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	Apr 8, 2019
REPORTING PERIOD	From: March 1, 2019 To: March 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 project is in a stage where data and conclusions from multiple tasks need to be incorporated together to get at 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, an outline of a final report has been prepared. This outline lays out current hypotheses and questions to answer and will now help direct research efforts towards concrete deliverables and core goals.

Task 1: High-Resolution (HR) Analysis

The Iodide Chemical Ionization Mass Spectrometer (ICIMS) data has been completely fit using an extensive peak list. This task was a major computational effort and has produced a large dataset that can now be used by several scientists at once. Upcoming tasks using this dataset include refinement of this peak list to identify those ions that show the most variability in intensity and/or respond to clean-air additions; use in positive matrix factorization approaches to identify interesting temporal trends; and comparison with ions identified in other instruments.

An analysis of the calibration results for the EC-PTR dataset has been done. This analysis focuses on understanding the response of individual compounds to the instrument, and will be crucial in determining response factors for the numerous chemical species that were not present in the calibration tank, including any newly identified species. These response factors depend on relating the rate of reaction of a given species with the water ion responsible for the chemical ionization at the heart of the PTR.

Additionally, the full high-resolution EC-PTR dataset has been examined to identify those species that respond to the addition of clean-air. This strategy aims to exclude any signals that are due to instrument artifacts and focus instead on real, detectable compounds in ambient air. Comparisons of certain EC-PTR data have also been undertaken with other available datasets for this campaign, for example the GC-ToF dataset, and stationary AutoGC sites run by the state.

Task 2: PMF Analysis

Two different approaches to PMF analysis of the GC-ToF dataset have been attempted. The data Has been grooped in two ways in an attempt to pull out notable factors. The targeted data are: 1) a comparison of the San Antonio vs Floresville sites using mid-day data and 2) diurnal variations at the San Antonio site, comparing nighttime vs daytime data for 3 consecutive days. This enables PMF analysis given the inherent data file size limitations of the current PMF program.

Task 3: 0D Box Model

The 0D Box Model is currently built and running on a server at Aerodyne. The first model runs leveraging measured concentrations of select species have been done. We have identified additional data input needs of the model (e.g. concentrations of certain alkanes). Depending on the identity of the desired input species, there may be data gaps during the campaign. One solution that has been developed is to determine ratios of species of interest versus certain common denominator species that have complete data coverage during the campaign. Such denominator species include ethane and carbon monoxide. Identifying representative ratios and their typical ranges will allow us to give the model reasonable input concentrations, even during periods where data coverage was poor.

Task 4: Back-Trajectory Footprint Analysis

Hysplit back-trajectories have been leveraged in an analysis aimed at linking the Hysplit footprint results to maps of Texas that include information about land cover. This is discussed in "preliminary analysis".

Preliminary Analysis

Ecological mapping information was obtained from the Ecological Mapping Systems of Texas database (EMST) published by the Texas Parks & Wildlife Department. The hundreds of individual ground cover classes were broadly sorted into three categories: urban, woods, and grass/marsh. This sorting is preliminary. Separately, the outlines of the Eagleford shale play were obtained from the EIA and plotted on the same map. Then, an overlap analysis was done with results from Hysplit footprint simulations. An example overlap figure is reproduced below.
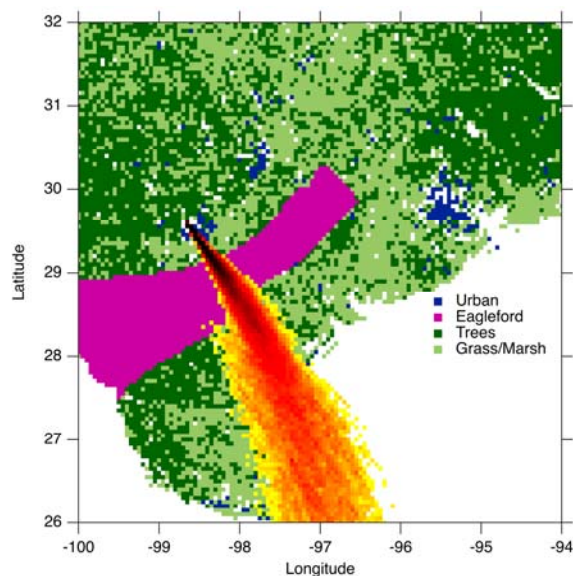

Figure 1. Example Hysplit overlap figure. The black/red/gold cloud shows the Hysplit footprint overlaid upon a map of Texas.

The overlap was calculated as a function of time. Example data is plotted below. This data makes it easier to identify periods of time where the sampled airmass does not originate from, for example, the Eagle Ford shale (e.g. on 5/13; or 5/22-5/23). It also shows relatively little variation in the biogenic sources (wood, Grass/Marsh). Now that this analysis has been developed, it will be simple alter to better suit the data in question. The maps can be re-classified to highlight a smaller subset of vegetation (e.g. oak trees, expected to produce isoprene), or to include additional areas of oil and gas exploration (e.g. the Barnett Shale play).
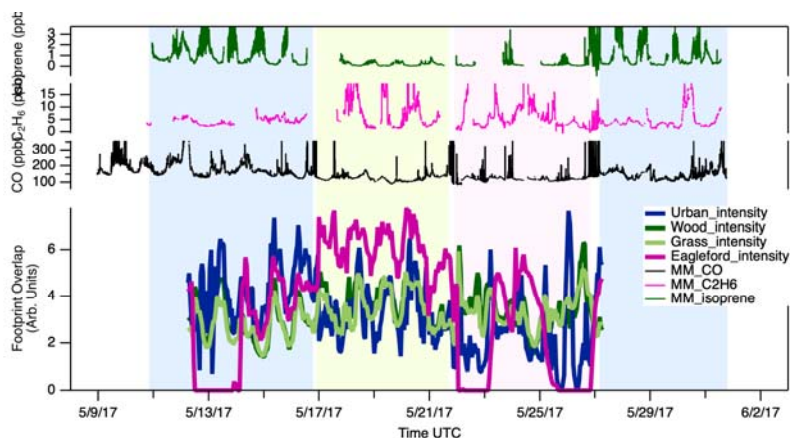

Figure 2. Hysplit footprint overlap with 4 different land cover types. Measured isoprene, ethane and carbon monoxide time traces are also shown. Shaded areas represent time spent at UTSA (blue), Floresville (green) and Corpus Christi State Park (pink).

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 1: Identify species of most interest in integrated high-resolution I-CIMS dataset.
- Task 2: Run PMF on I-CIMS 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: Incorporate additional real measurement data and/or ratios of tracers into the 0D model.
- Task 3: Refine tools to parse the output of the 0D model
- All Tasks: Tailor work towards answering main project goals and filling in the final report outline

No issues are anticipated.

Detailed Analysis of the Progress of the Task Order to Date

Progress continues on all tasks.

Task 1 has seen major progress on two instruments: the EC-PTR, where an analysis has been developed to help determine sensitivities for uncalibrated species; and the I-CIMS, where the full high-resolution fit has bene completed.

A final report outline has been written and discussed, which will serve as a guiding document to focus research towards the most important goals and questions.

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

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Submitted to AQRP by   Dr. Tara Yacovitch

Principal Investigator