

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	Feb 8, 2019
REPORTING PERIOD	From: Jan 1, 2019 To: Jan 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

A productive mini-meeting was held to discuss results from the EC-PTR PMF analysis. This meeting resulted in several action items for continued PMF exploration and HR fitting analysis. Much of the progress this month focused on those specific analysis pathways identified in this mini-meeting and during the last whole-project meeting.

Task 1: High-Resolution (HR) Analysis

High-resolution fitting of the I-CIMS dataset is in progress. Analogously to the PTR-ToF dataset, the plan is to use an automated peak-finding algorithm to augment pre-existing lists of known species, as was done for the PTR-ToF dataset. This step will be made faster than usual because the I-CIMS data have already been pre-averaged onto a 10-second time base. This is ample time resolution for subsequent PMF tasks.

Task 2: PMF Analysis

The first stages of PMF exploration of organic particulate matter measurements has been completed using data from the Aerosol Mass Spectrometer (AMS). Preliminary results show separate factors for newer and aged particles. The temporal analysis of these data and comparison with other factors is ongoing.

A mini-meeting was held on the topic of the GC-ToF dataset. Major strides have been made in the development of methodology for PMF of this two-dimensional dataset. These methodological advancements are results in and of themselves and will comprise a section of this project's final report.

Task 3: 0D Box Model

Prototype code has been written to output average concentrations for a given time interval into simple text files. Such simplified files are required as input to the 0D box model. Selected time periods for initial analysis have been selected based on the preliminary results of the PMF

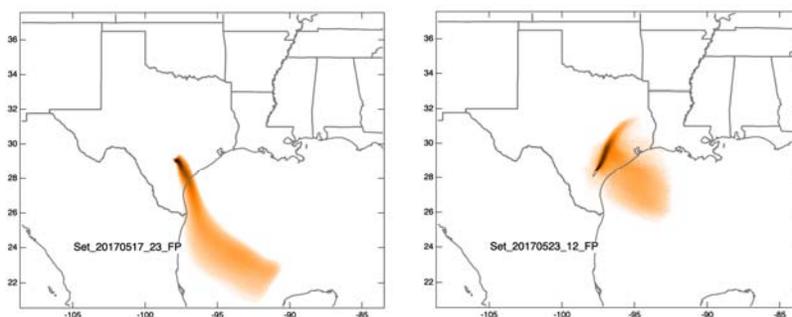
analysis. Two wrapper programs are being investigated, both of which can be used to run the master chemical mechanism model. The two options are DSMACC and BOXMOX.

Task 4: Back-Trajectory Footprint Analysis

A final computational run of back-trajectories is currently underway on a high-powered computational computer. This analysis leverages the best-available meteorological datasets and takes about 30 minutes to complete 1 hour of simulated time. This analysis is about 40% complete. 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 being output for ease of more qualitative analysis.

Preliminary Analysis

An example of the Hysplit back-trajectory footprint figures is shown below. These two simulations show the origin of the air mass sampled during the campaign during an hour-long period. The first, on 05/17/2017 shows clear influence from the ocean; the second, only a few days later on 05/23/2017, shows more influence from on-land surfaces. These two time periods are compared with measured tracers (like ethane and pentanes) as well as PMF factor results (which represent groupings of species), to better understand potential sources of observed species.



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

The magnitude of data present in the GC-ToF dataset has revealed limitations in using the currently-available version of the PMF program written by Dr. Paatero. With the current software, dataset, and methodology, analysis on a segment of GC-ToF data of about 7 hours is the current limit. For this project, PMF will be explored in 7-hour chunks for time periods of interest. However, discussions are also underway with Dr. Paatero on potential future improvements to the underlying codebase.

Goals and Anticipated Issues for the Succeeding Reporting Period

In the next reporting period, there are several goals:

- Hold a project-wide science meeting to share results, subject them to peer-review, and generate new action-items.
- Task 1: Generate a pseudo-HR dataset for the I-CIMS dataset.

- Tasks 1 and 2: Continue with peak identification efforts on PTR-ToF and I-CIMS data using results from Task 2. This task will be ongoing through the next few reporting periods.
- Task 2: Discuss the interpretation of PMF factors results between various datasets.
- Task 3: Evaluate MCM wrapper model programs and test the 0D box model.
- Task 4: Continue output of highest-quality HYSPLIT footprint results and associated figures.

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 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

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 Dr. Tara Yacovitch
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