of:

- A Quality Manual (document QM0002-08, referenced below), defining the Corporation's policy, organization and general responsibilities and statements of our quality policy and quality objectives;
- A second level of Operating Procedures (QOP's) referenced in the Quality Manual, which define organizational activities, designed to control operation of the Corporation;
- A third tier of Work Instructions (WI's), where necessary, which specify how processes are undertaken, contain product specifications, and define the documents used in these activities, where these are necessary to achieve adequate control of AER processes;
- Documents needed by the company to ensure the effective planning, operation and control of our processes;
- Records required by ISO9001.

The components of the QMS are described in Table 1, which also refers to a procedures document (or collection) within AER's QMS.

Referenced Documents

- AER Quality Manual-ISO 9001, QM0002-08
- National Risk Management Research Laboratory (NRMRL) QAPP Requirements for Research Model Development and Application Projects
- Project Work Plan for Work Order No. 582-16-62311-03
- QM-0002-08 Quality Manual
- QOP-0201 Project Implementation
- QOP-0201S01 Configuration Management (AER internal ISO 9001 procedure)
- QOP-030406 Document Numbering, Control, Retention, and Disposal and QOP-0403 Quality Documents
- QOP-030709 Computer Backup (AER internal ISO 9001 procedure)
- QOP-0405 Management Review

- QOP-0404 Internal Auditing
- QOP-0401 Corrective and Preventive Action

Table 1. Components of AER's Quality Management System

QMS Component	Description
Quality Manual	Defines the company's policy, organization and general responsibilities and statements of our quality policy and quality objectives *(QM-0002-08, Quality Manual)*
Management Responsibility	Statements of management's responsibilities to quality, management structure, chain of authority, quality policy (*QOP-0405, Management Review)*
Resource Management	Identifies resource requirements, including training, performance of work and verification activities including carrying out internal quality audits *(QOP-0201, Project Implementation)*
Product Realization	Processes and procedures that encompass all aspects of providing and maintaining services of highest quality to customers *(QOP-0201, Project Implementation)*
Measurement, Analysis, and Improvement	Description of AER's plans and procedures for monitoring, measuring, analyzing, and improving conformity of the product and the QMS *(QOP-0404, Internal Auditing* and *QOP-0401, Corrective and Preventive Action)*
Sequence and Interaction	Description of how QA procedures are applied as each activity is undertaken *(QM-0002-08, Quality Manual)*

1. Project Description and Objectives

The primary objective of this project is to use an advanced smoke plume chemistry model (AER's Aerosol Simulation Program, or ASP, Alvarado et al., 2015a) to improve understanding of the formation of O3 and PM2.5 in biomass burning plumes, and improve estimates of the impacts of in-state and out-of-state biomass burning on Texas air quality. Biomass burning (BB) is a major source of trace gases and aerosols that impact air quality. For example, in June 2012 the estimated median contribution of fires to maximum daily 8-hr average (MDA8) O_3 in Texas was 2 ppb, with maximum impacts of over 40 ppb (McDonald-Buller et al., 2015).

3D Eulerian chemical transport models like CAMx make estimates of the primary emissions from BB and unphysically "mix" them across large-scale grid boxes, which can lead to incorrect estimates of the impact of BB on air quality. For example, Baker (2015) found that the 3D Eulerian model CMAQ tended to overestimate the impact of BB on individual hourly ozone measurements at CASTNET monitoring sites near the fires by up to 40 ppb and underestimate it further downwind by up to 20 ppb. This behavior is consistent with an incorrect treatment of the sub-grid scale near-source O_3 and NO_y chemistry, where the model underestimates the loss of NO_x near the source due to formation of inorganic and organic nitrates, thus overestimating O_3 formation near the source (e.g., Alvarado et al., 2010). This same error leads to an underestimate of the amount of peroxy nitrates formed near the source, which then leads to an underestimate of O_3 formation downwind when the peroxy nitrates decompose, regenerating NO_x.

Plume-scale process models like ASP (Alvarado et al., 2015a) allow us to examine the chemical and physical transformations of trace gases and aerosols within BB smoke plumes and to develop parameterizations for this aging process in coarser grid-scale models. For example, McDonald-Buller et al. (2015) used a subset of the ASP-based parameterization of Lonsdale et al. (2014) to adjust the chemistry of biomass burning in CAMx, and found that this approach reduced the median impact of BB on MDA8 O_3 in Texas by 0.3 ppb, or 15%. However, McDonald-Buller et al. (2015) did not use the full Lonsdale et al. (2014, 2015) parameterization or examine the impact of BB organic aerosol (OA) on $PM_{2.5}$ in Texas.

