AQRP Monthly Technical Report

PROJECT TITLE	ANALYSIS OF SURFACE PARTICULATE MATTER AND TRACE GAS DATA GENERATED DURING THE HOUSTON OPERATIONS OF DISCOVER-AQ	**PROJECT #**	14-009
PROJECT PARTICIPANTS	R.J. Griffin, B.L. Lefer, and group members	**DATE SUBMITTED**	1/9/2015
REPORTING PERIOD	**From:** December 1, 2015 **To:** December 31, 2015	**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. We 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

This project is broken down into eleven tasks. Naturally, some of the work for an individual task will be complementary to the needs of other tasks. Based on the original schedule, at this point, Tasks 1 through 5, 8, and 9 should be complete, and the work for Tasks 6 and 10 should have begun. Tasks 1 through 5 are considered complete; this work was described in previous monthly technical reports, and no further information will be given here. Progress on Tasks 6 and 8-11 is described here. Task 7 is not yet considered; relevant work on Task 7 is scheduled to begin in March.

Task 6 – Relative Oxidation of Organic Aerosol (OA)
Preliminary analysis of the OA dataset generated during DISCOVER-AQ was conducted using positive matrix factorization (PMF) using PMF2 (v.4.2) running in robust mode. The main factors contributing to the organic fraction of the submicron aerosol were identified in a sub-dataset corresponding to a period where elevated PM_1 concentrations were observed (near the end of the field campaign). Multiple criteria such as the contribution of each factor to the observed variance and the residual levels for PMF solutions including different number of components were considered for selection of the number of factors contributing to the OA concentrations. Preliminary results indicate that three main factors explain most of the variance in the dataset: a component corresponding to hydrocarbon-like OA (HOA) and two oxygenated OA components (OOA-I and OOA-II). The identified factors agree with those reported by previous studies. The degree of oxidation follows the order HOA < OOA-I < OOA-II, with mass-to-charge ratio (m/z) 44 constituting 3.5, 7 and 12 % of the mass spectral signal, respectively. Moving forward, this categorization will be verified by investigating the correlation of the identified factors with tracers of primary combustion (for HOA) and particulate sulfate, nitrate, and chloride (for OOA-I and OOA-II).

PMF analysis on an organic aerosol dataset collected in Houston during August 2014 also was conducted for comparison purposes (Figure 2). Although results of this analysis require additional study, four factors can be identified. These factors exhibit a less oxidized character than those retained for the DISCOVER-AQ sub-dataset, suggesting a significant variation of the OA oxidation state as a function of space and time across Houston. The spatial and temporal variation of the contribution of the identified/selected factors to OA during DISCOVER-AQ will be further analyzed and presented in a future report.

Task 8 – Biogenic influence

Task 8 aims to evaluate the influence of biogenic volatile organic compounds (BVOCs) on ozone and PM formation. The research team continues to work to understand the FACSIMILE model, which was purchased using funds for this project and will be used for this effort. This model will require data inputs for BVOCs. Because data are not available for all periods of the mobile laboratory operation, alternative data sources have been identified. Community Multi-scale Air Quality (CMAQ) model output for isoprene, isoprene oxidation products, and monoterpenes has been received for the DISCOVER-AQ period. The CMAQ output will be used as input for FACSIMILE. The CMAQ data were obtained at the very end of the previous reporting period, and most effort on this Task over the current reporting period focused on understanding how to work with CMAQ output files to allow for their use as FACSIMILE input files.

Task 9 - Analysis of NO_2

NO_2 was measured in situ aboard the NASA P-3B and remotely sensed from the King Air B200 during the flights of DISCOVER-AQ. For these flights, the NO_2 measurements were compared to the NO_2 column measurements from the network of Pandora spectrometers in Houston when coincidences occurred.

The Airborne Compact Atmospheric Mapper (ACAM) was aboard the King Air B200 aircraft, measuring NO_2 slant columns nadir of the aircraft altitude (~9km). The instantaneous field of view for this instrument is reported as 0.35 x 1 km^2. Currently, the data still need to be post-processed to transform slant column to vertical column using its air mass factor (AMF). Therefore, ACAM slant columns are compared to Pandora slant columns (minus an OMI-measured stratospheric column) and normalized over the range of that day's ACAM measurements to get a relative comparison. Analysis has been done only for September 25^{th}, 2013, but will be expanded to the rest of the flights in the future. The spatial footprint of the ACAM and Pandora measurements are much more similar than when compared to OMI. The biggest deviations from a one-to-one relationship (with ACAM being in excess of Pandora) are in the more polluted regions (Channelview, Moody Tower, Deer Park) where the AMF calculation becomes more critical due to the spatial heterogeneity of pollution. This analysis shows that even though the ACAM data have yet to be converted to vertical columns, ACAM comparisons shows improvement in capturing the spatial variability of NO_2 in comparison to OMI because of its smaller spatial resolution.

In order to compare Pandora measurements to P-3B data, the in situ data must be binned and integrated to produce a lower tropospheric column. NO_2 was measured aboard the aircraft at one-second temporal resolution. Aircraft spiral data is averaged in 100m bins through the height of the profile and summed to derive a lower tropospheric column density (that is, data from above 5 km are not included). To fill in gaps of missing data interpolation was used. Profiles missing more than 5 bins were excluded from this analysis. Coincident Pandora measurements were averaged through the time of the spiral and the monthly averaged OMI stratosphere was subtracted to give a tropospheric estimate.

Aircraft data have information about the vertical distribution of NO_2, but the larger horizontal distribution of the spirals leads to the inclusion of areas not incorporated in the Pandora field of view. For this reason, the root-mean-squared error for this comparison increases with higher levels due to spatial variability and pollution. Moving forward, the aircraft spiral will be divided into subsets to incorporate data only within a threshold distance of the ground measurement location. Analyzing each profile also will allow for the analysis of vertical profile shape between upwind, source, and receptor regions, which will assist with the ground in situ analysis described in the previous report.

Tasks 10 and 11 – Ozone and radical production rate calculations
The FACSIMILE model described above also will be utilized to evaluate these parameters and provide an estimate of the uncertainty of the calculations by using multiple chemical mechanisms. Staff members continue to become familiar with FACSIMILE. In addition, the ratio technique described in previous reports continues to be explored as a viable means to generate model input.

Preliminary Analysis

No additional analysis beyond that described above has been performed.

Data Collected

No new data has been collected as part of this project as it is purely a data analysis project.

Identify Problems or Issues Encountered and Proposed Solutions or Adjustments

No significant problems have been identified beyond those described in previous reports. Work is proceeding as would be expected.

Goals and Anticipated Issues for the Succeeding Reporting Period

The goals for the next period are to continue work on Tasks 6 (characterization of oxidation state and similar metrics for OA using PMF), 8 (characterization of biogenic influence), 9 (analysis of NO_2), 10 (modeling of ozone production rate), and 11 (modeling of radical sources). According to the project plan, Tasks 1-5, 8, and 9 should be complete as of the end of January.

Detailed Analysis of the Progress of the Task Order to Date

Tasks 1-5 are considered complete. Although we are slated to have completed Tasks 8 and 9 but have not, we are ahead on Tasks 6, 10, and 11, as these activities have started ahead of schedule. We believe the progress on Tasks 6, 10, and 11 balances the delays in Tasks 8 and 9; therefore, we deem our progress appropriate.

Submitted to AQRP by: Robert J. Griffin
Principal Investigator: Robert J. Griffin