AQRP Monthly Technical Report

PROJECT TITLE	Analysis of Ozone Production Data from the San Antonio Field Study	**PROJECT #**	19-040
PROJECT PARTICIPANTS	Ezra Wood, Shannon Capps, Daniel Anderson	**DATE SUBMITTED**	4/8/2019
REPORTING PERIOD	**From:** 3/1/2019 **To:** 3/31/2019	**REPORT #**	6

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

The goal of Task #1 is to quantify the dependence of the ozone production rate on the concentrations of NOx, VOCs, and other measurements at the three SAFS sites where peroxy radical concentrations were measured. Most of this work has been collected into a paper which was submitted to the journal *Atmospheric Chemistry and Physics* in October of 2018. The final revised paper has been accepted and published and can be accessed at https://www.atmos-chem-phys-discuss.net/acp-2018-1083/. Remaining parts of Task #1 are to investigate the influence of biomass burning on ozone formation in the San Antonio area and to investigate to what extent the time averaging of the NO and peroxy radical measurements affects the calculated ozone production rates. We have not worked on these remaining aspects of Task #1 during the March period.

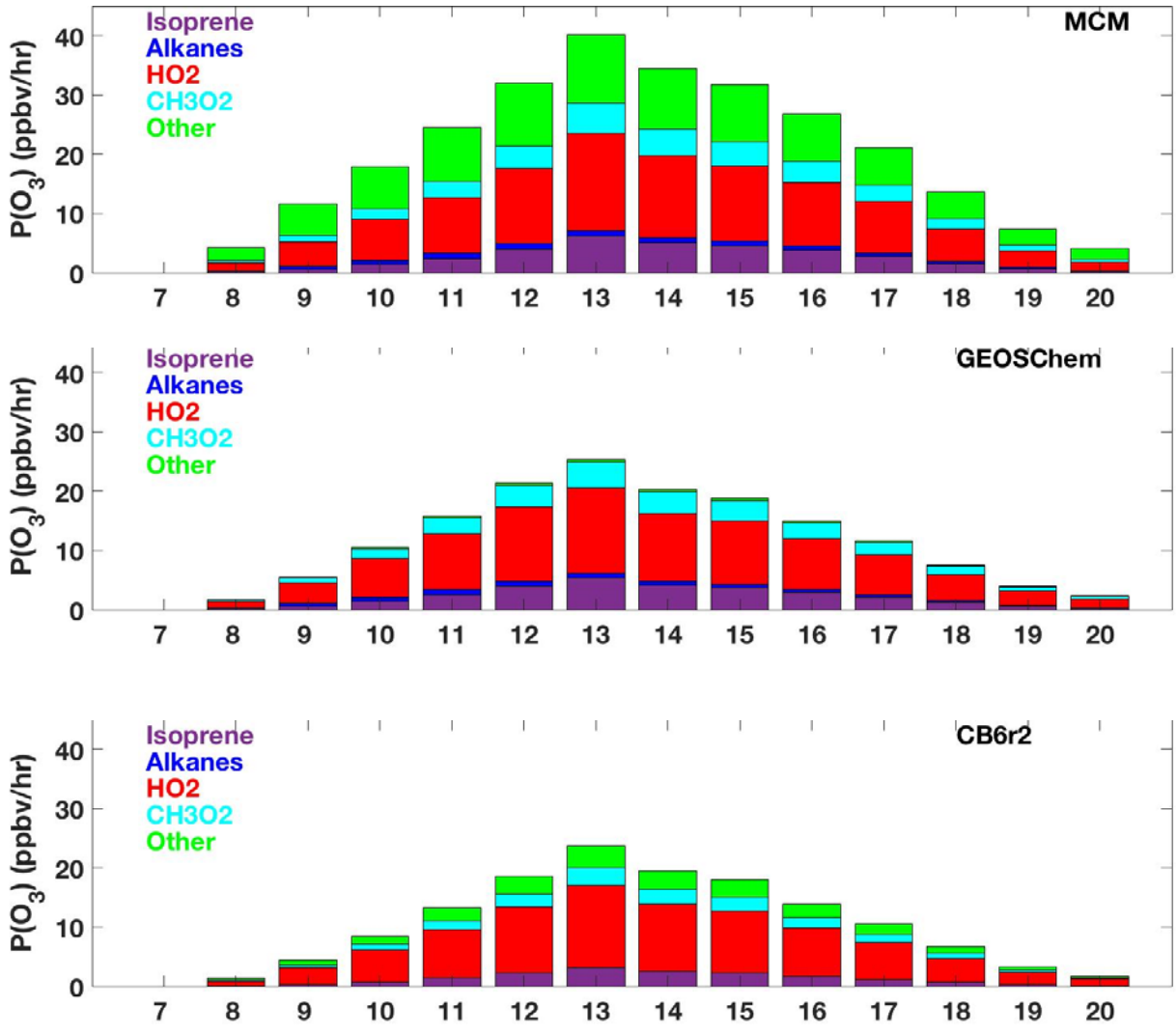
Task #2 consists of conducting 0-D photochemical modeling constrained by the Aerodyne/Drexel and Rice/Baylor/U. Houston measurements with several model chemical mechanisms for four SAFS measurement sites, spanning a large range of NOx values. Further details are described in the "preliminary analysis" section. Most interestingly, the different chemical mechanisms give different results for $P(O_3)$ at the Traveler's World site. The Master Chemical Mechanism (MCM) gave high $P(O_3)$ values, which happened to be very similar to the modeled values produced by the NASA LaRC model as conducted by the Rice/U.Houston/Baylor team. Work will continue on this during the next several months.

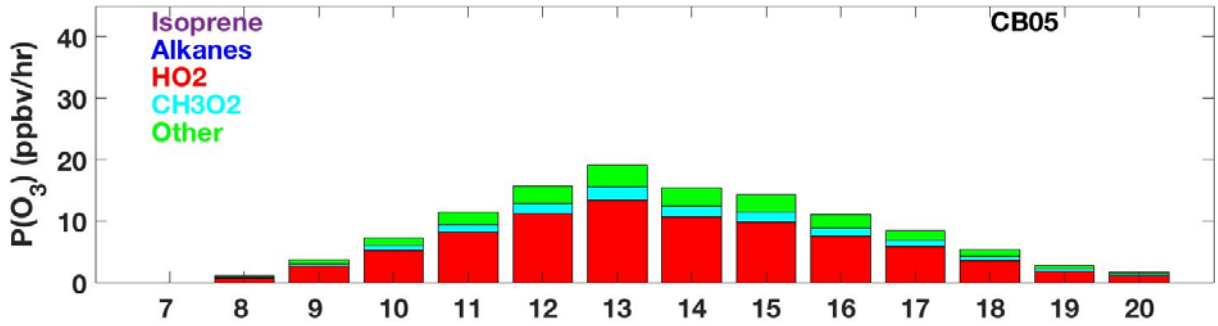
The goal of Task #3 is to apportion ozone concentrations to location-specific emission sources using 3-D air quality modeling with the instrumented Community Multiscale Air Quality model (CMAQ). We have begun spinning up a 2017 modeling platform provided by EPA OAQPS at Drexel. CMAQ v5.2.1 is running with the CB6r3 chemical mechanism and the aero6 treatment of aerosol with nonvolatile primary organic aerosol. The modeling episode will begin on March 28, 2017, to provide sufficient time for the influence of initial conditions to be reduced. In addition to area sources, emissions include point sources for commercial marine vehicles

(Category 3), wildfire, agricultural fires, electricity generating units, point sources not included in the Integrated Planning Model, and oil and gas point sources. BEIS3 was used for biogenic emissions.

Preliminary Analysis

We have used the F0AM 0-D photochemical model to investigate the contributions of different peroxy radical types to modeled ozone formation at the Traveler's World site. These results are summarized in the figure below for four different chemical mechanisms: MCM (Master Chemical Mechanism), GEOSChem, CB6r2 (Carbon bond v. 6r2) and CB05 (Carbon bond v 05). The MCM is a near-explicit model, whereas the other three include some amount of "lumping" of similar compounds.





As described in the prior monthly report, the MCM values were significantly (60+%) higher than the observation-based $P(O_3)$ at UTSA, which is surprising.

Data Collected

No additional data have been collected.

Identify Problems or Issues Encountered and Proposed Solutions or Adjustments

The federal government shutdown delayed our work on task 3 as described in an earlier report. We are slightly behind schedule on Task 3 but anticipate that we will be able to catch up given the progress on Tasks 1 and 2.

Goals and Anticipated Issues for the Succeeding Reporting Period

We will refine the 0-D modeling and begin first tests of CMAQ using the recently acquired 2017 emissions data.

Detailed Analysis of the Progress of the Task Order to Date

Task 1 is near-complete. Tasks 2 is making good progress and 3 has started.

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?

__X_Yes __ _No

The title is "Characterization of Ozone Production in San Antonio, Texas Using Observations of Total Peroxy Radicals", submitted and accepted to *Atmospheric Chemistry and Physics*, accessible at https://www.atmos-chem-phys-discuss.net/acp-2018-1083/. This manuscript was sent to Gary McGaughey (Project Manager for project 17-032, during which most of the analysis was conducted) and Mark Estes (TCEQ) prior to submission.

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).
___Yes __X_No

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.

___Yes _X__No

Submitted to AQRP by

Ezra Wood,
Principal Investigator