In this project, we will improve understanding of the impacts of local and out of state fires on air quality in Texas by: (a) implementing an improved version of the ASP-based sub-grid scale parameterization of the formation of O_3 and SOA in BB plumes into CAMx via the plume-in-grid (PiG) module (Karamchandani et al., 2011; Task 1); and (b) using ASP within the Lagrangian particle dispersion model STILT (Lin et al., 2003) to investigate the impact long-range transport of BB smoke could have on the boundary conditions of the CAMx modeling for Texas, and thus on the simulated air quality (Task 4.2). In Task 1, we will use ASP within the large eddy simulation model SAM (Khairoutdinov and Randall, 2003) along with aircraft measurements of the evolution of several North American smoke plumes from the Department of Energy (DOE) Biomass Burning Observation

Project (BBOP; Kleinman and Sedlacek, 2015), to develop the improved parameterization which will take advantage of the data on plume dilution provided by the PiG module. In order to minimize the computational expense, the PiG module will be used to explicitly simulate only the CO and CO_2 emissions from individual fires. The downwind concentrations of O_3, NO_y species, and organic aerosol (OA) transferred from the individual plumes to the grid will be determined by the parameterization based on fire and environmental conditions. In Task 2, we will use the STILT-ASP model to determine if the impacts of fires on the CAMx boundary conditions for CO, O_3, NO_y species, OA, etc., from GEOS-Chem have significant errors due to numerical diffusion or incorrect treatment of BB chemistry. We will then assess the impact these errors have on simulated air quality in Texas.

The objectives of this project are thus to:

1. **Develop and evaluate an improved sub-grid scale parameterization of biomass burning for CAMx based on SAM-ASP and an analysis of O3 and SOA production in fire plumes observed during BBOP.**
2. **Explore the impact of BB plumes on the boundary conditions used for CAMx and the resulting impact on Texas air quality with STILT-ASP.**

Note that, for the purposes of this QAPP, we are treating Task 1 as a Model Development project and Task 2 as a Model Application project.

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 QAPP are also identified.

A project organization chart is provided in Figure 1. The AER persons shown in Figure 1 are divided into two main groups: those shown in the blue boxes (President, R&D Division VP, ACR Section Lead, 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), Matt Alvarado, is also the Project Quality Assurance Officer and will have responsibility for maintaining and updating this QAPP via communication with the AQRP Project Manager, Elena McDonald-Buller. Updates to this document will be coordinated with the AER Quality Officer, Susan Cline, who serves independently in this role from the project.

The technical individuals shown in Figure 1 will 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) described in the Introduction Section.

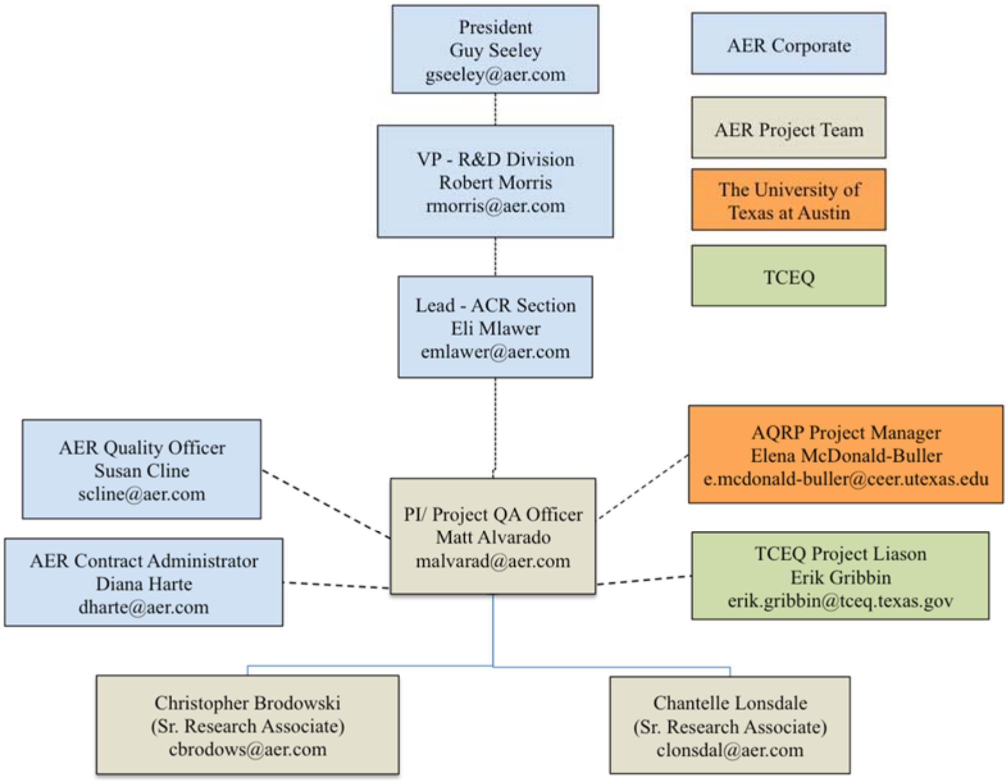

Figure 1. AER organization chart for AQRP project 16-024. Persons with direct charging authority to the project are indicated in brown; persons serving in a corporate capacity are indicated in blue. AQRP project manager is shown in orange and TCEQ liaison is shown in green. Solid blue lines indicate the reporting for this project only, while dotted lines indicate AER's corporate hierarchy. Dashed lines are used to connect the PM to AER administrative support, the AQRP project manager, and the TCEQ liaison.

