AQRP Monthly Technical Report

PROJECT TITLE	Apportioning the Sources of Ozone Production during the San Antonio Field Study	**PROJECT #**	19-025
PROJECT PARTICIPANTS	Aerodyne Research, Inc.	**DATE SUBMITTED**	Mar 8, 2019
REPORTING PERIOD	**From:** Feb 1, 2019 **To:** Feb 28, 2019	**REPORT #**	5

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

A full project meeting was held and all scientists presented updates on their tasks. This meeting spurred progress on several fronts, and resulted in additional action items.

The project is getting to the stage where data and conclusions from multiple tasks need to be viewed together to try to answer the scientific questions at the center of the project. Progress on this big-picture analysis will be more difficult to quantify. In an effort to focus this synthesis effort, we will prepare, in the coming month, a document that lays out current hypotheses and questions to answer. This document will also serve as a working outline for the final report.

Task 1: High-Resolution (HR) Analysis

The Iodide Chemical Ionization Mass Spectrometer (ICIMS) data has been further analyzed during this reporting period. Specifically, the full mass spectrum has been calibrated, and peaks have been identified from 60 amu to 700 amu. Upcoming analysis will include refinement of this peak list for use in positive matrix factorization approaches to identify interesting temporal trends.

An in-depth investigation of the high-resolution spectra for the EC-PTR has been done. Several classes of compounds have been identified, drawing from the literature results and by comparison with other known species. These classes are preliminary but include: biomass burning, photochemistry involving nitrogen, biogenic emissions from conifers, and isoprene oxidation products. The photochemical products are of particular interest.

Task 2: PMF Analysis

Individual time periods of interest for PMF analysis of the GC-ToF dataset have been identified and discussed in a project meeting. The size of this dataset mean that only selected times can be processed in a given PMF run.

Task 3: 0D Box Model

The Dynamically Simple Model of Atmospheric Chemical Complexity (DSMACC) model was designed as a multipurpose chemical mechanism integrator with relevant submodules. This model has been chosen for use in 0D photochemical simulations. Dr. Barron Henderson, one of the architects and current maintainers of DSMACC, has graciously provided both technical support in getting the model properly compiled and advice on modifications to the model to allow it to run in with our desired options.

DSMACC is built and running on an Aerodyne computer. The base GEOS-CHEM chemistry model has been successfully supplanted by the explicit Master Chemical Mechanism (MCM) version 3.3. An Igor code that converts the SAFS measurement data into an input file(s) has been developed and tested. The model, running with the photochemical control using the out-of-the-box options, runs and produces output files. An Igor code that parses the output files has been developed but not fully tested. Next steps will involve getting the intended photolysis rate mechanism into the code before continuing with the assimilation of output into Igor.

