

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 Vizquete Jason Surratt	DATE SUBMITTED	4/30/17
REPORTING PERIOD	From: 4/1/17 To: 4/30/17	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

Task 1 Updated SAPRC-07 and Aerosol Module for Isoprene Oxidation

Preliminary Analysis

We have completed the development of the input files needed to evaluate the updates in the SAPRC16 mechanism.

Data Collected

Files needed for modeling of the SAPRC16 chemical mechanism and production of input files needed for the UNC box model.

Identify Problems or Issues Encountered and Proposed Solutions or Adjustments

N/A

Goals and Anticipated Issues for the Succeeding Reporting Period

We will QA model with the SAPRC16 mechanism and begin to produce simulation of UNC chamber data.

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

Continue to collect data from coating experiments and familiarizing ourselves with the Potential Aerosol Mass (PAM) Oxidation Flow Reactor (Aerodyne Research, Inc)

Data Collected

Densities were obtained for ABS as well as α -pinene SOA, toluene SOA, dodecane SOA and naphthalene SOA in various concentrations of VOCs and oxidants.

Identify Problems or Issues Encountered and Proposed Solutions or Adjustments

Continue to adjust CIMS to improve performance.

Goals and Anticipated Issues for the Succeeding Reporting Period

We plan to conduct kinetic measurements using Flow Tube Reactor to derive IEPOX uptake coefficient onto aerosols coated with organic matters produced by oxidation of α -pinene, toluene, and naphthalene under various relative humidity

Detailed Analysis of the Progress of the Task Order to Date

When our measurement equipment was out of operation we were unable to make any progress, but we are now trying to complete our proposed experimental schedule.

Task 3 Implementation in a regulatory air quality model

Preliminary Analysis

Completed detailed investigation of key parameters that could affect IEPOX-SOA yield calculation and implementations in various box and regional scale models. Quality assured the output data to ensure our ability to change IEPOX uptake parameters in CMAQ modeling system.

Data Collected

Produced modeling output as a sensitivity analysis on IEPOX-SOA yield and aerosol phase diffusivity.

Identify Problems or Issues Encountered and Proposed Solutions or Adjustments

N/A

Goals and Anticipated Issues for the Succeeding Reporting Period

We will visualize and analyze the results of our first sensitivity run ensuring our ability to compare with previous simulations and observational data. Based on preliminary data from the experiments proposed we will develop a series of sensitivity runs for future analysis.

Detailed Analysis of the Progress of the Task Order to Date

We are on schedule.

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

William Vizuete

Jason Surratt