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) will assist with the preparation of the Work Plan and ensure that all reporting requirements are being met.

Erik Gribbin, TCEQ Liaison (erik.gribbin@tceq.texas.gov, 512-239-2590) is responsible for the approval of the Work Plan and final authorization for funding. During the life of the Project, he will receive and approve all technical reports.

Matthew Alvarado, AER Principal Investigator and Project Quality Assurance Officer (malvarad@aer.com. 781-761-2330) is the lead developer of

ASP and has extensive experience in the modeling of the chemistry of BB smoke plumes. He will lead all of the studies of the chemistry and impacts of BB to be carried out in this project and 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 will ensure the project implementation follows all contract requirements and that project quality standards are met on all deliverables. He will assist in interactions with AQRP project management as required.

Chantelle Lonsdale, AER Senior Research Associate (clonsdal@aer.com, 781-761-2327) developed the ASP-based parameterization of BB chemistry. Ms. Lonsdale also has experience with the SAM model (Lonsdale et al., 2012) and is leading our efforts to couple SAM and ASP. Ms. Lonsdale will incorporate the improved ASP-based parameterizations into CAMx and evaluate the impacts of BB on Texas air quality (Task 1).

Christopher Brodowski, AER Senior Research Associate (cbrodows@aer.com, 781-761-2369) has detailed experience with the STILT-ASP model from his work on coupling the two models. Mr. Brodowski will perform the STILT-ASP simulations to evaluate the impact of long-range transport of BB pollution on Texas air quality (Task 2) as well as assist with the incorporation of the updated parameterization into CAMx (Task 1).

Susan Cline, AER QA Officer (scline@aer.com, 781-761-2288), will provide independent quality assurance to the project. She is familiar with all aspects of AER's quality control standards, procedures and policies.

Diana Harte, AER Contract Administrator (dharte@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 are shown in Table 2 below. As necessary, AER will propose revised milestone dates. AER will commence work upon receipt of the Notice to Proceed from the TCEQ and AQRP.

Table 2. Project work schedule and deliverables.

2016	
Start of project through Q4	Modify CAMx to simulate fires using PiG with CO and CO_2 tracers (Task 1).
	Use STILT to see how well GEOS-Chem boundary conditions represent BB CO (Task 2).
	Determine input variables and sampling hypercube for improved parameterization (Task 1).
	Perform STILT-ASP runs with full chemistry to see how well GEOS-Chem BCs represent O_3, NO_y, and OA emissions and secondary production from fires (Task 2).
2017	
Q1	Use SAM-ASP and BBOP data to develop an improved sub-grid parameterization (Task 1)
	Determine how an improved representation of fire impacts on the boundary conditions alters the CAMx simulations (Task 2).
	Use STILT-ASP to investigate potential errors in biomass burning chemistry due to numerical diffusion in coarser CAMx grids (Task 2)
Q2	Incorporate improved parameterization into CAMx (Task 1)
	Run CAMx tests to determine impact of parameterization on O_3 and $PM_{2.5}$ (Task 1).
Q3	Complete evaluation of improved parameterization in CAMx (Task 1).
	Deliverable 1: Modified CAMx code that includes the improved ASP-based parameterization for BB chemistry. **Due:** August 31, 2017 (as a separate but concurrent submission with the Final Report)
	Deliverable 2: Draft journal article summarizing result of Tasks 1 and 2. **Due:** August 31, 2017 (as a separate but concurrent submission with the with Final Report)

3. Model Selection

This section only applies to the selection of the STILT-ASP model for Task 2.

3.1. Model Use in Task 2

As stated in the Work Plan, we will use a Lagrangian chemical transport model to assess the errors in the impacts of fires on CAMx boundary conditions due to numerical diffusion. One danger of using global 3D Eulerian chemical transport models like GEOS-Chem and MOZART to estimate the impact of inter-hemispheric transport of BB is that the numerical diffusion in these models tends to reduce the plume concentrations, thus potentially altering the chemistry and leading to incorrect boundary conditions for regional air quality studies (Rastigejev et al., 2010). Lagrangian models, like STILT-ASP (Alvarado et al., 2016), are not subject to this numerical diffusion and thus can be a useful check on the predictions of the 3D CTMs. In this task, we will examine the CAMx boundary conditions produced from GEOS-Chem for the 2012 CAMx modeling episode, along with satellite observation of CO (from the NASA Atmospheric Infrared Sounder (AIRS) instrument) and aerosols (from the Moderate Resolution Imaging Spectroradiometers (MODIS) flown on the NASA Terra and Aqua satellites) from BB, for periods where the boundaries of the North American (36 km) nest were impacted by long-range transport of biomass from, for example, Siberian fires. The details of these satellite data sources, including where the data were obtained, references for protocols for QA/QC, and validation by sources, will be included in the Final Report. We will run a CAMx simulation with the boundary concentrations impacted by BB perturbed by ~20% and assess the impact on Texas and North American air quality. We will then run a Lagrangian chemical transport model for a selected set of these "boundary" receptors that have a relatively high impact on Texas air quality to determine how this "Lagrangian" estimate of the impact of fires on the boundary conditions for CO, O_3, NO_y species, OA, etc., differs from the "Eulerian" estimate from GEOS-Chem. This will include both a qualitative evaluation of the location and horizontal and vertical extent of the wildfire impacts as well as a quantitative comparison of the excess concentrations (i.e., concentrations in the fire plume relative to a non-fire influenced background) along the boundaries.

