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 Vizuete Jason Surratt	**DATE SUBMITTED**	11/30/16
REPORTING PERIOD	**From:** 10/18/16 **To:** 11/30/16	**REPORT #**	1

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
We have begun the collection of our archived digital files of the experimental data needed for the evaluation of updates in the SAPRC-07 mechanism. We have begun the training of the GRA on the software needed to complete the task. The GRA is also conducting literature reviews of any relevant publications and attended the recent 2016 Community Modeling and Analysis System annual conference in Chapel Hill, NC. This conference provided an opportunity to view the latest gas phase changes that maybe relevant for the project.

Identify Problems or Issues Encountered and Proposed Solutions or Adjustments
N/A

Goals and Anticipated Issues for the Succeeding Reporting Period
We will continue with training on the modeling software such that the GRA is able to successfully replicate past UNC modeling applications. This will ensure the installation of the software and training. The next step will be training on the software needed to visualize the modeling results to provide meaningful analysis.

Detailed Analysis of the Progress of the Task Order to Date
We are currently in the startup phase of this task and have begun gathering relevant data and information and training of the GRA on the tools needed for the task. 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 have reviewed protocols and supplies needed for the synthesized organic materials needed for the indoor chamber experiments. We have obtained and analyzed the synthesized organic materials needed for the indoor chamber experiments. Based on this we have determined we can begin the first round of indoor chamber experiments.

Data Collected

From our first round of indoor chamber experiments we have obtained particle concentration time profiles and size distributions. This data was collected for all three types of particles in our experiments: acidified ammonium sulfate seed particle, seed particle coated by **α**-pinene ozonolysis products (AP SOA), and IEPOX-AP SOA. 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 μg 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

Issue: **α**-pinene ozonolysis products tend to nucleate instead of condensing onto inorganic seed particles
Adjustments: reduce volume of each **α**-pinene injection, use higher injection flow rate to avoid localized high concentration and wait for longer time for reaction to finish before next injection.

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 **α**-pinene ozonolysis and a control experiment with IEPOX uptake onto acidified ammonium sulfate. Three coating experiments were done with incremental **α**-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
In collaboration with EPA scientists we have obtained a regulatory CMAQ modeling episode developed to explore isoprene oxidation chemistry. EPA developed the CMAQ modeling episode for a 12 km grid resolution and spans May through June 2013. This CMAQ source code and all relevant input files have been transferred to UNC computing. Further, modeling output from EPA was also obtained for QA/QC of our installation. We have also obtained SOAS2013 data needed for evaluation of results.

Identify Problems or Issues Encountered and Proposed Solutions or Adjustments
There were several technical issues in compiling the CMAQ source code onto the UNC computing cluster. To overcome this we relied on internal expertise to debug the issue and were able to compile a version of CMAQ on the cluster. The data transfer of input files for CMAQ from EPA resulted in a flattened directory structure. Time was spent rebuilding the file structure. Currently, we are dealing with run time bugs due to inconsistency input data structure and missing files. We are working with EPA to identify these missing files.

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. We will also begin to compile observational PM data relevant to Houston.

Detailed Analysis of the Progress of the Task Order to Date
We have spent time training the GRA on the CMAQ modeling system. The GRA is also being familiarized with both explicit and CMAQ model representations of isoprene to PM reaction pathways. In parallel with these efforts we have successfully compiled CMAQ 5.2 onto the UNC computing cluster.

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 _X__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 _X__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 __X_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 __X_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 __X_No

Submitted to AQRP by

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