Scope of Work For

Project #16-031
Project Title
Condensed Chemical Mechanisms for Ozone and Particulate Matter Incorporating the Latest in
Isoprene Chemistry

Prepared for

Air Quality Research Program (AQRP)
The University of Texas at Austin

By

William Vizuete, Jason Surratt
University of North Carolina at Chapel Hill

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QA Requirements: Audits of Data Quality: 10% Required
Report of QA Findings: Required in Final Report

NOTE: The workplan package consists of three independent documents: Scope of Work, Quality Assurance Project Plan (QAPP), and budget and justification.

Approvals

This Scope of Work was approved electronically on **October 13, 2016** by Elena McDonald-Buller, The University of Texas at Austin

Elena McDonald-Buller
Project Manager, Texas Air Quality Research Program

This Scope of Work was recommended electronically on **October 17, 2016** by Jim Price, Texas Commission on Environmental Quality

Jim Price
Project Liaison, Texas Commission on Environmental Quality

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1.0 Abstract

Isoprene, the most emitted non-methane hydrocarbon on the planet, is known to influence ozone (O_3) formation in Houston, Texas. Eastern Texas and northern Louisiana feature some of the largest biogenic emission sources of isoprene in the United States. It is also now known that the photochemical oxidation of isoprene, when mixed with anthropogenic emissions from urban areas like those found in Houston, can produce significant yields of fine particulate matter ($PM_{2.5}$) through acid-catalyzed multiphase chemistry of isoprene epoxydiols (IEPOX) that leads to secondary organic aerosol (SOA) formation. Next-generation regulatory models in Houston will attempt to capture this recent discovery even though there exists great uncertainty in both gas-phase isoprene oxidation and SOA formation chemistry. This work will produce a fully updated condensed gas-phase mechanism based on SAPRC-07 and PM formation parameters suitable for use in a regulatory air quality model. The updated parameters will be evaluated against an archive of UNC smog chamber experiments, including new isoprene SOA experiments that investigate the effect of organic coatings/mixtures on the acid-catalyzed multiphase chemistry of IEPOX. Our previously funded Air Quality Research Program (AQRP) work has directly derived the multiphase kinetics of IEPOX only on pure inorganic aerosols. In the atmosphere, however, IEPOX will more likely encounter mixed particles containing both pre-existing organics and acidic sulfate. As a result, there is a need to constrain the impact of pre-existing organics within acidic sulfate aerosol on the kinetics of IEPOX multiphase chemistry. We will also produce a regulatory air quality modeling episode focused on Houston to test these new updates in a simulated urban environment. This work directly addresses the stated priority area of improving the understanding of O_3 and PM formation and the interaction with PM precursors. Further, the regulatory air quality modeling system developed by this work can begin to address the stated priority of quantifying the impacts of uncertainty due to the treatment of atmospheric chemical processes by condensed models.

2.0 Background

Isoprene (2-methyl-1, 3-butadiene, C_5H_8) is the most abundant non-methane hydrocarbon emitted from vegetation[1] and has a significant impact on atmospheric chemistry. Isoprene is known to influence ground-level ozone (O_3) formation in urban areas rich with biogenic emissions[2,3]. **Recently, it has been discovered that the formation of secondary organic aerosol (SOA) from photochemical oxidation of isoprene represents a significant source of fine aerosol mass ($PM_{2.5}$)[4,5].** Measurements have shown this to be especially true in the southeastern United States during the summer[6-11] where isoprene emissions approach those of Eastern Texas. Epoxides formed from isoprene oxidation have been shown to be critical precursors of isoprene-derived SOA[12,13]. Isoprene epoxydiols (IEPOX) and methacrylic acid epoxide (MAE), as shown in Figure 1, have the capability of producing SOA through acid-catalyzed reactive uptake (or multiphase chemistry) to atmospheric $PM_{2.5}$[11]. Subsequent condensed-phase (or multiphase) reactions form SOA constituents "tracer" species

(organosulfates, 2-methyltetrols, C₅-alkene triols, 2-methylglyceric acid, oligomers, and brown carbon) that contribute to the SOA burden[14,15].

