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**	4/6/17
REPORTING PERIOD	**From:** 3/1/17 **To:** 3/31/17	**REPORT #**	4

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
Produced and have completed our quality assurance of the input files needed for our box modeling system of the SAPRC16 chemical mechanism.

Data Collected
Documentation 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

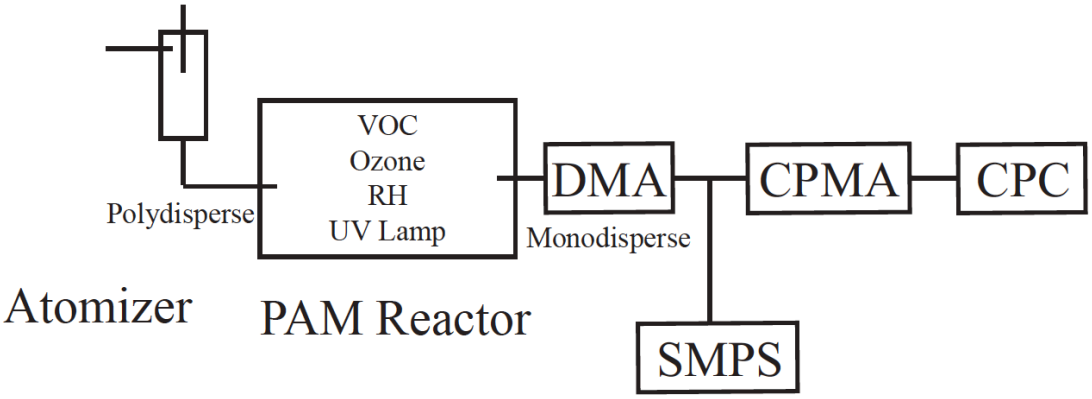
Goals and Anticipated Issues for the Succeeding Reporting Period
We will investigate the new changes made in the SAPRC16 mechanism and begin to produce simulation of UNC chamber data.

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

Coating experiments were conducted using Potential Aerosol Mass (PAM) Oxidation Flow Reactor (Aerodyne Research, Inc) with additional VOC precursors to generate organic coatings. Namely, dodecane and naphthalene. The experimental setup is shown below.



The thickness of the organic layer is calculated by eq 1, where $\boldsymbol{\rho}_{\text{total}}$ is the density of coated aerosol as a whole and $\boldsymbol{\rho}_{\text{org}}$ is the density of the organic PM measured in experiments without seed aerosols. Generally, uniform coating thickness can be achieved for toluene and **α**-pinene. However, coating thicknesses of dodecane SOA and naphthalene SOA are size dependent. This suggests we will have to size select aerosols for the two types of SOA. We also confirmed that using a DMA to size select monodisperse ABS aerosol can produce enough aerosol surface area for IEPOX uptake within the flow tube.

$$d_{thickness} = d_{total}\left[1 - \sqrt[3]{\frac{\rho_{total} - \rho_{org}}{\rho_{inorg} - \rho_{org}}}\right] \qquad \textbf{(eq 1)}$$

Data Collected

Densities are obtained for ABS as well as **α**-pinene SOA, toluene SOA, dodecane SOA and naphthalene SOA in various concentrations of VOCs and oxidants. They can be potentially used to calculate coating thickness in experiments to be conducted at UNC.

Identify Problems or Issues Encountered and Proposed Solutions or Adjustments

Although CIMS TPS module have been fixed and ions could be seen, sensitivity and resolution keep dropping over time. The software used for autotuning the voltages in the ion transmission region failed to improve CIMS performance.

Adjustment
We had to manually adjust the voltages including Lens, Deflector and Deflector Flange. They seemed to have shifted a lot from old tuning, i.e., out of the constraints of range of change set in the autotune. This is probably caused by replacement of TPS module and/or rough handling of shipping during the FIREX campaign last year.

Goals and Anticipated Issues for the Succeeding Reporting Period
PAM is set up in the Surratt Lab at UNC and ready to run experiments. We are setting out to run several flow tube experiments of IEPOX uptake onto inorganic seed and see if we can reproduce the results described in Gaston et al., ES&T, 2014 and Riedel et al., ES&TL, 2015. Since CIMS has undergone substantial instrumental changes, it requires fine tunings to optimize IEPOX response for flow tube measurements.

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 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 discuss this month and 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 _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

Principal Investigator
William Vizuete
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