

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	1/8/2015
REPORTING PERIOD	From: December 1, 2014 To: December 31, 2014	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.

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 December we had limited availability for experiments due to holidays. Nevertheless we made some progress and will continue to conduct experiments in January.

Table 1. Indoor experiments to be conducted at UNC.

Expt. #	[Epoxide]		Seed Aerosol Type	Initial Seed Aerosol ($\mu\text{g}/\text{m}^3$)	RH	
	Epoxide	(ppb)			(%)	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 $(\text{NH}_4)_2\text{SO}_4 + 0.6 \text{ M } \text{H}_2\text{SO}_4$

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 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 focused in December in submitting a manuscript describing our first modeling analysis used to constrain two uncertain parameters central to secondary organic aerosol (SOA) formation from isoprene-derived epoxides: (1) the rate of epoxide heterogeneous reaction with the particle phase and (2) the molar fraction of uptaken epoxides that go on to contribute to the SOA burden – the SOA yield (α_{SOA}).

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 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:
William Vizquete

Principal Investigator: