Scope of Work For

AQRP 17-024

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

Prepared for

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

By

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QA Requirements: Audits of Data Quality: 10% Required
Report of QA Findings: Required in Final Report

Approvals

This Scope of Work was approved electronically on September 15, 2016 by Elena McDonald-Buller, The University of Texas at Austin

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

This Scope of Work was recommended electronically on October 12, 2016 by Erik Gribbin, Texas Commission on Environmental Quality

Erik Gribbin
Project Liaison, Texas Commission on Environmental Quality

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1.0 Abstract

Fires can have a large impact on ozone and particulate matter concentrations, and thus air quality, in Texas. Three-dimensional Eulerian models like CAMx take estimates of the primary emissions from biomass burning and unphysically "mix" them across large-scale grid boxes, leading to inaccurate chemical modeling and incorrect estimates of the impact of biomass burning on air quality. Plume-scale process models like AER's Aerosol Simulation Program allow us to examine the chemical and physical transformations of trace gases and aerosols within biomass burning plumes and to develop parameterizations for this aging process in coarser grid-scale models. In this project, we will improve our understanding of the impacts of local and out-of-state fires on air quality in Texas by implementing an improved ASP-based sub-grid scale parameterization of the formation of ozone and secondary organic aerosols in biomass burning plumes into CAMx via the plume-in-grid (PiG) module. We will also investigate the impact that long-range transport of wildfire smoke has on air quality in Texas. This project thus addresses two strategic topics of the AQRP program: "Improving the understanding of ozone and particulate matter (PM) formation [and] the interactions of ozone and PM precursors" and "Investigating global, international, and regional transport of pollutants using data and modeling analyses."

2.0 Background

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 O_3 and $PM_{2.5}$ 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 4.1); 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 4.1, 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.

3.0 Objectives

The objectives of this project are thus to:

- **Develop and evaluate an improved sub-grid scale parameterization of biomass burning for CAMx based on SAM-ASP and an analysis of O_3 and SOA production in fire plumes observed during BBOP.**
- **Explore the impact of BB plumes on the boundary conditions used for CAMx and the resulting impact on Texas air quality with STILT-ASP.**

4.0 Task Descriptions

Task 4.1: Develop improved parameterization and assess the impact on Texas air quality

The Lonsdale et al. (2015) parameterization was originally designed for global CTMs like GEOS-Chem, and thus does not take full advantage of the information on plume concentrations and dispersion that are available from the PiG module within CAMx. In addition, there have been several recent field studies of biomass-burning plume chemistry, like BBOP, that can be used to refine the chemistry within ASP, which will lead to an improved parameterization.

In this task, we will refine the chemistry in ASP and improve our sub-grid scale parameterization using the output of the SAM-ASP model runs of the wildfire and agricultural fires measured during the BBOP campaign that will be performed in our companion NSF project. We expect this output to be available at the beginning of 2017; if it is not, we can proceed with the parameterization development by using ASP within a single Lagrangian parcel model as in Alvarado et al. (2015a). We will then perform a set of SAM-ASP runs to expand our parameterization to account for the variation in plume chemistry with fire size, plume height, and dispersion rates. We will use a quasi-random Latin hypercube (Lee et al., 2011) to choose the input parameters for a statistically appropriate number (~100) of plume-model simulations.

We will then use 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. Note that by sampling in a Latin hypercube and fitting using GEM, we will require far fewer simulations for fitting than sampling at evenly spaced increments in all dimensions.

We will then implement this improved parameterization into CAMx and determine how the parameterization alters estimates of the impacts of BB on Texas air quality. Our evaluation will focus on the 2012 CAMx modeling episode from TCEQ (May 16 – June 30, 2012), as this episode was used in the previous study of McDonald-Buller et al. (2015) and thus has the most up-to-date FINN fire emissions. Other model input files for this episode are publically available at https://www.tceq.texas.gov/airquality/airmod/data/tx2012. This work will be a significant advance on the previous study of McDonald-Buller et al. (2015) in that our study will: (a) use the updated version of the parameterization developed above; (b) account for the full set of variables from the parameterization that can affect the O_3 and SOA formation in plumes (e.g. fire size, dispersion rates, temperature, overhead ozone column, starting and ending SZA) rather than just fuel type; and (c) will incorporate the parameterization into the CAMx model via the PiG module, rather than assuming direct emission of the 1-hour aged smoke to the model grid.