The results of these Lagrangian runs will be used to scale the concentrations at these "boundary" receptors, with the scaling selected to minimize (in a least-squares sense) the differences in the excess concentrations between the Lagrangian runs and the CAMx boundary conditions (i.e., minimize the root-mean-square error of the excess concentrations, where root-mean-square error is defined in Section 5). We will run CAMx again to assess the sensitivity of Texas air quality to errors in the impacts of fires on the boundary conditions.

In addition to examining the impact of BB on the North American boundary conditions, we will perform similar investigations of the impact of BB on the boundaries of the Texas (12 km) and SE Texas (4 km) domains for the 2012 episode from McDonald-Buller et al. (2015). This test will look for consistency of the predicted boundary impacts between the CAMx simulations for the outer domains and those of the Lagrangian model, thus quantifying potential errors in the modeling impact of BB emission in CAMx due to numerical diffusion in the coarser grids. These errors will be quantified in terms of the mean bias (MB) and root-mean-square error (RMSE) of the predicted Eulerian excess concentrations relative to the Lagrangian predictions.

3.2. Required Attributes

To accomplish the above objectives, we need a Lagrangian chemical transport model that is capable of being run in a time-reversed, receptor-focused framework, and which is capable of simulating the complex chemistry of biomass-burning plumes.

3.3. Selected Model

Based on the above requirements, we have selected the STILT-ASP model (Alvarado et al., 2016) for this task. The STILT model (http://www.stilt-model.org; Lin et al., 2003) is a Lagrangian particle dispersion model derived from HYSPLIT but which includes additional modifications that improve the mass-conservation of the simulations and allow the use of customized WRF meteorological fields (Nehrkorn et al., 2010), which have been shown to improve the model performance when compared with tracer-release studies (e.g., Hegarty et al., 2013). STILT has been extensively used at AER in inverse modeling to improve emission estimates for greenhouse gases (e.g., McKain et al., 2012, 2015; Henderson et al., 2015).

STILT-ASP (Alvarado et al., 2016) is an extension of STILT that includes the gas-phase chemistry of the ASP model, which has been validated against observations of O_3 and $PM_{2.5}$ formation in biomass burning plumes (e.g., Alvarado and Prinn, 2009; Alvarado et al., 2015a). In this project, we will use STILT-ASP to better account for the impacts of long-range transport of BB emissions on CO, O_3, and other pollutants on the boundary conditions of the CAMx modeling of Texas air quality (Task 2).

3.4. Application Requirements

Most of the required input files for STILT-ASP are constant between runs and are supplied with the model. Default values for number of particles and other parameters will be used as described in Alvarado et al. (2016). The input files that vary between cases include:

Meteorological inputs: Meteorological inputs to STILT-ASP v1.0 must be in “Air Resources Laboratory” (“ARL”), or Hybrid Single-Particle Lagrangian Integrated Trajectory (HYSPLIT), format. STILT-ASP v1.0 can be run with either the National Centers for Environmental Prediction/National Center for Atmospheric Research Reanalysis (NARR) 32 km wind fields or the North American Mesoscale (NAM) 12 km wind fields supplied on the NOAA Air Resources Laboratory (ARL) web site (e.g., http://ready.arl.noaa.gov/archives.php).

Chemical boundary and initial conditions: STILT-ASP v1.0 can use CMAQ ICON/BCON files to specify initial/boundary conditions, or it can use output from a run of the global chemical transport models MOZART-4 or GEOS-Chem. One publically available source of such output is the MOZART-4/GEOS-5 output from the NCAR Chemical Forecasts (http://www.acom.ucar.edu/acresp/forecast/).

Chemical emissions files: STILT-ASP v1.0 can use 4D emission files similar to those used in CAMx or "default" emissions generated from the Fire INventory from NCAR (FINN, Wiedinmyer et al., 2011, the HTAP v2 inventory (http://edgar.jrc.ec.europa.eu/htap_v2/index.php), and MEGAN v2 (Guenther et al., 2006) model output, as described in Alvarado et al. (2016).

4. Model Design

This section only applies to the selection of the development of the sub-grid scale parameterization of biomass burning chemistry for the CAMx model (Task 1).

4.1. Conceptual Model

The conceptual model for this system is that the O_3 and $PM_{2.5}$ concentrations in biomass burning smoke plumes are due to a combination of the initial emissions from biomass burning and the complex chemical and physical changes that take place in the young, concentrated smoke plume. Accurate simulation of this near-source chemistry is necessary to determine the contributions of fires to the O_3 and $PM_{2.5}$ concentrations measured at a receptor.

