AQRP Monthly Technical Report

PROJECT TITLE	**Improving the Modeling of Wildfire Impacts on Ozone and Particulate Matter for Texas Air Quality Planning**	**PROJECT #**	AQRP 16-024
PROJECT PARTICIPANTS	Matthew Alvarado (AER) Chantelle Lonsdale (AER) Christopher Brodowski (AER)	**DATE SUBMITTED**	08/08/2017
REPORTING PERIOD	**From:** 07/01/2017 **To:** 07/31/2017	**REPORT #**	10

A Financial Status Report (FSR) and Invoice will be submitted separately from each of the Project Participants reflecting charges for this Reporting Period. I understand that the FSR and Invoice are due to the AQRP by the 15th of the month following the reporting period shown above.

Detailed Accomplishments by Task

Task 1: Develop improved parameterization and assess the impact on Texas air quality

In this reporting period we performed QA/QC of the GEM parameterization we have developed. However, our evaluation of the GEM parameterization showed that our current GEM training approach does not result in a parameterization of sufficient quality for use in regional air quality modeling. The GEM parameterization is able to represent the dependence of O_3 formation in the plume on fuel type, temperature, day of year, and latitude reasonably well, but the dependence on time of day is unrealistic, as the GEM prediction for the O_3 enhancement ratio ($\Delta O_3/\Delta CO$) is negative for plumes emitted at 14:00 local time in the summer, when these plumes should still be forming O_3 at the end of the simulation at 17:00 (5 PM) local time in the summer. Comparisons of the parameterization to the observations from the Williams Fire show that the GEM parameterization underestimates the measured $\Delta O_3/\Delta CO$ for these conditions (GEM value of 0.04 mol/mol, as opposed to measurements of 0.10 mol/mol), and underestimated the results of a custom SAM-ASP simulation for these conditions (0.07 mol/mol). The GEM predictions for NO_x and other NO_y species have more serious deficiencies, with the GEM parameterization overestimating the NO_x downwind in the Williams Fire relative to both observations and SAM-ASP simulations, and GEM predictions of the formation of PAN and HNO_3 being inconsistent with the GEM predictions of the loss rate of NO_x. Further work on the GEM parameterization training would be needed to identify the source of these errors and correct them.

Thus, rather than implement the GEM parameterization into CAMx, we instead implemented the parameterization of Lonsdale et al. (2015) into CAMx. This parameterization modifies the emissions of O_3, NO_y species, and OA from fires based on a look-up-table (LUT) that is built from many runs of the ASP model within a simple Lagrangian parcel dispersion model. We continued debugging the CAMx code changes to incorporate the Lonsdale et al. (2015) parameterization results into the CAMx plume-in-grid (PiG) module, as described in our last monthly report.

We also summarized our evaluation of the SAM-ASP model and the GEM parameterization in the Draft Final Report, along with a description of our plans for the CAMx model evaluation.

Task 2: Investigate the impact of long-range transport of BB pollution on Texas air quality

We examined the 36-km CAMx boundary condition files (derived from the GEOS-Chem model) of the 2012 base case TCEQ modeling episode for potential episodes of biomass burning influence. Regions with CO concentration ≥ 120 ppbv along the southern boundary in May and June, which are sensitive to fires in Mexico and Central America, were simulated with STILT-ASP v2.0. The STILT-ASP v2.0 simulations show a lot of fine structure in the impacts of fires on CO along the boundaries that is not captured by the low-resolution boundary conditions from GEOS-Chem. In addition, the STILT-ASP v2.0 estimate of the $\Delta O_3/\Delta CO$ ratio during these events (mean of 0.15 mol/mol) is consistent with the review of Jaffe and Wigder (2012), which found that the average $\Delta O_3/\Delta CO$ for smoke aged about 1-2 days was 0.2 ± 0.1 mol/mol. However, the STILT-ASP v2.0 prediction of O_3 was high relative to GEOS-Chem (Figure 1), which appears to be due to an error in the simulation of the diurnal cycle of O_3, especially at night. Predictions of NO_x and PAN were both much lower than the GEOS-Chem values, and this appears to be due to the chemistry of SVOCs used in ASP v2.1, which were derived from measurements of a biomass burning plume for the first 0-5 hours of aging. Thus the SVOC chemical mechanism of ASP v2.1 may need to be re-examined for the longer one to seven day runs of STILT-ASP v2.0.

