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**	3/11/2015
REPORTING PERIOD	**From:** February 1, 2015 **To:** February 28, 2015	**REPORT #**	9

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.

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

Preliminary Analysis
We are confident in the QA/QC testing of the algorithms for the predicted uptake of gaseous IEPOX onto an aerosol of variable acidity, temperature, and relative humidity.

Data Collected
We have generated simulations necessary for QA of data from the model including the predicted bulk SOA formation in our indoor chamber using reactive uptake coefficients we recently derived in flow tube studies (Gaston et al., 2014, ES&T).

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

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

Preliminary Analysis
We have completed all syntheses needed for the project including dealing with the impurity of the organosulfate standards.

Data Collected

QA/QC data verifying synthesis.

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

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

Preliminary Analysis
Our experimental plan is listed in Table 1. In the month of February we continued to conduct experiments listed in Table 1.

Table 1. Indoor experiments to be conducted at UNC.

Expt. #	Epoxide	[Epoxide] (ppb)	Seed Aerosol Type	Initial Seed Aerosol ($\mu g/m^3$)	RH (%)	T (°C)
1	IEPOX	300	$(NH_4)_2SO_4$	~20-30	~50-60	~20-25
2		300	$(NH_4)_2SO_4 + H_2SO_4$	~20-30	~50-60	~20-25
3	MAE	300	$(NH_4)_2SO_4$	~20-30	~50-60	~20-25
4		300	$(NH_4)_2SO_4 + H_2SO_4$	~20-30	~50-60	~20-25
5	none		$(NH_4)_2SO_4$	~20-30	~50-60	~20-25
6	none		$(NH_4)_2SO_4 + H_2SO_4$	~20-30	~50-60	~20-25
7	IEPOX	300	none	none	~50-60	~20-25
8	MAE	300	none	none	~50-60	~20-25

0.6 M (NH4)2SO4 + 0.6 M H2SO4

Data Collected
We continue to collect, process, and quality assure our data for completed experiments. Some of this data has been released for preliminary modeling as described in the next task.

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 1-2 months will yield enough experimental data to evaluate with the model. This will mean completing all experiments outlined in Table 1.

Detailed Analysis of the Progress of the Task Order to Date
We are currently on schedule to complete this task in time allocated.

Task

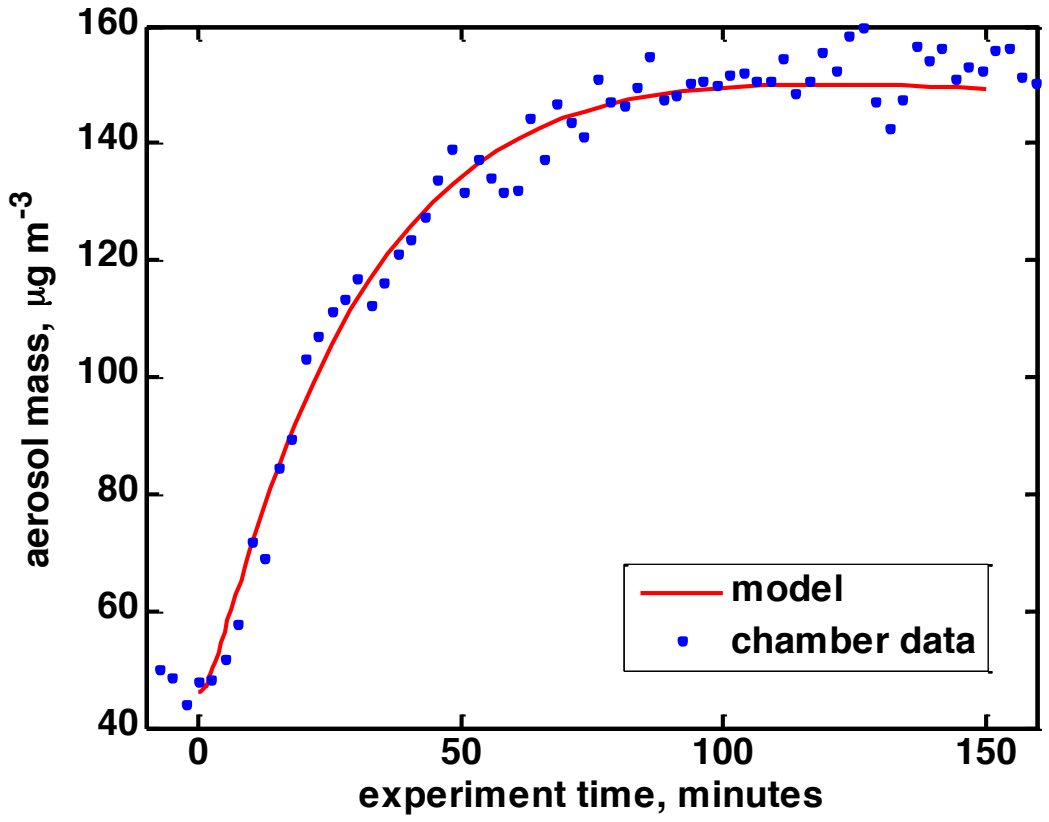
4. Modeling of Isoprene-derived SOA Formation From Environmental Simulation Chambers

Preliminary Analysis

We have designed a model to explicitly simulate both gas- and aqueous- phase reactions that lead to SOA from IEPOX heterogeneous reactions. We have just completed our first test of this model using data from an IEPOX-SOA experiment with ammonium sulfate seed aerosol doped with sulfuric acid. This experiment was completed as part of task 3.