The secondary chemical formation of O_3 in biomass burning plumes is generally determined by the ratio of the fire emissions of NO_x to the fire emissions of non-methane organic compounds (NMOCs), which is in turn determined by the combustion efficiency and the amount of nitrogen in the fuel (e.g., Jaffe and Widger, 2012; Jaffe et al., 2013; Baylon et al., 2014; Alvarado et al., 2015a). Other environmental parameters, such as temperature and shortwave (solar) actinic flux, also alter the amount of O_3 that can be formed as the parcel is transported. This chemistry can be adequately simulated with small adjustments to current atmospheric chemical mechanisms (e.g., Alvarado et al., 2015a).

Primary emissions of $PM_{2.5}$ from fires are dominated by organic aerosol (OA), with smaller contributions from black carbon (BC) and inorganic salts (e.g., Akagi et al., 2011). The secondary production of $PM_{2.5}$ in parcels influenced by fire emissions is generally determined by the oxidation chemistry of the semi-volatile and intermediate volatility organic compounds (S/IVOCs) present in the fire emissions. This chemistry can be adequately simulated using a set of "average" reaction rates with OH and product yields for a small set of S/IVOC compounds (e.g., Alvarado et al., 2015a).

4.2. Model Algorithm Development

The proposed parameterization will be developed using output of the coupled SAM-ASP model from a companion project. The System for Atmospheric Modeling (SAM; Khairoutdinov and Randall, 2003) is a large-eddy simulation/cloud-resolving model. In Sakamoto (2015), as will be done in this proposed work, SAM was configured as a moving Lagrangian wall oriented normal to the mean wind in the layer of smoke injection.

ASP has been extensively used to study the chemical and physical transformations of gases and aerosols within BB smoke plumes (e.g., Alvarado and Prinn, 2009; Alvarado et al., 2009; 2010). Recently Alvarado et al. (2015) evaluated ASP simulations for a fire in California (Williams fire, Akagi et al., 2012). This study showed that ASP could simulate most of the observations (e.g., OA, O_3, NO_x, OH) using appropriate assumptions about the chemistry of the unidentified organic compounds. The algorithms and equations of ASP v1.0 are fully documented in Alvarado (2008). Modifications to the current version of ASP v2.1 are documented in Alvarado et al. (2015). In general, improvements were made to the chemical mechanism and other input files used in ASP, rather than to the model equations and algorithms themselves.

In this project, we will develop a new sub-grid scale parameterization for biomass burning that links into the PiG module in CAMx. The algorithms and equations for this new capability will be generated using the statistical package, the Gaussian Emulator Machine (Lee et al., 2011), which fits the training data points using multidimensional Gaussian curves, to create a computationally efficient parameterization, to fit the results of a statistically appropriate number (~100) of SAM-ASP runs selected via quasi-random Latin hypercube (Lee et al., 2011). This parameterization will take into account the variation in plume chemistry with fire size, plume height, and dispersion rates. All new CAMx model routines, equations, and algorithms will be fully documented in the Technical Memo describing the model updates and in the project final report.

4.3. Required Data Sources

The required data sources for the model runs that will be performed in this project are primarily the input files needed for the CAMx and STILT-ASP models. The required input files for CAMx are supplied as part of the 2012 CAMx modeling episode from TCEQ[1].

5. Model Coding

This section only applies to the selection of the development of the sub-grid scale parameterization of biomass burning chemistry for the CAMx model (Task 1).

5.1. Requirements for Model Code Development

The SAM-ASP and CAMx model source code is in Fortran. All source code generated in this project will be well documented within the code itself and will follow best-practices for Fortran software development. Any additional CAMx source code developed in this project will be designed to be compatible with a number of Fortran compilers, including the GNU (gfortran), PGI (pgf90), and Intel (ifort) compilers.

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[1] https://www.tceq.texas.gov/airquality/airmod/data/tx2012

5.2. Computer Hardware and Software Requirements

We will design the sub-grid scale parameterization such that the computer hardware and software requirements of the updated CAMx model will not be appreciably different than the requirements for the current model. The tests of model timing and memory usage with and without the parameterization will be reported in the final report.

5.3. Requirements for Code Verification

A team member who did not write the code will review all source code generated or modified in this project in order to ensure that the code is written correctly. Tests will be performed to ensure the output of the sub-grid scale parameterization, as implemented in CAMx, is consistent with the output of the SAM-ASP model used for training. This consistency will be evaluated in terms of the mean bias (MB) and root-mean-square error (RMSE) in the predictions of O_3, $PM_{2.5}$, PAN, and other critical species between the parameterization and the SAM-ASP output. MB is defined as:

$$MB \equiv \frac{1}{n}\sum_{i=1}^{n} P_i - S_i$$

where P_i is the output for the parameterization for a given species under different times and conditions *i* and S_i is the original SAM-ASP output for the same species, time, and conditions. A small value of this metric ensures that, averaged over all times and conditions, the parameterization output is unbiased relative to the original SAM-ASP output. However, the MB can be low due to positive and negative errors cancelling each other out. Thus we will also examine the RMSE, defined as:

$$RMSE \equiv \sqrt{\frac{1}{n}\sum_{i=1}^{n}(P_i - S_i)^2}$$

where a low value of this metric implies both a small mean bias and a small variance in the errors.