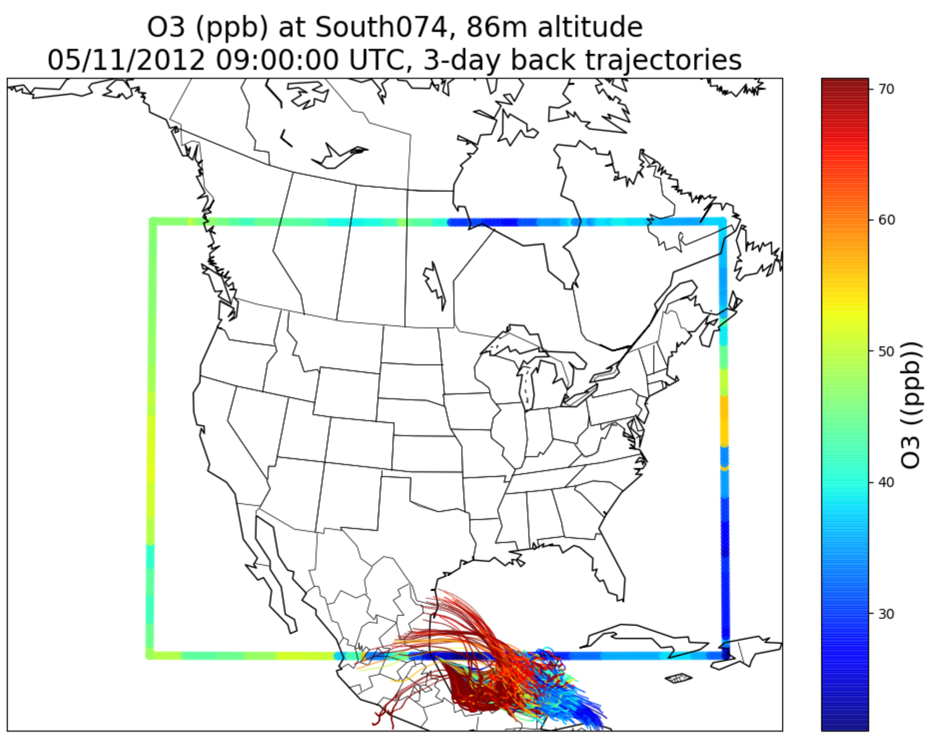

Figure 1. O_3 (ppbv) from a 3-day back trajectory run of STILT-ASP v2.0 for May 11th, 2012 at 09:00 UTC (03:00 CST) fire-influenced box of the southern boundary of the CAMx modeling domain. The GEOS-Chem boundary conditions are also shown.

We also used STILT-ASP v2.0 to examine the impact of fires on CO, O_3, NO_x, and $PM_{2.5}$ during a small fire event in the Austin/Round Rock urban area. The model predictions of O_3, CO, and NO_x were all consistent with the observations, with O_3 overestimated (MB of 7.3 ppbv, RMSE of 7.7 ppbv) and NO_x generally underestimated (MB of -0.5 ppbv, RMSE of 1.0 ppbv). However, $PM_{2.5}$ was substantially overestimated, likely due to the assumption in STILT-ASP v2.0 that all aerosol are emitted with a monodisperse size distribution diameter of 0.1 μm, which is reasonable for biomass burning aerosols but is not when applied to anthropogenic aerosols. Thus deposition of $PM_{2.5}$ to the surface is underestimated. However, as deposition should affect all aerosol sources relatively evenly, and for these cases the fire contributions are further upwind than the local anthropogenic emissions, the STILT-ASP v2.0 results can be used to estimate the relative fraction of $PM_{2.5}$ at the receptor that is due to fires, which for these cases was 12-14%.

Preliminary Analysis See the accomplishments described above.

Data Collected None.

Identify Problems or Issues Encountered and Proposed Solutions or Adjustments

Nothing to report

Goals and Anticipated Issues for the Succeeding Reporting Period

Task 1:

- Complete work to add the Lonsdale et al. (2015) parameterization as a subroutine within CAMx and analyze results.
- Complete Final Report.

Task 2:

- Run full chemistry STILT-ASP runs for June episodes when in domain fires impacted El Paso, TX.
- Complete Final Report.