We will first adjust the PiG module within CAMx to simulate only the dispersion of the CO_2 and CO emissions from fires, as this will minimize the computational expense of simulating the fire plumes. The PiG module will store the mixing time scale of the plume and other environmental and fire parameters needed by the sub-grid scale parameterization. When mass is transferred from the plume to the grid (either through slow “leaking” of the plume pollutants to the grid while the plume is still sub-grid scale or through sudden “dumping” when the puff horizontal size is greater than the grid cell area, see Emery et al., 2013), the parameterization function will calculate the correct ratio of plume O_3, NO_y species, and OA to the total carbon emissions (estimated as the sum of CO and CO_2) for the plume age and conditions, and these ratios will be used to determine the correct amount of these species to add to the grid.

We will then compare the results of this 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 $PM_{2.5}$).

Deliverable 1: Modified CAMx code that includes the improved ASP-based parameterization for BB chemistry.

Schedule: Due August 31, 2017 (with Final Report)

Task 4.2: Investigate the impact of long-range transport of BB pollution on Texas air quality

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, 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 and aerosols 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. 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 the STILT-ASP 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. The results of these STILT-ASP runs will be used to scale the concentrations at these "boundary" receptors, and 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 STILT-ASP, thus quantifying potential errors in the modeling impact of BB emission in CAMx due to numerical diffusion in the coarser grids.

Deliverable 2: Draft journal article summarizing result of Tasks 1 and 2.

Schedule: Due August 31, 2017 (with Final Report)

Task 4.3 Project Reporting and Presentation

As specified in Section 7.0 "Deliverables" of this Scope of Work, AQRP requires the regular and timely submission of monthly technical, monthly financial status and quarterly reports as well as an abstract at project initiation and, near the end of the project, submission of the draft final and final reports. Additionally, at least one member of the project team will attend and present at the AQRP data workshop. For each reporting deliverable, 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 (or their designee) will electronically submit each report to both the AQRP and TCEQ liaisons and will follow the State of Texas accessibility requirements as set forth by the Texas State Department of Information Resources. The report templates and accessibility guidelines found on the AQRP website at http://aqrp.ceer.utexas.edu/ will be followed. ****Draft copies of any planned presentations (such as at technical conferences) or manuscripts to be submitted for publication resulting from this project will be provided to both the AQRP and TCEQ liaisons per the Publication/Publicity Guidelines included in Attachment G of the subaward.**** Finally, our team will prepare and submit our final project data and associated metadata to the AQRP archive.

Deliverables: Abstract, monthly technical reports, monthly financial status reports, quarterly reports, draft final report, final report, attendance and presentation at AQRP data workshop, submissions of presentations and manuscripts, project data and associated metadata

Schedule: The schedule for Task 4.3 Deliverables is shown in Section 7.

5.0 Project Participants and Responsibilities

- Dr. Matthew Alvarado of AER will be the Principal Investigator and will lead all of the studies of the chemistry and impacts of BB to be carried out in this project. Dr. Alvarado is the lead developer of ASP and has extensive experience in the modeling of the chemistry of BB smoke plumes.
- Ms. Chantelle Lonsdale of AER 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).
- Mr. Christopher Brodowski of AER 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).

6.0 Timeline

The proposed work schedule and deliverables for this project are summarized in Table 1 below. The required monthly and quarterly progress reports are listed in Section 7.

Table 1. 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 Final Report)

7.0 Deliverables

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.

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.

8.0 References

Alvarado, M. J., J. A. Logan, J. Mao, *et al.* (2010), Nitrogen oxides and PAN in plumes from boreal fires during ARCTAS-B and their impact on ozone: an integrated analysis of aircraft and satellite observations, *Atmos. Chem. Phys.,* 10*,* 9739-9760, doi:10.5194/acp-10-9739-2010.

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Lonsdale, C. R., M. J. Alvarado, R. J. Yokelson, S. K. Akagi, E. Fischer, K. Travis, T. Soni, J. S. Craven. J. W. Taylor, G. R. McMeeking, I. R. Burling, S. P. Urbanski, C. E. Wold, J. H. Seinfeld, H. Coe, and D. R. Weise (2015), Using the Aerosol Simulation Program to parameterize biomass-burning plumes for global air quality models, American Association for Aerosol Research, Minneapolis, MN, October 12-16.

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Rastigejev, Y., R. Park, M. P. Brenner, and D. J. Jacob (2010), Resolving intercontinental pollution plumes in global models of atmospheric transport, *J. Geophys. Res., 115*, D02302, doi:10.1029/2009JD012568.