Current understanding of the full isoprene SOA formation mechanism is shown in Figure 1[13,15-18]. IEPOX and MAE, and more recently hydroxymethyl-methyl- -lactone (HMML)[19] have been identified as direct precursors to isoprene SOA formation. **The formation of SOA from these precursors is heavily affected by controllable anthropogenic emissions such as oxides of nitrogen (NOx) and sulfur dioxide (SO₂).** Atmospheric oxidation of SO₂ contributes to particle acidity, which enhances isoprene SOA formation through acid-catalyzed reactive uptake and multiphase chemistry of IEPOX and MAE,[15,17,20-22] while NOx determines whether the oxidation pathway leading to IEPOX or MAE predominates.[17,18,23] Recent work has shown that the IEPOX pathway dominates
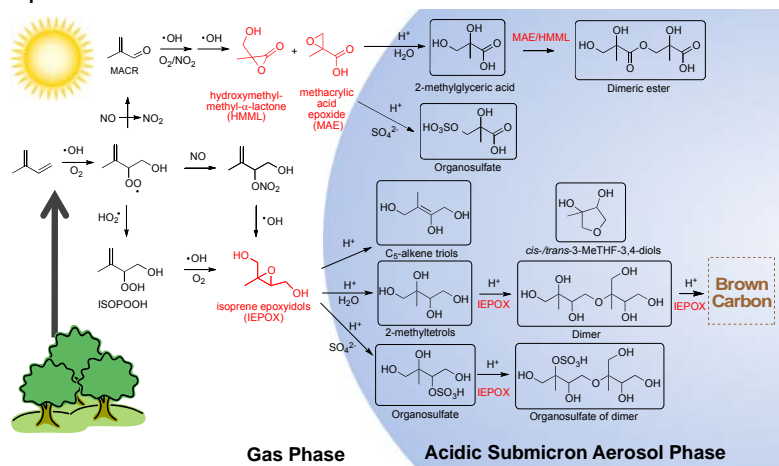

Figure 1. Acid-catalyzed multiphase chemical mechanism of isoprene-derived epoxides leading to SOA formation from isoprene oxidation under low- and high-NOₓ conditions. Aerosol phase components shown in this figure have been observed in both lab-generated and ambient aerosols.

SOA production in the southern U.S., even in urban areas[6,9,24]. This is due to the fact that the IEPOX pathway in Figure 1 is more favored in the presence of acidic sulfate aerosol; where as wet acidic aerosol can actually suppress the high-NOₓ pathway (HMML and MAE), as recently demonstrated by Nguyen et al, 2015. Globally, it has been recently demonstrated that multiphase chemistry of IEPOX accounts for up to 33% of organic aerosol mass in rural and urban areas where isoprene emissions combine with anthropogenic pollutants[24].

With previous funding provided by the Air Quality Research Program (AQRP) our team was able to make great strides in our understanding of the chemical processes that produce this source of PM. Our evaluation of two gas-phase chemical mechanisms: the regulatory version of the condensed SAPRC-07[25] and an updated version that included isoprene SOA gas-phase precursors for isoprene SOA[26]. **Our analysis found that the updated SAPRC-07 mechanism produces more O₃ and predicts an earlier nitrous oxide (NO)/nitrous dioxide (NO₂) crossover time than SAPRC-07 for all chamber experiments[27].** Overall, the updated mechanism reacts more volatile organic compounds (VOCs) due to a more explicit representation of isoprene oxidation products that increases subsequent hydroxyl radical (OH) formation[27]. The updated mechanism also increases NO₂ recycling from nitrogen termination species, which accounts for

the increase in the afternoon O_3 peak concentrations in the lower-NO_X experiments. This data suggests more work is needed to balance the production of radical and oxidation species to improve O_3 chemistry while maintaining explicit gas-phase precursors for isoprene SOA.

Through AQRP funding we have also generated new experimental data that quantitatively measures the reactive uptake of two predominant isoprene-derived gas-phase intermediates (IEPOX and MAE, shown in Figure 1) to pure inorganic aerosols of varying composition and aerosol acidity[28,29]. **These new fundamental aerosol measurements provide, for the first time, the data needed to directly evaluate the aerosol-phase processes in a regulatory air quality model.** The explicit chemistry shown in Figure 1 is starting to be incorporated into EPA's CMAQ model, however, in this version of EPA's air quality model it only assumes multiphase chemistry in pure inorganic aerosols (i.e., acidic sulfate aerosols). There remains a critical need for further experiments to determine the effect of pre-existing organic mixtures/coatings within inorganic aerosols on multiphase chemistry of isoprene-derived epoxides, especially for IEPOX since it appears to dominate isoprene SOA in urban areas of the southern U.S.

Given the location of Houston, isoprene oxidation chemistry is critical for accurate model predictions of O_3 and PM. Although our recent publications provide exciting new data to help constrain these important parameters, work is still needed prior to its use in a regulatory model.

3.0 Objectives

The proposed work will make full use of our previous AQRP project, and with the new proposed experimental data, we will be able to provide the most state of the science estimate for isoprene derived SOA parameters and gas-phase reactions. This work directly addresses the stated priority area of improving the understanding of O_3 and PM formation and the interaction with PM precursors. The gas-phase mechanism created here will produce critical PM precursors and yet will be relatively unchanged in terms of ozone chemistry. The PM rate constant data is needed to help modelers decide whether the effects of organic coatings/mixtures are needed to include with acidic sulfate aerosol. Preliminary laboratory data presented within Gaston et al. 2014[21] using a single-component organic molecule mixed within acidic sulfate aerosol suggests that this effect could be quite dramatic. These best estimates are also implemented in a regulatory model to provide a preliminary quantification of the relative importance of this uncertainty to other model processes. This can begin to address the stated priority of quantifying the impacts of uncertainty due to the treatment of atmospheric chemical processes by condensed models. It is beyond the scope of this project to produce an official chemical mechanism suitable for regulatory applications, but this work provides a start and should be continued with evaluations with other chambers to ensure against experimental bias.