In addition, during the CAMx code development, “benchmark” tests will be used to ensure that the model results for a fixed set of inputs and outputs do not change significantly during the model development. A set of timing and memory requirement tests will also be performed on the revised code. Version control (through Subversion) will be used to ensure any errors detected in these benchmark tests can be quickly identified and fixed.

6. Model Calibration

Model calibration is 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.”

For Task 1, uncertain parameters in the chemistry within the SAM-ASP model (e.g., the chemistry of S/IVOCs from fires) may be adjusted based on the outcome of the comparisons with data from the BBOP campaign as described in Section 8.1. In addition, an automatic "calibration" will be done as part of the Gaussian Emulator Machine fit to the SAM-ASP output to develop the parameterization. The degree of fit to the original SAM-ASP output will be assessed in terms of the bias and RMS errors of the parameterization relative to the SAM-ASP observations of O_3, $PM_{2.5}$, and other species. For both, the acceptance criteria will be that, in our expert judgment, the selected parameters minimize the mean bias and root-mean-square errors relative to the 2011 smoke events while remaining consistent with the scientific literature.

For Task 2, no changes to the default settings of the STILT-ASP model are planned in this project. However, we may adjust some parameters (e.g., number of particles simulated, height below which the particles deposit to the surface or pick up emissions) and assess the sensitivity of our conclusions to a range of physically defensible choices of these parameters. This will thus represent an estimate of the uncertainty of our results – thus there is no specific acceptance criteria needed.

7. Model Verification

Model verification is defined as "comparing the predictions of a calibrated model with data that were not used in the model development and calibration." For Task 1, the model verification of the SAM-ASP model with the BBOP data will be performed as discussed in Section 8.1. The uncertainty of the parameterizations predictions relative to the SAM-ASP simulations will be assessed as described in Section 6. We will then compare the results of the new treatment of BB plume chemistry in CAMx to the "traditional" approach of simply adding the fresh emissions directly to the model gridbox as well as the previous parameterization approach of McDonald-Buller et al. (2015). We will determine the change in the model simulations and evaluate these simulations versus observations from EPA (e.g., CASTNET for O_3, IMPROVE for OA) and TCEQ (e.g., monitor data on O_3, NO_x, and $PM_{2.5}$). The metrics used will be MB, RMSE, and the mean normalized bias (MNB). MNB is defined as

$$MNB \equiv \frac{1}{nm}\sum_{i=1}^{n}\sum_{j=1}^{m}\frac{PRED_{i,j} - OBS_{i,j}}{OBS_{i,j}}$$

where $PRED_i$ is the CAMx predictied concentration at location i and time interval j and $OBS_{i,j}$ is the observed (measured) value. MB and RMSE are defined as in Section 5, but with $PRED_{i,j}$ and $OBS_{i,j}$ replacing P_i and S_i, respectively. The model will be considered verified if the new parameterization reduces the absolute value of all three metrics relative to the current CAMx model predictions. This would indicate that the updated model does a better job of predicting the impact of fires on O_3 and $PM_{2.5}$.

The uncertainty in the STILT-ASP simulations for Task 2 will be assessed as described in Section 6. The performance relative to satellite observations, surface observations, and literature estimates of O_3 and $PM_{2.5}$ formation will be assessed as described in Section 8.1.

8. Model Evaluation

8.1. Model Assessment Process

AER shall determine what data sources would be most useful in evaluating the simulated impact of biomass burning on Texas air quality. At a minimum, this will include observations from EPA (e.g., CASTNET for O_3, IMPROVE for OA) and TCEQ (e.g., monitor data on O_3, NO_x, and $PM_{2.5}$), and may include other relevant data sources (e.g., NASA and NOAA satellite data). Details on all data used in the evaluation, including where the data were obtained, references for protocols for QA/QC, and validation by sources, will be included in the final report.

We will use data from the BBOP campaign (Kleinman and Sedlacek, 2015) to evaluate our SAM-ASP simulations by determining the bias and RMS errors relative to the BBOP observations of O3, PM2.5, and other species. BBOP used the DOE G-1 aircraft to perform quasi-Lagrangian sampling of BB plumes between ~0–5 hours downwind of the fire source with the goal of quantifying the downwind time evolution of smoke generated by BB. The G-1 BBOP payload included measurements of many reactive trace gases (including VOCs from PTR-MS, NO, NO_2, O_3, SO_2, and CO), as well as extensive measurements of the aerosol size distribution, composition, optical properties, and CCN activity. This large dataset will provide a strict test of the formation of O_3 and SOA within the SAM-ASP model, thus allowing us to improve our parameterization of the sub-grid scale chemistry of BB plumes for use in CAMx.

We will then compare the results of the new treatment of BB plume chemistry in CAMx to the "traditional" approach of simply adding the fresh emissions directly to the model gridbox as well as the previous parameterization approach of McDonald-Buller et al. (2015). We will determine the change in the model simulations and evaluate these simulations versus observations from EPA (e.g., CASTNET for O_3, IMPROVE for OA) and TCEQ (e.g., monitor data on O_3, NO_x, and $PM_{2.5}$) as described in Section 7. The above evaluations of the SAM-ASP model and the CAMx model will be performed for at least 10% of the days in the 2012 O_3 modeling episode, thus satisfying the requirement to audit at least 10% of the data produced in the project.

