

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	10/8/2014
REPORTING PERIOD	From: September 1, 2014 To: September 30, 2014	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.

Task

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

Preliminary Analysis

This month we have completed our implementation of a modeling framework that can predict the multiphase chemistry of isoprene-derived epoxides. 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 SOA formation. We have also generated QA 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). We are finalizing these plots and will include in the following report.

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 test the entire box model to verify that all portions are working together. We will use the QA code to model experiments listed in the Table 1. 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.

Table 1. Indoor experiments to be conducted at UNC.

Expt. #	[Epoxide]		Initial Seed		RH	
	Epoxide	(ppb)	Seed Aerosol Type	Aerosol ($\mu\text{g}/\text{m}^3$)	(%)	T ($^{\circ}\text{C}$)
1	IEPOX	300	$(\text{NH}_4)_2\text{SO}_4$	~20-30	~50-60	~20-25
2		300	$(\text{NH}_4)_2\text{SO}_4 + \text{H}_2\text{SO}_4$	~20-30	~50-60	~20-25
3	MAE	300	$(\text{NH}_4)_2\text{SO}_4$	~20-30	~50-60	~20-25
4		300	$(\text{NH}_4)_2\text{SO}_4 + \text{H}_2\text{SO}_4$	~20-30	~50-60	~20-25
5	none		$(\text{NH}_4)_2\text{SO}_4$	~20-30	~50-60	~20-25
6	none		$(\text{NH}_4)_2\text{SO}_4 + \text{H}_2\text{SO}_4$	~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 $(\text{NH}_4)_2\text{SO}_4 + 0.6 \text{ M H}_2\text{SO}_4$

Detailed Analysis of the Progress of the Task Order to Date

We will continue development of the box model to include more speciated products that can be used for performance evaluation. This task is progressing as expected.

Task

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

Preliminary Analysis

We have completed all syntheses needed for the project.

Data Collected

QA/QC data verifying synthesis.

Identify Problems or Issues Encountered and Proposed Solutions or Adjustments

There are some purification issues in the synthesis of the organosulfate standards. These are being addressed and methods have been proposed.

Goals and Anticipated Issues for the Succeeding Reporting Period

We hope to have a purified organosulfate standard.

Detailed Analysis of the Progress of the Task Order to Date

We are confident that this task will be completed in time.

Task

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

Preliminary Analysis

Our experimental plan is listed in Table 1. We continued to complete more experiments.

Data Collected

We have collected data for completed 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 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

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

Submitted to AQRP by:
William Vizquete

Principal Investigator: