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**	6/5/2015
REPORTING PERIOD	**From:** May 1, 2015 **To:** May 30, 2015	**REPORT #**	12

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
We have completed the 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 have completed the collection, processing, and quality assurance our data from the completed experiments.

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

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

Preliminary Analysis

We have completed our chemical box model simulations that explicitly predict the gas- and aqueous-phase reactions during chamber experiments of SOA growth from IEPOX uptake onto acidic sulfate aerosol. Specifically, the model is constrained by recent measurements of the IEPOX reactive uptake coefficient (Gaston et al., 2014; Riedel et al., 2015), the aforementioned experimentally obtained aqueous-phase rate constants (Eddingsaas et al., 2010), chamber-measured aerosol mass and surface area concentrations, aerosol thermodynamic model calculations (E-AIM III) (Wexler and Clegg, 2002), and offline filter measurements of SOA of a number of the aforementioned tracers. Figure 1 shows a tracer-specific model simulation and the corresponding offline filter measurements from the chamber experiment. Through the use of offline filter measurements collected during the chamber experiments, we are able to place estimates on the tracer formation reaction rate constants that have yet to be measured for bulk solutions. By varying the aqueous-phase reaction rate constants in the model that lack experimental constraints until the modeled SOA tracer mass loadings closely match those of the filter measurements we are able to constrain the kinetics of the aerosol-phase species that have been quantified through offline techniques but lack formation rate information. Additionally, those species that are not quantified through filter analyses, which we term “other SOA”, are also examined and a preliminary formation rate constant for the sum of those species can be obtained.

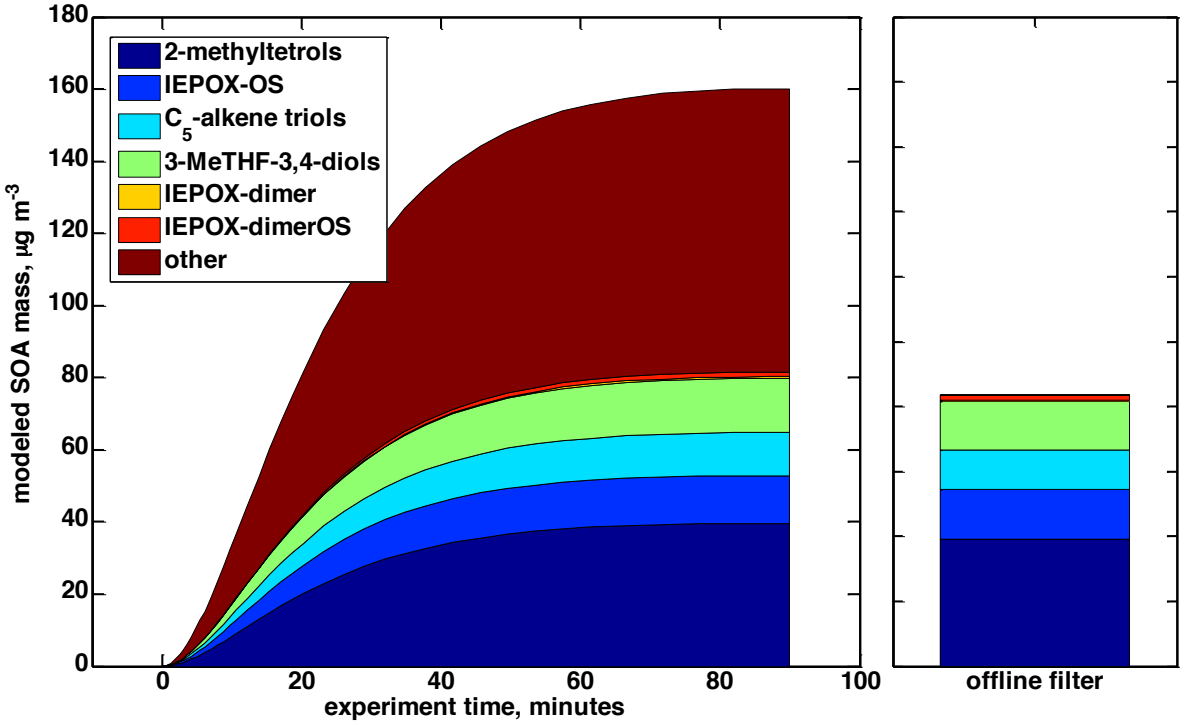

Figure 1: Model simulation of speciated SOA growth during a chamber experiment (left panel). Corresponding filter measurements during the chamber experiment (right panel). "other SOA" represents tracers not quantified by the filter analyses.

Eddingsaas, N. C., VanderVelde, D. G., and Wennberg, P. O.: Kinetics and Products of the Acid-Catalyzed Ring-Opening of Atmospherically Relevant Butyl Epoxy Alcohols, The Journal of Physical Chemistry A, 114, 8106-8113, doi: 10.1021/jp103907c, 2010.

Gaston, C. J., Riedel, T. P., Zhang, Z., Gold, A., Surratt, J. D., and Thornton, J. A.: Reactive Uptake of an Isoprene-Derived Epoxydiol to Submicron Aerosol Particles, Environmental Science & Technology, 48, 11178-11186, doi: 10.1021/es5034266, 2014.

Riedel, T. P., Lin, Y.-H., Budisulistiorini, S. H., Gaston, C. J., Thornton, J. A., Zhang, Z., Vizuete, W., Gold, A., and Surratt, J. D.: Heterogeneous Reactions of Isoprene-Derived Epoxides: Reaction Probabilities and Molar Secondary Organic Aerosol Yield Estimates, Environmental Science & Technology Letters, 2, 38-42, doi: 10.1021/ez500406f, 2015.

Wexler, A. S., and Clegg, S. L.: Atmospheric aerosol models for systems including the ions H^+, NH_4^+, Na^+, SO_4^{2-}, NO_3^-,Cl^-, Br^-, and H_2O, Journal of Geophysical Research-Atmospheres, 107, doi: 10.1029/2001jd000451, 2002.

Data Collected

We have processed and quality assured the new modeling data.

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

Goals and Anticipated Issues for the Succeeding Reporting Period
We will focus our efforts on writing up these recent results in a manuscript.

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 Vizuete

Principal Investigator: