

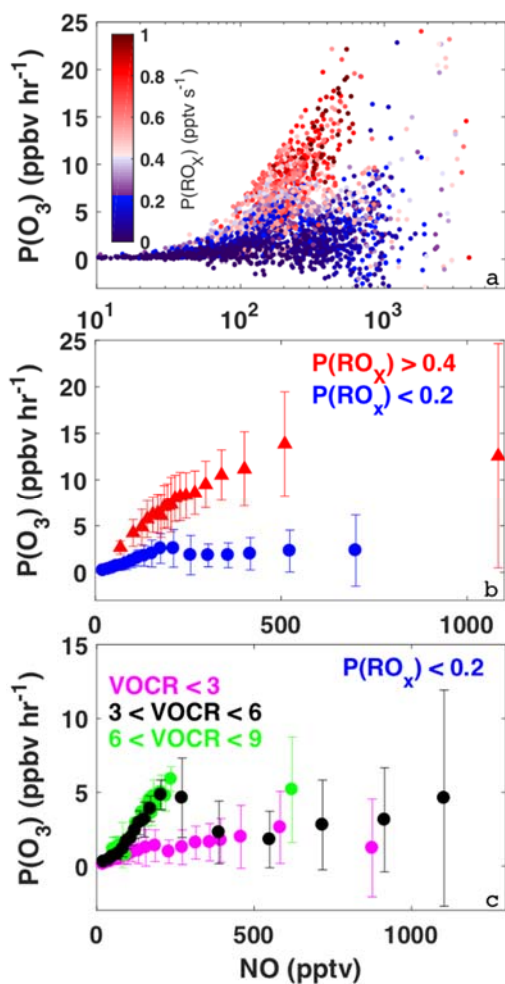
AQRP Monthly Technical Report

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	2/8/2019
REPORTING PERIOD	From: 1/1/2019 To: 1/31/2019	REPORT #	4

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 NO_x, VOCs, and other measurements at the three SAFS sites where peroxy radical concentrations were measured. Some of the preliminary aspects of this work have been collected into a paper which was submitted to the journal *Atmospheric Chemistry and Physics* in October of 2018. The paper and open review process can be accessed at <https://www.atmos-chem-phys-discuss.net/acp-2018-1083/>. We have completed the revision for the paper currently in ACPD based on reviewer comments. The revision mainly consisted of clarifying various aspects of the VOC measurements and other minor items. In the revision we also updated Figure 6 which shows the relationship between the ozone production rate P(O₃) and NO concentrations (next page). Panel c of the new version of the figures divides the P(O₃) data under low P(RO_x) conditions into three different classes of VOC reactivity, defined as $\Sigma_{\text{KOH}+\text{VOC}}[\text{VOC}]$ for all VOCs measured. This clarifies the point made in the paper that ozone formation at the SAFS measurement sites (UTSA, Floresville, and Lake Corpus Christi) was usually NO_x-limited, and only possibly VOC-limited under low P(RO_x) conditions (days that were not sunny), evident by the apparent “turnover” in the black and green points in panel c. The figure also helps to demonstrate that even when VOC-limited, P(O₃) values were relatively low – always less than 6 ppb/hr.



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 NO_x values. In this last month we have acquired the final proton transfer reaction – mass spectrometer (PTR-MS) dataset from Baylor University. A key issue is the formaldehyde data, which is a crucial HO_x precursor. The Baylor team measured formaldehyde using a relatively new method with the PTR-MS in which the sampled air is dried prior to sampling. The Baylor team scaled the raw formaldehyde measurements based on a comparison to the Aerodyne infrared absorption measurement when both instruments were co-located at UTSA. Comparisons of other measurements during the co-located sampling period showed acceptable agreement (e.g., NO_x, ethane, O₃). We have conducted 0-D modeling with the FOAM model and the GEOS-CHEM chemical mechanism with formaldehyde unconstrained in order to compare to the measured formaldehyde at UTSA. For the modeling of the Traveler’s World data, we will conduct the modeling both with the scaled, PTR-MS based formaldehyde data and with formaldehyde data unconstrained.

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). Prior to this reporting period, CMAQ version 5.2.1 was installed on the Drexel high performance computing cluster and Daniel Anderson was trained in its use by Shannon Capps, and a benchmark run was performed and compared to model output provided by EPA. We have

finally received the 2017 emissions data from our contact at the EPA (this was delayed due to the government shut-down). We have started to upload the data into the computing cluster.

Preliminary Analysis

No preliminary analysis has been conducted beyond that summarized in the paper submitted to the journal *Atmospheric Chemistry and Physics* and described above.

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 above. Now that we have the 2017 emissions data we do not anticipate that a possible second shutdown will adversely affect our progress.

Goals and Anticipated Issues for the Succeeding Reporting Period

Daniel Anderson (postdoc), with guidance from Dr. Wood and Dr. Capps, will fully run the F0AM 0-D photochemical model for all four measurement locations as described above. Furthermore, we will 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 and 3 have 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 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 No

The title is “Characterization of Ozone Production in San Antonio, Texas Using Observations of Total Peroxy Radicals”, submitted 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 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 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 No

Submitted to AQRP by

Ezra Wood,
Principal Investigator