The STILT-ASP simulations used to quantify the impact of biomass burning on model boundary conditions, and thus Texas air quality, will be assessed in two phases. First, the calculated back-trajectories will be evaluated using satellite data and surface observations of biomass burning tracers such as CO, EC/BC, NO_y, and other species as available. This evaluation will include both a subjective evaluation (i.e., how well does the smoke transport predicted by the tool match the observed transport pattern from satellites) and an objective/quantitative evaluation (e.g., mean bias, root-mean-square error, and model-measurement regression slope). This evaluation of the STILT-ASP model will be performed for at least 10% of the days in 2012 O_3 modeling episode, thus satisfying the requirement to audit at least 10% of the data produced in the project.

Second, AER will evaluate the performance of STILT-ASP for O_3 and $PM_{2.5}$. This will include subjective and quantitative evaluations using surface and satellite O_3 and $PM_{2.5}$ data as described above. The model predictions of the additional O_3 and $PM_{2.5}$ generated by biomass burning will be compared with previous literature estimates for similar North American fires.

8.2. Peer Review and Reconciliation with User Requirements

The information collected from the exercises described in Section 8.1 will be used to make a final, overall assessment of the model and data usability that will be included in the final report. Project Manager Elena McDonald-Buller will also provide an independent review of the model output and evaluation results, and our results will be submitted to a peer-reviewed journal for further review.

For Task 1, the development of an improved sub-grid scale parameterization of biomass burning for CAMx, this assessment will address the following questions:

- What are the software and hardware requirements for the updated CAMx model using the new sub-grid scale parameterization? How long should a reference model run take?
- What is the magnitude of the change in the model simulations when the sub-grid scale parameterization is used? Do these changes improve the agreement of the simulations with observations from EPA (e.g., CASTNET for O_3, IMPROVE for OA) and TCEQ (e.g., monitor data on O_3, NO_x, and $PM_{2.5}$).
- Is the simulated chemical formation of O_3, $PM_{2.5}$, and other chemical species in the PiG module reasonable? Are these predictions consistent with the original SAM-ASP model? Are these predictions consistent with the scientific literature on the impacts of wildfires on O_3 and $PM_{2.5}$?
- Under what conditions is the updated model expected to be valid?

For Task 2, the analysis of the impact of BB plumes on the boundary conditions used for CAMx and the resulting impact on Texas air quality, this assessment will address the following questions:

- What is the impact on CAMx simulations of Texas and North American air quality of perturbing boundary concentrations impacted by BB by ~20%? Is this simulated impact consistent with the scientific literature?
- How does the “Lagrangian” estimate of the impact of fires on the boundary conditions for CO, O_3, NO_y species, OA, etc., from STILT-ASP differ from the “Eulerian” estimate from GEOS-Chem? Is this difference consistent with our

understanding of the impact of numerical diffusion on the transport of biomass burning plumes in Eulerian models?

- How consistent are the CAMx (Eulerian) and STILT-ASP (Lagrangian) estimated impacts of remote North American biomass burning on Texas air quality? Is this difference consistent with our understanding of the impact of numerical diffusion on the transport of biomass burning plumes in Eulerian models?

9. Model Documentation

In the Final Report AER will describe and document the sub-grid scale parameterization added to CAMx. The details on the STILT-ASP simulations for Task 2 will also be included in the Final Report. As described in the NRMRL QAPP Requirements this documentation will include:

- The final model description, final model specifications, 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 of the models
- 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
- Boundary conditions used in the model
- 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
- Output of model runs and interpretation
- User's guide (electronic or paper)
- Instructions for preparing data files
- Example problems complete with input and output
- Programmer’s instructions
- Computer operator’s instructions
- A report of the model calibration, validation, and evaluation

- Documentation of significant changes to the model
- Procedures for maintenance and user support, if applicable.

In addition, AER will produce a Final Report that includes thorough documentation of our findings and recommendations for future work (see Section 10). All scripts and methods used in the project will be documented in the Final Report.

10. Reporting

AQRP requires certain reports to be submitted on a timely basis and at regular intervals. A description of the specific reports to be submitted and their due dates are outlined below. One report per project will be submitted (collaborators will not submit separate reports), with the exception of the Financial Status Reports (FSRs). The lead PI will submit the reports, unless that responsibility is otherwise delegated with the approval of the Project Manager. All reports will be written in third person and will follow the State of Texas accessibility requirements as set forth by the Texas State Department of Information Resources. Report templates and accessibility guidelines found on the AQRP website at http://aqrp.ceer.utexas.edu/ will be followed.

Abstract: At the beginning of the project, an Abstract will be submitted to the Project Manager for use on the AQRP website. The Abstract will provide a brief description of the planned project activities, and will be written for a non-technical audience.