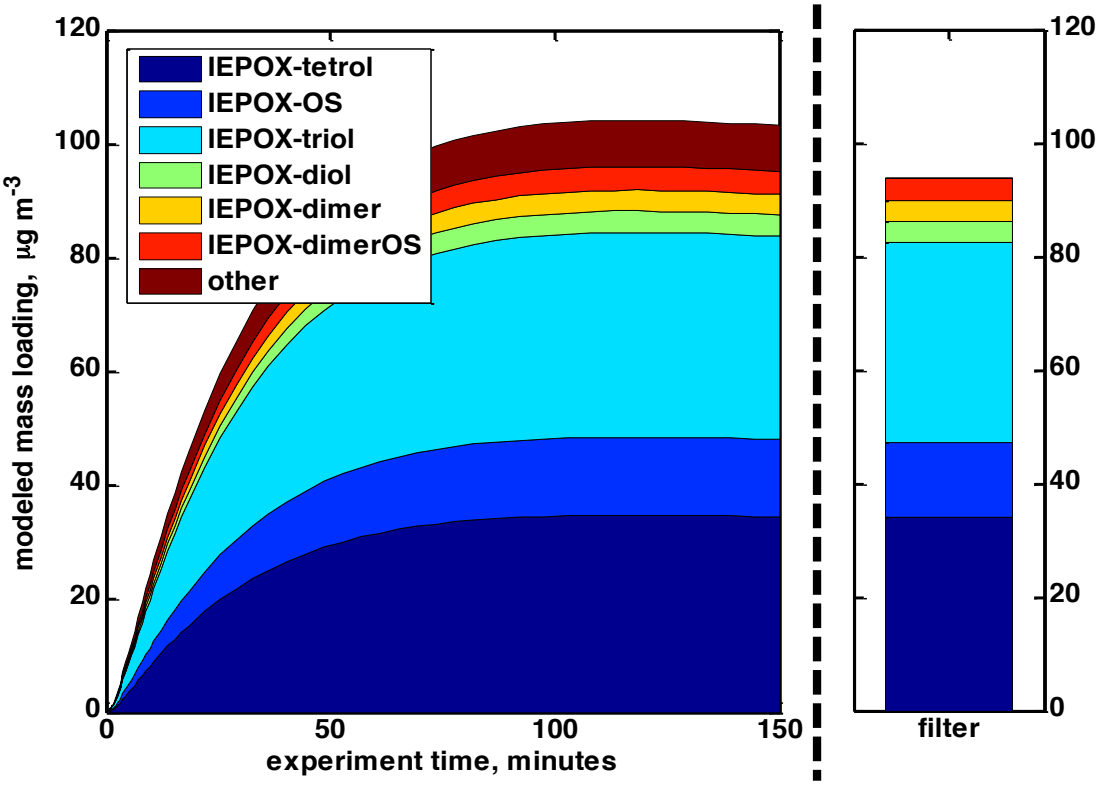
Data Collected

As shown in the following figure we predicted (red line) the change in chamber-measured aerosol mass loadings (shown as blue dots). The model SOA mass growth is obtained from heterogeneous IEPOX uptake constrained by flow reactor measurements of the gas-aerosol reaction probability for the seed aerosol. The resulting aerosol-phase IEPOX then reacts with the aqueous aerosol constituents to form the SOA-tracers that contribute to the modeled aerosol mass loadings.



Using collected filters we are also able to evaluate the model's ability to predict IEPOX-SOA tracers. The figure below shows both the model predicted and filter speciated SOA tracers. On the right we show the measured tracer mass loadings obtained from offline analysis of filters collected during the SOA chamber experiment. The modeled SOA tracer loadings are constrained by these filter measurements. We also constrain the aqueous-phase reaction rate constants for IEPOX tetrol and IEPOX organosulfate formation as these have been measured for

bulk solutions. Given these constraints we vary the remaining aqueous-phase reaction rate constants until the modeled SOA tracer loadings match those of the filter measurements. In this way we obtain an estimate of the SOA tracer formation aqueous-phase reaction rate constants that have yet to be measured for bulk solutions. The SOA tracers termed "other" represent the remaining SOA mass that is not captured by the offline filter measurements.



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

Goals and Anticipated Issues for the Succeeding Reporting Period
We will continue to simulate experiments as they become available from Task 3.

Detailed Analysis of the Progress of the Task Order to Date
We are currently on schedule to complete this task in time allocated.

Submitted to AQRP by:
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Principal Investigator: