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**	9/8/2014
REPORTING PERIOD	**From:** August 1, 2014 **To:** August 31, 2014	**REPORT #**	2

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

The University of Houston (UH) group was still awaiting funds and final approval to purchase well into August 2014; therefore, they were unable to perform significant work during the period covered by this report. As such, a description of the work for Task 8 (which focuses on assessing the importance of biogenic activity and is the first task for which primary responsibility lies with UH) is not included despite the original work plan specifying that effort in this area would be made during this period. They have, however, received funding and ordered the requisite code to allow them to perform their analysis. Additional information will be provided in the next monthly report.

This project is broken down into several tasks, and some of the work for an individual task may be complementary to other tasks. The only Rice-focused tasks on which progress was expected during this period are Task 1 and 2, which focus on determination of particle emission factors from motor vehicular sources and characterization of large particle mass concentration events, respectively. Progress was made on each of these tasks, as well as on Tasks 3 and 6 (slightly out of order). Tasks 4 and 5 will require sharing of data.

For Task 1, a protocol for determination of motor vehicular particulate emission factors was described previously. A ratio of enhancements in organic aerosol to enhancements in either carbon monoxide (CO) or nitric oxide (NO) will be compared to known emission factors for CO or NO (to be taken from Environmental Protection Agency (EPA) modeling). Enhancements (over three standard deviations) are defined relative to the background immediately before and after the plume sampling. Plumes of organic aerosol while the mobile laboratory was on-road sampling vehicles have been identified for the DISCOVER-AQ period, and the corresponding enhancements in organic aerosol have been calculated. Including the eight events that were described in the last report, eleven specific episodes have been identified for on-road emissions;

enhancements in sub-micron organic aerosol ranged from 14 to 215 micrograms per cubic meter. On-road sources were confirmed through a meticulous review of the video footage, which also allowed for an estimate of the nearby fleet distribution (amount of diesel versus gasoline, amount of light-duty versus heavy-duty, etc.). Final NO and CO data averaged to a more appropriate time-scale are expected soon from UH to allow calculation of the emission factors. The EPA model (MOVES2014) has been problematic; efforts in the group to run MOVES2014 have proven impossible, and assistance from EPA staff to debug has been sought.

With regard to Task 2, thirteen additional particle mass events not associated with motor vehicle emissions have been identified. Five were associated with biomass burning, with a range of organic aerosol enhancements of 22 to 105 micrograms per cubic meter. An additional event is attributable to a passing tanker ship, with an enhancement of organic aerosol of 9 micrograms per cubic meter. Additional chemical characterization of the organic aerosol mass spectra associated with these events continues. In contrast, eight particle mass events were observed near petrochemical facilities, with the nature of the particles depending on the near-by operations. Storage tanks and activities associated with general operations showed organic aerosol enhancements up to 15 micrograms per cubic meter. Flaring and other operations appeared to lead to sulfate enhancements of up to 30 micrograms per cubic meter.

Task 3 is focused on the preparation of data for sharing with investigators at other Texas institutions. As part of this process, an individual in our research group who was not involved in the generation or initial analysis has audited our data. A comparison between data inclusion, flags that described mobile or stationary sampling, and GPS coordinates is being made to ensure appropriateness and completeness of data prior to sharing the data before the end of September 2014.

For Task 6, the focus is on determination of organic aerosol oxidation state (and similar metrics) during the campaign. In addition to the application of factor analysis by positive matrix factorization (PMF) for identification of aerosol components (e.g. hydrocarbon-like organic aerosol versus oxidized organic aerosol), the feasibility of conducting a three-dimensional (3-D) factorization technique, specifically parallel factor analysis (PARAFAC), is being evaluated. The extension of the two-dimensional analysis (PMF) to a 3-D analysis of size resolved organic composition data set has been recently reported. Only a few studies have employed this technique for analysis of high-resolution aerosol mass spectrometer data sets. Application of PARAFAC (sometimes referred to as PMF3) on the high-resolution data set generated during DISCOVER-AQ would likely allow the identification of additional aerosol components and will provide more robust information of the size distribution of these. Compilation/rearrangement of the data set is being conducted, and preliminary PARAFAC application will be performed after this stage is completed.

Preliminary Analysis

No true analysis beyond the calculations described above has been performed to date.

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

Beyond the lack of funds in place for the UH team (already resolved), only two minor problems have been identified so far. First, the currently available time-averaged CO and NO data are too low in temporal resolution for the emissions effort; the UH team is working to rectify this situation. The Rice team has struggled to perform MOBILE2014 modeling; an expert from EPA has been sought to assist with debugging of the model.

Goals and Anticipated Issues for the Succeeding Reporting Period

With the higher resolution CO and NO data, it will be possible to calculate the enhancement ratios for each event. Multiple points can be combined to provide data across vehicle type or location type. The appropriate emission factor for vehicle type or location will be determined by regression between the enhancement ratios and the EPA estimates once the MOBILE2014 model is working appropriately. This will complete Task 1. In addition, analyses focused on characterization of the organic aerosol in high concentration events are proceeding; this will complete Task 2. Data should be shared prior to the end of the next reporting period; this will complete Task 3. Task 6 will continue as planned. UH should obtain the necessary code to enable initiation of its modeling activities, allowing initiation of Task 8.

Detailed Analysis of the Progress of the Task Order to Date

Progress on Task 1 has been slowed over the second month of the project, as UH works on its data and as MOBILE2014 is debugged. Faster progress will be made in the next month. Appropriate progress on Task 2 has been made during the second month of the project and will continue in the third month as well. Data will be sharable with collaborators by the end of the next reporting period. The Rice team is ahead of schedule on Task 6. Due to delays in funding, the project team will need to find a way to make up the lost time for Task 8 during the second month of the project.

Submitted to AQRP by: Robert J. Griffin

Principal Investigator: Robert J. Griffin