

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	5/8/2019
REPORTING PERIOD	From: 4/1/2019 To: 4/30/2019	REPORT #	7

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

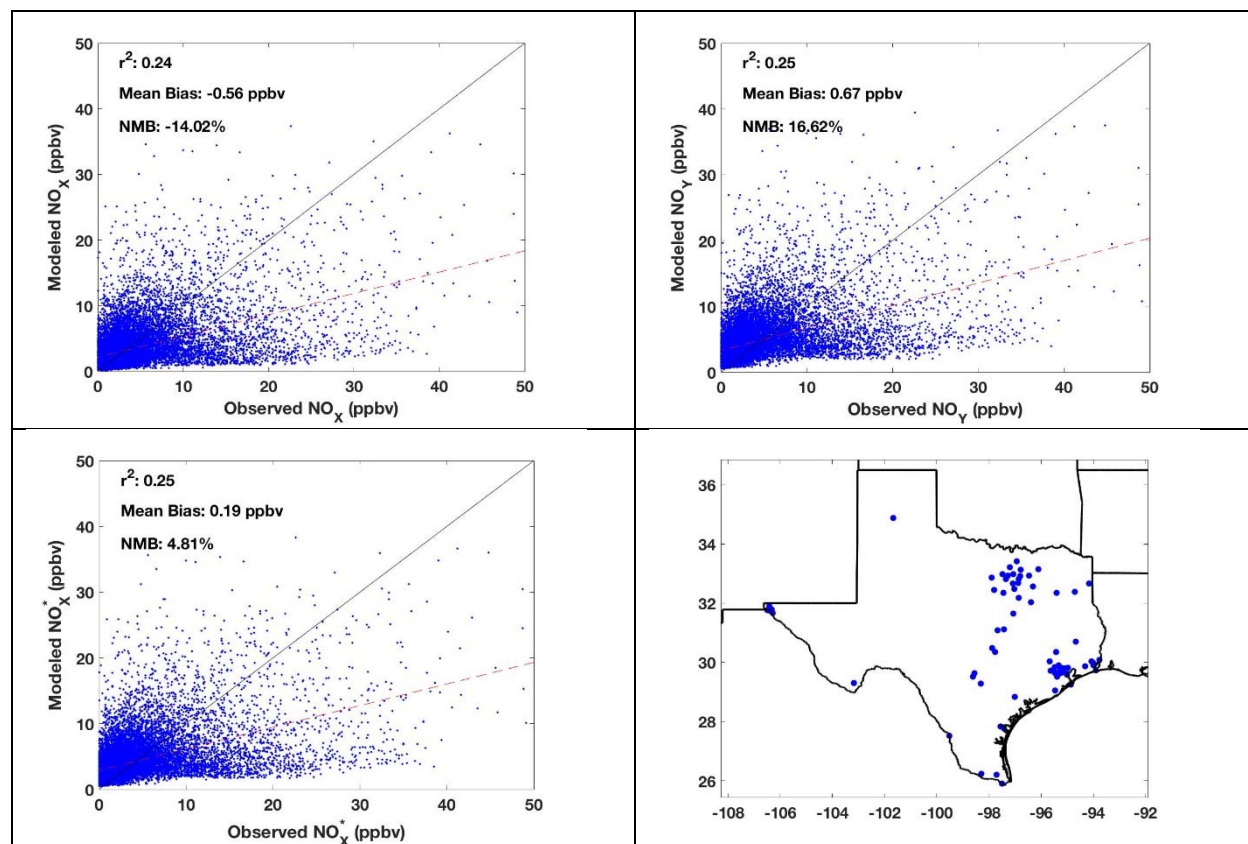
The goal of Task #1 is to quantify the dependence of the ozone production rate on the concentrations of NO_x, VOCs, and other measurements at the three SAFS sites where peroxy radical concentrations were measured. Most of this work has been collected into a paper which was submitted to the journal *Atmospheric 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 April 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 NO_x values. We have continued the modeling at the centrally-located Traveler's World site (more results are below). As described last time, the different chemical mechanisms give a range of modeled P(O₃) values, with the Master Chemical Mechanism (MCM) giving the high P(O₃) values.

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 spun up a 2017 modeling platform provided by EPA OAQPS at Drexel and have initial (preliminary) results from CMAQ v5.2.1 as described below in the "preliminary analysis" section.

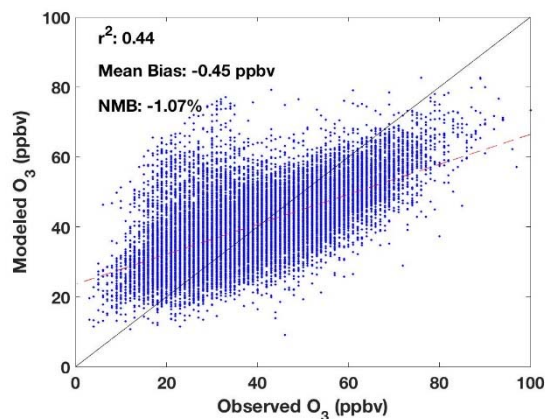
Preliminary Analysis

Preliminary first outputs from the 3-dimensional photochemical model CMAQ are shown below.

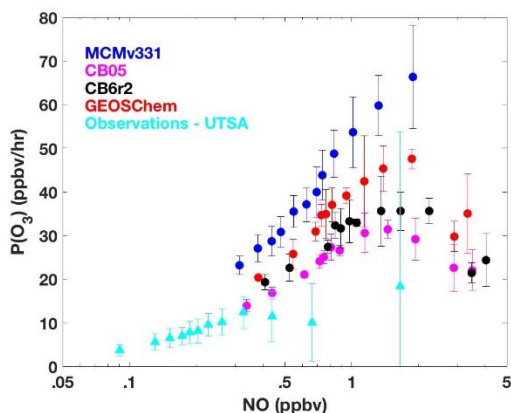


The three graphs above compare nitrogen oxide measurements to modeled (CMAQ) nitrogen oxides at all TCEQ monitoring sites (in the entire state). Most monitoring sites' measurements of NO₂ are subject to photochemical interferences (because of the non-selective method of converting NO₂ into NO using a hot molybdenum catalyst), and so we are unable to conduct a direct comparison of modeled NO_x to measured NO_x. The "Observed" quantity on the x-axis is the same quantity for each graph (though labeled differently) – the chemiluminescence-based measurements of NO_x. We compare those measurements to model outputs for NO_y (= sum of NO, NO₂, and oxidation products, including HNO₃ and organic nitrates), "NO_x*" which is the sum of NO, NO₂ and organic nitrates but excluding HNO₃, HONO, HO₂NO₂, NO₃, and N₂O₅, and NO_x*. Regardless of the quantity used, the correlation coefficients are low (R^2 values of 0.25), but the mean bias values are under 1 ppb. "NBM" values are the normalized mean bias values, which vary from -14% to +17%.

The figure below shows the comparison of modeled to measured O₃ values:



A summary of P(O₃) values from the 0-D models is shown below using the Traveler's World data. The observation-based P(O₃) values using the peroxy radical measurements from UTSA are included for comparison.



CMAQ uses the CB6r3 mechanism, which is very similar to the CB6r2 mechanism. The large variation in results between the models continues to be 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 continue to refine the 0-D modeling and the CMAQ modeling. In particular we will continue to compare the CMAQ output to measurements from numerous monitoring sites, and to satellite 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 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 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 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