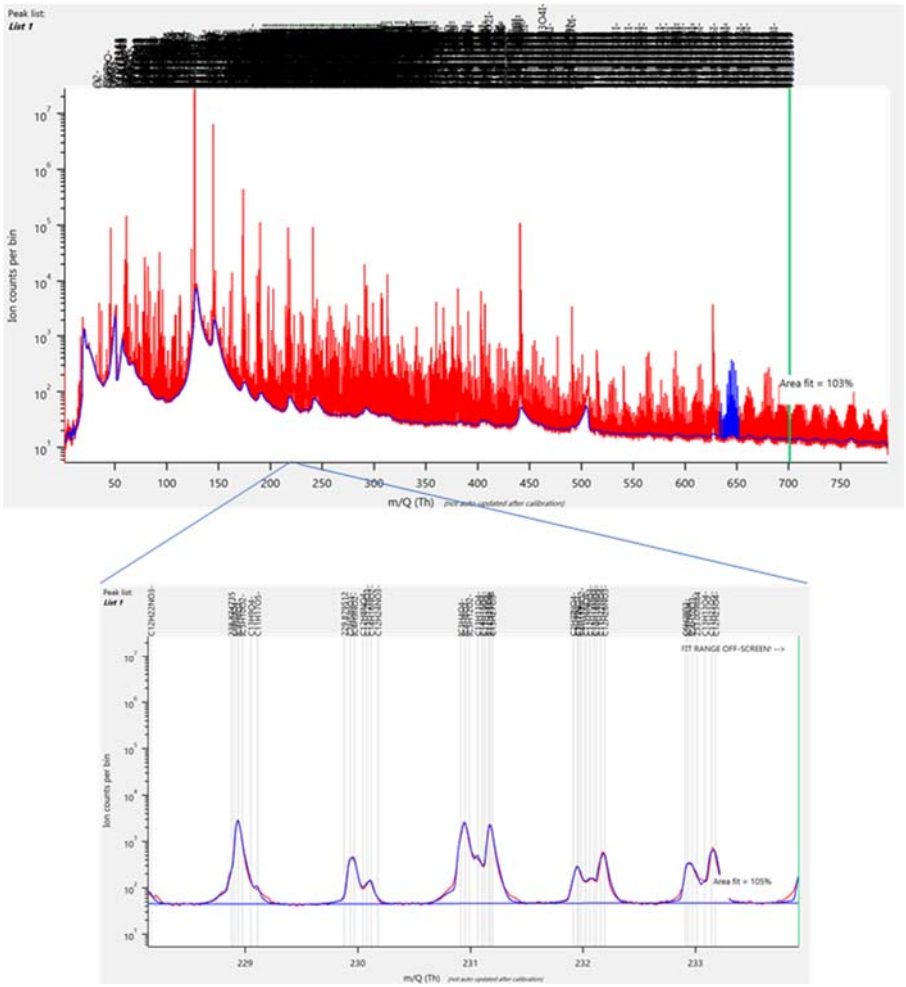
The current activity is centered on modifications to the model source code. We need it operate in a mode where $j(NO_2)$ is constrained to the measured value, but all other j values are computed via lookup in the NCAR Tropospheric UltraViolet model (TUV). Additionally, we have a scheme in mind to interrogate the model output for sum OH reactivity.

Task 4: Back-Trajectory Footprint Analysis

The full set of Hysplit back-trajectories has been run. This analysis leverages the best-available meteorological datasets. The results are output in a format that is accessible in the analysis software of choice, Igor Pro, and summary .PNG figures (see "Preliminary Analysis") are stored on a shared project drive to facilitate qualitative analysis by all project members.

Preliminary Analysis

A reference spectrum for the I-CIMS dataset has been compiled. It is based upon representative spectra (shown below) taken across the entire SAFS dataset. It reveals the presence of 2446 potential mass peaks, of which 1700 are chemically identified, and another 825 are currently unknown. The top panel shows an overview of the entire mass spectrum; the bottom panel zooms in to just a few masses showing multiple peaks.



Data Collected

No data will be collected as part of this project. However, data will be generated after completion of Task 1, HR analysis.

Identify Problems or Issues Encountered and Proposed Solutions or Adjustments

No specific issues have come up in the most recent reporting period.

Goals and Anticipated Issues for the Succeeding Reporting Period

In the next reporting period, there are several goals:

- Task 2: Run PMF on selected time periods for the GC-ToF dataset.
- Tasks 1 and 2: Continue with peak identification efforts on PTR-ToF and I-CIMS data using results from Task 2. Include other existing SAFS data to help in identification (e.g. isoprene). This task will be ongoing through the next few reporting periods.
- Task 3: Run the 0D model using appropriate photochemical parameters.
- Task 3: Develop tools to parse output of the 0D model.
- All Tasks: Begin outlining major project hypotheses. Make a draft report outline to guide analysis.

No issues are anticipated.

Detailed Analysis of the Progress of the Task Order to Date

Progress continues on all tasks.

Task 4, HYSPLIT back-trajectories, is on its way to completion and will help with interpretation of PMF results.

Task 2, PMF analysis, has seen notable developments in methodology for the two-dimensional GC-ToF dataset.

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).

___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 Dr. Tara Yacovitch

Principal Investigator