Abstract Due Date: Wednesday, August 31, 2016

Quarterly Reports: Each Quarterly Report will provide a summary of the project status for each reporting period. It will be submitted to the Project Manager as a Microsoft Word file. It will not exceed 2 pages and will be text only. No cover page is required. This document will be inserted into an AQRP compiled report to the TCEQ.

Quarterly Report Due Dates:

Report	**Period Covered**	**Due Date**
Aug2016 Quarterly Report	June, July, August 2016	Wednesday, August 31, 2016
Nov2016 Quarterly Report	September, October, November 2016	Wednesday, November 30, 2016
Feb2017 Quarterly Report	December 2016, January & February 2017	Tuesday, February 28, 2017
May2017 Quarterly Report	March, April, May 2017	Friday, May 31, 2017
Aug2017 Quarterly Report	June, July, August 2017	Thursday, August 31, 2017
Nov2017 Quarterly Report	September, October, November 2017	Thursday, November 30, 2017

Monthly Technical Reports (MTRs): Technical Reports will be submitted monthly to the Project Manager and TCEQ Liaison in Microsoft Word format using the AQRP FY16-17 MTR Template found on the AQRP website.

MTR Due Dates:

Report	**Period Covered**	**Due Date**
Aug2016 MTR	Project Start - August 31, 2016	Thursday, September 8, 2016
Sep2016 MTR	September 1 - 30, 2016	Monday, October 10, 2016
Oct2016 MTR	October 1 - 31, 2016	Tuesday, November 8, 2016
Nov2016 MTR	November 1 - 30 2016	Thursday, December 8, 2016
Dec2016 MTR	December 1 - 31, 2016	Monday, January 9, 2017
Jan2017 MTR	January 1 - 31, 2017	Wednesday, February 8, 2017
Feb2017 MTR	February 1 - 28, 2017	Wednesday, March 8, 2017
Mar2017 MTR	March 1 - 31, 2017	Monday, April 10, 2017
Apr2017 MTR	April 1 - 28, 2017	Monday, May 8, 2017
May2017 MTR	May 1 - 31, 2017	Thursday, June 8, 2017
Jun2017 MTR	June 1 - 30, 2017	Monday, July 10, 2017
Jul2017 MTR	July 1 - 31, 2017	Tuesday, August 8, 2017

Financial Status Reports (FSRs): Financial Status Reports will be submitted monthly to the AQRP Grant Manager (Maria Stanzione) by each institution on the project using the AQRP FY16-17 FSR Template found on the AQRP website.

FSR Due Dates:

Report	Period Covered	Due Date
Aug2016 FSR	Project Start - August 31	Thursday, September 15, 2016
Sep2016 FSR	September 1 - 30, 2016	Monday, October 17, 2016
Oct2016 FSR	October 1 - 31, 2016	Tuesday, November 15, 2016
Nov2016 FSR	November 1 - 30 2016	Thursday, December 15, 2016
Dec2016 FSR	December 1 - 31, 2016	Tuesday, January 17, 2017
Jan2017 FSR	January 1 - 31, 2017	Wednesday, February 15, 2017
Feb2017 FSR	February 1 - 28, 2017	Wednesday, March 15, 2017
Mar2017 FSR	March 1 - 31, 2017	Monday, April 17, 2017
Apr2017 FSR	April 1 - 28, 2017	Monday, May 15, 2017
May2017 FSR	May 1 - 31, 2017	Thursday, June 15, 2017
Jun2017 FSR	June 1 - 30, 2017	Monday, July 17, 2017
Jul2017 FSR	July 1 - 31, 2017	Tuesday, August 15, 2017
Aug2017 FSR	August 1 - 31, 2017	Friday, September 15, 2017
FINAL FSR	Final FSR	Monday, October 16, 2017

Draft Final Report: A Draft Final Report will be submitted to the Project Manager and the TCEQ Liaison. It will include an Executive Summary. It will be written in third person and will follow the State of Texas accessibility requirements as set forth by the Texas State Department of Information Resources. It will also include a report of the QA findings.

Draft Final Report Due Date: Tuesday, August 1, 2017

Final Report: A Final Report incorporating comments from the AQRP and TCEQ review of the Draft Final Report will be submitted to the Project Manager and the TCEQ Liaison. It will be written in third person and will follow the State of Texas accessibility requirements as set forth by the Texas State Department of Information Resources.

Final Report Due Date: Thursday, August 31, 2017

Project Data: All project data including but not limited to QA/QC measurement data, metadata, databases, modeling inputs and outputs, etc., will be submitted to the AQRP Project Manager within 30 days of project completion (September 29, 2017). The data will be submitted in a format that will allow AQRP or TCEQ or other outside parties to utilize the information. It will also include a report of the QA findings. AER will retain all project data for a minimum of five years.

AQRP Workshop: A representative from the project will present at the AQRP Workshop in the first half of August 2017.

Presentations and Publications/Posters: All data and other information developed under this project which is included in **published papers, symposia, presentations, press releases, websites and/or other publications** shall be submitted to the AQRP Project Manager and the TCEQ Liaison per the Publication/Publicity Guidelines included in Attachment G of the Subaward.

11. References

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