

# AQRP Monthly Technical Report

<b>PROJECT TITLE</b>	Condensed Chemical Mechanisms for Ozone and Particulate Matter Incorporating the Latest in Isoprene Chemistry	<b>PROJECT #</b>	16-031
<b>PROJECT PARTICIPANTS</b>	William Vizuete Jason Surratt	<b>DATE SUBMITTED</b>	1/5/17
<b>REPORTING PERIOD</b>	<b>From:</b> 12/1/16 <b>To:</b> 12/31/16	<b>REPORT #</b>	2

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 15<sup>th</sup> of the month following the reporting period shown above.

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## Detailed Accomplishments by Task

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

#### Preliminary Analysis

N/A

#### Data Collected

We have completed the collection of our archived digital files of the experimental data needed for the evaluation of updates in the SAPRC-07 mechanism. We have completed the training of the GRA on the software needed to complete the task. We are in the process of inquiring and evaluating the latest SAPRC release.

#### 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**

We are currently processing the obtained data from our first round of indoor chamber experiments for all three types of particles: acidified ammonium sulfate seed particle, seed particle coated by  $\alpha$ -pinene ozonolysis products (AP SOA), and IEPOX-AP SOA..

### **Data Collected**

Both online and offline instrumentation was used to collect data as detailed below.

**Online:** particle number, surface, volume concentrations and size distribution measured by Differential Mobility Analyzer; IEPOX concentrations measured by Chemical Ionization Mass Spectrometer; real time particle bulk composition measurement by Aerosol Chemical Speciation Monitor; real time ozone concentration; real time relative humidity and temperature.

**Offline:** two filters of 50  $\mu\text{g}$  submicron particles each for each experiment for chemical characterization of particulate tracers in molecular level by GC/MS, LC/MS and UV-Vis Spectrophotometer.

### **Identify Problems or Issues Encountered and Proposed Solutions or Adjustments**

N/A

### **Goals and Anticipated Issues for the Succeeding Reporting Period**

We will continue to finish processing all obtained data from various instruments during this first round of indoor chamber experiments. Once processed we will then analyze the resulting observational data set and decide whether to proceed with chamber modeling.

### **Detailed Analysis of the Progress of the Task Order to Date**

We have completed 3 sets of indoor chamber experiments. Each set includes an experiment with IEPOX uptake onto acidified ammonium sulfate particles coated with organic products from  $\alpha$ -pinene ozonolysis and a control experiment with IEPOX uptake onto acidified ammonium sulfate. Three coating experiments were done with incremental  $\alpha$ -pinene injections and hence increased particulate organic matter/organic coating thickness prior to IEPOX uptake. An acidified ammonium sulfate particle only experiment and a IEPOX only experiment were conducted to characterize the loss rates of particles and gaseous IEPOX to the chamber wall. The progress on the task is on schedule.

## **Task 3 Implementation in a regulatory air quality model**

### **Preliminary Analysis**

N/A

### **Data Collected**

We have completed collecting and quality assuring all input data for CMAQ model base run from the EPA. We continue to gather from the literature the latest modifications to potential modeling parameters that could affect output from literature reviews. We have also received source code from the EPA to help aid in our visualization of model data.

### **Identify Problems or Issues Encountered and Proposed Solutions or Adjustments**

There were several technical issues in running the EPA episode on the UNC super computing cluster that resulting in infinity loops. We are conducting line-by-line debugging of the run file to determine the problem.

### **Goals and Anticipated Issues for the Succeeding Reporting Period**

We will continue to debug the run time issues and will produce a base simulation run. We will then begin to QA/QC this base run by comparing to EPA simulation output produced by the EPA computing clusters.

### **Detailed Analysis of the Progress of the Task Order to Date**

We have spent time over the past month trying to complete a CMAQ simulation run. The GRA is also being familiarized with both explicit and CMAQ model representations of isoprene to PM reaction pathways.

**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

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Submitted to AQRP by

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