Detailed Analysis of the Progress of the Task Order to Date

As of the end of this reporting period, the following milestones have been completed for each task:

Task 1:

- Coupling of SAM-ASP completed.
- Preliminary runs and evaluation against Alvarado et al. (2015) completed, with dilution error identified and fixed.
- Verified that our CAMx simulation can reproduce the 2012 TCEQ modeling episode.
- Wrote code for CAMx to read FINN fire emission files directly.
- Built a Gaussian Emulator Machine (GEM) based on the original biomass-burning parameterization of Lonsdale et al. (2014) as a test case for the updated parameterization to be developed in this project.
- Ran SAM-ASP simulations for the new parameterization and chose input variables.
- Developed first GEM based on the SAM-ASP runs and investigated results.

- Revised GEM parameterization based on above analysis.
- Designed the file structure of parameterization that is to be read into CAMx
- Fixed SZA and wind speed/direction bugs and reran parameterization runs for all fuel types.
- Analyzed GEM parameterization, found it wasn't of sufficient quality, switched to Lonsdale et al. (2015) parameterization for CAMx.
- Identified method for incorporating Lonsdale et al. (2015) parameterization into CAMx.
- Ran CAMx for May 16-June 30 for no fire emissions.

Task 2:

- Examined of boundary condition files for potential episodes of biomass burning influence.
- Performed STILT-ASP simulations along TCEQ grid boundary and compared predicted CO levels to GEOS-Chem values.
- Expanded number of receptors for no-chemistry STILT-ASP runs along boundaries, focusing on CO plumes.
- Ran full chemistry runs of STILT-ASP for selected boundary receptors and compared results with GEOS-Chem.
- Ran full chemistry STILT-ASP run for episodes when out of domain fires impacted Austin, TX.

Do you have any publications related to this project currently under development? If so, please provide a working title, and the journals you plan to submit to.

___Yes __X_No

Do you have any publications related to this project currently under review by a journal? If so, what is the working title and the journal name? Have you sent a copy of the article to your AQRP Project Manager and your TCEQ Liaison?

___Yes __X_No

Do you have any bibliographic publications related to this project that have been published? If so, please list the reference information. List all items for the lifetime of the project.

___Yes __X_No

Do you have any presentations related to this project currently under development? If so, please provide working title, and the conference you plan to present it (this does not include presentations for the AQRP Workshop).

__X_Yes ___No

M. Alvarado, C. Lonsdale, and C. Brodowski (2017), Using Lagrangian Chemical Transport Modeling to Assess the Impact of Biomass Burning on Ozone and $PM_{2.5}$, to be presented at the AGU Fall Meeting, New Orleans, LA, Dec. 11-15.

C. Lonsdale, C. Brodowski, M. Alvarado, J. Henderson, J. Pierce, E. Ramnarine, J. Lin, and A. Kochanski (2017), New Developments in the Eulerian and Lagrangian Modeling of the Chemistry of Biomass-Burning Plumes, to be presented at the 15^{th} CMAS Conference, Chapel Hill, NC, 24-26 Oct.

Do you have any presentations related to this project that have been published? If so, please list reference information. List all items for the lifetime of the project.

__X_Yes ___No

C.M. Brodowski, M.J. Alvarado, C.R. Lonsdale, J.C. Lin, A.K. Kochanski (2017), An Eulerian vs. Lagrangian Comparison of Modeled Carbon Monoxide in Texas during Biomass Burning Events, presented at the 8^{th} International GEOS-Chem Meeting, Cambridge, MA, May 1-4.

Lonsdale, C. R., C. Brodowski, M. Alvarado, J. Henderson, J. R. Pierce, and J. Lin (2016), Regional Modeling of Biomass-Burning Aerosol Impacts, Abstract GC51E-1225, presented at the 2016 AGU Fall Meeting, San Francisco, CA, Dec. 12-16.

C. Lonsdale, C. Brodowski, M. Alvarado, J. Henderson, J. Pierce, E. Ramnarine, J. Lin, and A. Kochanski (2017), Recent Advances in Modeling the Near-Source Chemistry of Biomass-Burning Plumes in Photochemical Transport Models, presented at the EGU General Assembly 2017, Vienna, Austria, 23-28 April.

Submitted to AQRP by Matthew J. Alvarado (AER)

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