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**	5/31/17
REPORTING PERIOD	**From:** 5/1/17 **To:** 5/31/17	**REPORT #**	7

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
This month has been focused on finishing the experimental data while certain equipment was available to us. As a result, we had to move all resources to complete task 2 and postponed progress on Task 1 until next month.

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 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
We have completed 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. Ammonium bisulfate seed aerosols are generated by atomizing a solution mix of ammonium sulfate and sulfuric acid.

Upon generation, seed aerosols pass through a diffusion dryer before entering the Potential Aerosol Mass (PAM) Oxidation Flow Reactor (Aerodyne Research, Inc.). The injection rate of pure precursor VOCs is controlled by a syringe pump. Depending on the precursors, ozonolysis and/or photo-oxidation of the VOCs takes place in the PAM to form organic coatings on existing seed aerosols by condensational growth. A carbon strip denuder is introduced downstream to the PAM to remove excess gas phase species to prevent secondary reactions inside the flow tube as well as suppression of IEPOX detected by High Resolution Time-Of-Flight Chemical Ionization Mass Spectrometer (ToF-CIMS, Aerodyne Research, Inc.).

Data Collected
Aerosol size and bulk composition were measured in real time by scanning mobility particle sizer (SMPS, TSI Inc.) and aerosol chemical speciation monitor (ACSM, Aerodyne Research, Inc.). Filters (Teflo 47mm, 1 μm poresize, PALL Corp.) and Multi-Plate Sampler samples were collected for offline analyses to gain detailed chemical and morphological information of aerosols.

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

Goals and Anticipated Issues for the Succeeding Reporting Period
We expect to begin calculations of uptake coefficeints from the flow tube reactor data. By varying the axial position of the injector along the flow tube reactor, IEPOX is allowed to interact with aerosols for different period of time, and hence the heterogeneous reaction rate, k_{het}, of IEPOX with aerosols can be calculated by subtracting IEPOX loss rate to the wall, k_{wall}, from the total loss rate, k_{total}, i.e.,

$$k_{het} = k_{total} - k_{wall} \qquad (1)$$

After correcting k_{het} for non-plug flow condition, the uptake coefficient, γ, is calculated by

$$\gamma = \frac{4k_{het}}{S_a\omega} \qquad (2)$$

where Sa is the total surface area of the sulfate aerosols and ω is the mean molecular speed of gaseous IEPOX molecule in the air.

Detailed Analysis of the Progress of the Task Order to Date
We are now on schedule.

Task 3 Implementation in a regulatory air quality model

Preliminary Analysis
We have produced results from our CMAQ-BOX model simulations and are now QA those data. In addition, we have collected the Look Rock Site observational data from the SOAS campaign for a model performance evaluation.

Data Collected
Produced modeling output from a box model to predict the formation of IEPOX-SOA.

Identify Problems or Issues Encountered and Proposed Solutions or Adjustments
In our QA tests, we found several discrepancies in our model output compared with data found in the peer reviewed literature. We have contacted the corresponding author and are adjusting our methodology.

Goals and Anticipated Issues for the Succeeding Reporting Period
We will complete our QA tests to ensure a robust installation of our CMAQ-Box model.

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
Jason Surratt