# AQRP Monthly Technical Report

| PROJECT TITLE | Update and evaluation of model algorithms needed to predict particulate matter from isoprene | PROJECT # | 14-003 |
|---|---|---|---|
| PROJECT PARTICIPANTS | UNC-CH | DATE SUBMITTED | 7/8/2014 |
| REPORTING PERIOD | From: June 1, 2014<br>To: June 30, 2014 | REPORT # | 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 15th 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**
We have begun gathering the data concerning the SAPAC07TC gas phase chemical mechanism and initialized the integration into our MORPHO box model. We have consulted with EPA scientists to ensure we have the latest version of the chemical mechanism. We have also readied our modeling files for simulating our characterization experiments. These simulations will be used to fix the wall reaction rate constants and is needed for future simulations of experiments.

We have begun implementation of the multiphase chemistry of isoprene-derived epoxides. We have spent the month reviewing the underlying science and formulating a plan for implementation. We are also reviewing whether to code these updates separately using the python programming language or fully integrate into MORPHO. We are also investigating the use of ISOROPIA for calculating some of the parameters needed for the implementation.

**Data Collected**
We have collected reaction files needed to build the SAPRAC07TC chemical mechanism. We have also processed our characterization experiments and began compiling existing isoprene experiments.

**Identify Problems or Issues Encountered and Proposed Solutions or Adjustments**
We have to ensure that the same chemical reactions used in the research version of CMAQ were used in the MORPHO model. This was solved through interactions with EPA scientists. We also had issues locating correct versions of actinic flux files. File content investigations and discussions with former MORPHO users clarified the correct versions to use.

**Goals and Anticipated Issues for the Succeeding Reporting Period**
We will fix wall parameters analyzing results from characterization experiment simulations.

**Detailed Analysis of the Progress of the Task Order to Date**
We have begun the process of setting up 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 begun meeting with Dr. Avram Gold to review synthesis protocols and begin discussing scheduling when we would like the Epoxides ready for our experiments. We have now synthesized both IEPOX and MAE and have done some preliminary calibrations with our chemical ionization mass spectrometer (CIMS), which detects these epoxides in real- time from our chamber experiment.  These data are presented below in Task 2.  For the SOA constituents, the synthesis will be conducted over the next month.

**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 have completed maintenance and preparation of our UNC indoor 10-$m^3$ 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.

**Data Collected**

As an example of calibrations performed on the chamber, we have injected known quantities of both synthetic IEPOX and MAE into our indoor 10-m3 chamber for calibration of the CIMS. The CIMS calibrations are needed in order to carefully track and measure IEPOX and MAE, which are the DIRECT precursors to SOA. Figure 1 below shows our IEPOX (left panel) and MAE (right panel) calibrations obtained from measuring known quantities of these synthetic standards injected into the chamber by using our CIMS instrument. These results clearly show we are getting a linear response, giving us confidence we will be able to measure these compounds for the actual experiments we will conduct.
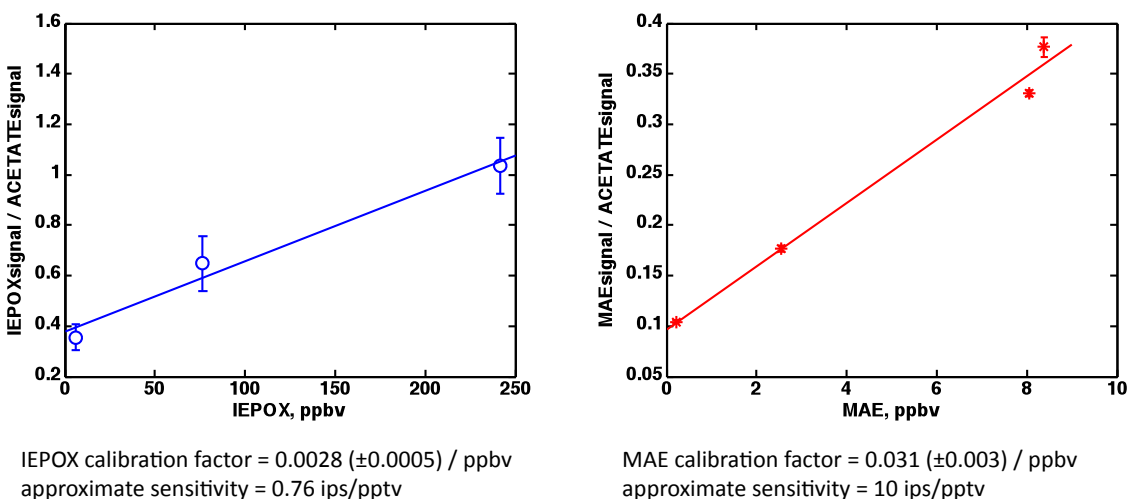


IEPOX calibration factor = 0.0028 (±0.0005) / ppbv
approximate sensitivity = 0.76 ips/pptv

MAE calibration factor = 0.031 (±0.003) / ppbv
approximate sensitivity = 10 ips/pptv

**Figure 1.** Calibrations of IEPOX and MAE standards injected into our 10-m3 indoor Teflon chamber and measured by CIMS.

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

**Goals and Anticipated Issues for the Succeeding Reporting Period**
Based on the progress in the other tasks we will use the next month to settle on a schedule of experiments and have personnel and materials prepared. 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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Submitted to AQRP by:
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Principal Investigator: