

AQRP Monthly Technical Report

PROJECT TITLE	Sources of Organic Particulate Matter in Houston: Evidence from DISCOVER-AQ data Modeling and Experiments	PROJECT #	14-024
PROJECT PARTICIPANTS	Lea Hildebrandt Ruiz and Ying Xu (The University of Texas at Austin) Greg Yarwood Bonyoung Koo (ENVIRON) Gookyoung Heo (University of California, Riverside)	DATE SUBMITTED	9/8/2014
REPORTING PERIOD	From: August 1, 2014 To: August 31, 2014	REPORT #	3

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

Task 1 – Inventory Analysis:

Based on literature reviews, EPA’s speciation data, and speciated point source emissions data for Houston from the STARS database, we have prepared a preliminary list of IVOCs to study in the chamber experiments (Task 2)

Task 2 – Environmental Chamber Experiments and Box Modeling:

Dr. Heo at UCR provided technical support to the UT-Austin team in regard to using the SAPRC chamber simulation software, designing chamber characterization experiments and analyzing data from characterization experiments. Dr. Heo started to implement the 1.5 dimensional (1.5D) volatility basis set (VBS) approach into the current version of the SAPRC software.

The UT-Austin team conducted and analyzed results from chamber characterization experiments.

The body of the thermodenuder was built by Swagelok and recently delivered to UT-Austin. The UT-Austin team has requested a quote for a controller which could be used to control the temperature of three heating tapes and also switch two valves (which will be used to switch between the thermodenuder and bypass lines) for operation of the thermodenuder. The heated injector was ordered and will be constructed by a machine shop at UT-Austin within the next reporting period.

Task 5 – DISCOVER-AQ Data analysis:

The UT-Austin team has begun PMF analysis of the organic aerosol mass spectra measured during DISCOVER-AQ.

Identify Problems or Issues Encountered and Proposed Solutions or Adjustments

Task 2 – Box Modeling:

In the Carbon Bond chemical mechanism (CB6r2), saturated alkanes such as n-C₁₄H₃₀ are represented by the PAR chemistry. However, using only the model species PAR to map an intermediate-volatility alkane is not enough to describe secondary organic aerosol (SOA) formation because the model species PAR is a lumped model species for various paraffinic carbon bonds. This issue can be addressed by mapping such an SOA precursor into PAR for ozone formation chemistry and also into a separate model species (e.g., IVOC1) for SOA formation chemistry.

Because we do not know the gas-phase chemistry of intermediate-volatility organic compounds (IVOCs), modeled OH concentrations may not be accurate. Measurement-based estimated OH concentrations can be fed to the model and these OH concentrations can be used to reduce the uncertainty in estimating SOA parameters.

Goals and Anticipated Issues for the Succeeding Reporting Period

Dr. Heo received a job offer from the National Institute of Environmental Research of the Republic of Korea and he needs to wrap up his work at UCR by the end of September, 2014. In response to this, he will focus on developing an operational version of the SAPRC software in which the 1.5D VBS method is available, give a training session to the UT-Austin team on September 24, 2014, and provide Dr. Lea Hildebrandt Ruiz with a document on his work for this project.

The UT-Austin team will purchase the selected IVOCs and develop GC analysis methods for them. After the heated injector has been built, the IVOCs will be injected into the chamber in trial experiments and their loss rates will be measured and characterized.

The UT-Austin team will also continue quality assurance of data collected during DISCOVER-AQ as well as positive matrix factorization analysis of the organic aerosol mass spectra.

Detailed Analysis of the Progress of the Task Order to Date

Progress to date has been appropriate. Some changes have been made to the project timeline, for example, positive matrix factorization (PMF) analysis was started earlier than anticipated, and Dr. Heo intends to complete his contributions to the project by the end of September 2014. Overall, we do not anticipate problems completing all project tasks by the end of the project period (June 30, 2015).

Submitted to AQRP by: Lea Hildebrandt Ruiz

Principal Investigator: Lea Hildebrandt Ruiz