

## AQRP Monthly Technical Report

<b>PROJECT TITLE</b>	<b>Update and evaluation of model algorithms needed to predict particulate matter from isoprene</b>	<b>PROJECT #</b>	14-003
<b>PROJECT PARTICIPANTS</b>	UNC-CH	<b>DATE SUBMITTED</b>	8/12/2014
<b>REPORTING PERIOD</b>	<b>From:</b> July 1, 2014 <b>To:</b> July 30, 2014	<b>REPORT #</b>	3

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**

*1. Integration of Gas-Phase Epoxide Formation and Subsequent SOA Formation into UNC MORPHO Box Model*

### **Preliminary Analysis**

This month we have simulated using the SAPRAC07TC chemical mechanism our characterization experiments. We have analyzed these simulations and decided on wall reaction rate constants.

We have continued our implementation of the multiphase chemistry of isoprene-derived epoxides. In the past month we have been debugging and refining the box model which simulates the uptake of gaseous IEPOX onto an aerosol of variable acidity, temperature, and relative humidity. In particular, we have implemented a time stepping algorithm that finds a time step that is small enough to keep the solution error within a particular tolerance while keeping it large enough so that the solution is found within a reasonable amount of computing time. Additionally, we have corrected errors in the code related to wall loss calculations.

### **Data Collected**

We have generated simulations necessary for the wall chemistry of our chamber. We have also generated QA data for the multiphase box model.

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

We had performance issues with the characterization runs that have been linked to incorrect actinic flux files. These files have been corrected and made model performance more consistent. There some debugging errors we had to deal with in the box model implementation.

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

We will continue to test individual portions of our box model code for error. We will also verify that all portions are working together by checking the solution to one time step given a set of initial conditions.

We will use the QA code to model five different IEPOX uptake experiments where aerosols of varying composition and relative humidity were injected into a chamber and gaseous IEPOX was injected and the resulting aerosol phase components of the IEPOX products were measured. We plan to compare the final measured concentrations of these aerosol species to the model using different proposed rate constants for the acid-catalyzed ring opening reactions.

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

We are finishing the development of the box model needed for the rest of the project. This task is progressing as expected.

## **Detailed Accomplishments by Task**

### *2. Synthesis of Isoprene-derived Epoxides and Known SOA Tracers*

## **Preliminary Analysis**

We have completed our discussions with Dr. Avram Gold concerning synthesis protocols. As a result of these meetings we have finalized the synthesis protocols for SOA constituents and placed them on schedule.

## **Data Collected**

We have ordered starting materials for concerning synthesis of SOA constituents.

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

None

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

Finalize synthesis protocols for SOA constituents and place on schedule.

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

Given the synthesis protocol in timing we are confident this task being completed in time for our experiments.

## **Detailed Accomplishments by Task**

### *3. Indoor Chamber Experiments Generating SOA Formation Directly from Isoprene-Derived Epoxides*

**Preliminary Analysis**

We continue our preparation of our UNC indoor 10-m<sup>3</sup> flexible Teflon chamber for use in this project. We have also used the month to train students, prepared our teflon filters, and calibrated our GC/MS, IC, CIMS, and LC/DAD-ESI-QTOFMS instruments. Finally, we have proposed a experimental plan and placed experiments on the calendar.

**Data Collected**

We have collected publications and scoped out materials needed for experiments.

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

N/A

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

We expect the next 2-3 months will yield enough experimental data to evaluate by the model. These will include wall-loss experiments (including for IEPOX and MAE), as well as actual experiments outlined in the work plan.

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

We are currently on schedule to complete this task in time allocated.

**Detailed Accomplishments by Task**

*4. Modeling of Isoprene-derived SOA Formation From Environmental Simulation Chambers*

**Preliminary Analysis**

N/A

**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**

N/A

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

N/A

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