

AQRP Monthly Technical Report

PROJECT TITLE	Condensed Chemical Mechanisms for Ozone and Particulate Matter Incorporating the Latest in Isoprene Chemistry	PROJECT #	16-031
PROJECT PARTICIPANTS	William Vizueté Jason Surratt	DATE SUBMITTED	2/6/17
REPORTING PERIOD	From: 1/1/17 To: 1/31/17	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 Updated SAPRC-07 and Aerosol Module for Isoprene Oxidation

Preliminary Analysis

N/A

Data Collected

N/A

Identify Problems or Issues Encountered and Proposed Solutions or Adjustments

N/A

Goals and Anticipated Issues for the Succeeding Reporting Period

We will investigate the possible latest version of SAPRC and inquire how to interface with our modeling system.

Detailed Analysis of the Progress of the Task Order to Date

The progress on the task is on schedule.

Task 2 Chamber Experiments: Interplay of Particle-Phase Composition, Phase, and Viscosity on IEPOX Multiphase Chemistry

Preliminary Analysis

N/A

Data Collected

N/A

Identify Problems or Issues Encountered and Proposed Solutions or Adjustments

Both the CIMS and ACSM instruments need to be repaired before further chamber experiments can proceed.

Goals and Anticipated Issues for the Succeeding Reporting Period

We will be tweaking certain aspects of our experimental approach to better constrain the uptake kinetics in the chamber. Potential Aerosol Mass (PAM) Oxidation Flow Reactor (Aerodyne Research, Inc) will likely be used to generate monodisperse organic aerosols, which will then be fed into the indoor chamber until targeting particle concentration is attained prior to IEPOX uptake. Two differential mobility analyzers are used to select aerosols by size, one for acidified sulfate aerosols entering the PAM and one for the organic aerosols output from PAM. With this approach, the coating thickness and size of the aerosol are in theory evenly distributed across aerosol population and therefore the modeled uptake coefficient can better represent the heterogeneous reaction probability with respect to the thickness and type of the organic layers enwrapping the acidified sulfate seeds. We have yet to put this experimental design into execution so trials and errors are expected until repeatability is confirmed.

Detailed Analysis of the Progress of the Task Order to Date

Given that our measurement equipment was out of operation we were unable to make any progress. We feel, however, that instrument should be ready in February and our progress will remain on schedule.

Task 3 Implementation in a regulatory air quality model

Preliminary Analysis

Comparison between EPA output (reference) and our data showed unacceptable difference in speciation concentrations.

Data Collected

Sample output received from EPA that was used as reference/benchmark.

Identify Problems or Issues Encountered and Proposed Solutions or Adjustments

The previous compiled CMAQ5.2 model predictions were different when compared to reference sample output obtained from EPA. We suspect unsuccessful installation of CMAQ on our cluster thus we are installing newer version of CMAQ 5.2 which is updated and uploaded on EPA-GITHUB site. The newer version of CMAQ 5.2 has compilation issue which ties to the IOAPI library.

Goals and Anticipated Issues for the Succeeding Reporting Period

Resolve compilation errors and run data with newer CMAQ model. Output data comparison to confirm successful installation. Then to start the full episode base run. Generate visualization tool to compare SOAS field data and output data.

Detailed Analysis of the Progress of the Task Order to Date

First day run output generated from CMAQ. Tools for our output to reference output comparison and visualization were generated.

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

Principal Investigator

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Jason Surratt