4.0 Task Descriptions

Task 1 Updated SAPRC-07 and Aerosol Module for Isoprene Oxidation

Condensed mechanisms such as the condensed versions of SAPRC-07[25,30-33] used in regulatory air quality models have parameters that are highly tuned and any changes may upset the delicate balance of radical and O_3 chemistry. Instead of adding new reactions to this condensed mechanism, we propose to make additions to the more explicit version of SAPRC-07 mechanism and then evaluate against smog chamber data with the goal of replicating the original model performance[32,33]. Once satisfied with the model performance, we will then begin the methodic process of producing a condensed version of the mechanism suitable for use in a regional scale model. This is the same method used by UC-Riverside in the development of the condensed version of SAPRC-07 currently used in the Community Modeling and Analysis (CMAQ) model[34].

Quarter	1	2	3	4
Task 1	■	■		
Task 2	■	■		
Task 3			■	■
Final Report				■

Figure 2. Timeline to complete the proposed tasks.

Condensing explicit mechanisms requires the integration of data from measurements and a kinetics model. For this work the Morphocule kinetics simulation software (Morpho) will simulate all archived and new (Task 4.2) UNC smog chamber experiments. The software also includes simulations of experiments from Caltech chambers and the large outdoor European (EUPHORE) chambers[35]. The system can readily incorporate any new experimental data sources as they become available and the software already has the capability to track the source and fate of all species within the mechanism. The Morpho system can also interface with our process analysis software allowing us to generate radical and nitrogen budget data as shown in Table 1[36-41]. This data will provide information needed to guide the formulation of the mechanism. We have already demonstrated our ability to conduct this type of detailed analysis as shown in a recent publication we evaluated seven chemical mechanisms across more than 70 experiments and provided a detailed statistical analysis[42]. This software and database infrastructure is built and ready for this proposed task.

Table 1. Example of process analysis output quantifying radical initiation, radical propagation, and major oxidation reactions.

Radical initiation	
OH	6.16
HO_2	7.46
RO_2	11.70
Radical propagation	
OH	49.84
HO_2	27.52
other HO_2	2.58
RO_2	9.00
Oxidation reactions	
HC/CO + OH	44.36
$NO \rightarrow NO_2$	80.58
Ox production	84.25

We will first use the most explicit version of SAPRC-07 and add the necessary isoprene oxidation reactions. Using Morpho we will then evaluate changes from the original explicit SAPRC-07 mechanism in radical budget, nitrogen distribution, OH/NO cycling, and other processes that influence O_3 formation. Once satisfied with maintaining model performance as closely as the base explicit mechanism we will then follow a "hierarchy of species" approach originally developed by Gery et al, 1989 to condense our updated explicit chemical mechanism[43]. We will use the Morpho model to first simulate chamber experiments with simple inorganic NOx and hydrogen oxide radical chemistry. Once replication of observations is found the mechanism parameters are fixed for those reactions. The next step is to simulate an experiment with the addition of formaldehyde and then the addition of a single VOC species like methane or ethene. At every step once model performance is deemed to adequately replicate the original condensed SAPRC-07 mechanism the chemical parameters will be fixed and then proceed with increasing complexity in chemistry. Throughout this process we will follow as many of the assumptions and condensations made by UC-Riverside involving the lumping or removal of species[30-33].

The expectation is that the majority of the mechanism will remain unchanged, but this technique will very quickly identify the critical reactions that our analysis will focus on. We anticipate this focus will be on the production of intermediate aldehydes in the isoprene oxidation reactions and the recycling of nitrogen from reservoir species.

In a regulatory air quality model aerosol formation chemistry is commonly parameterized such as with the Odum 2-product parameterization. We have already developed a "stand-alone" code that emulates all parameterized aerosol algorithms found in all regulatory models. This software is integrated with the Morpho gas-phase kinetics model, allowing UNC to replicate the full gas and PM chemistry found in regulatory models. Using this coupled model we can simulate all our gas- and particle-phase chamber data. As demonstrated in our published work we have the ability to efficiently simulate any number of gas-phase and particle phase chemistry in a regulatory framework and analyze in great detail against a large number of chamber experiments[27-29,44,45].

We will first evaluate a SOA module that is currently being used in a regulatory air quality model in conjunction with a SAPRC-07 condensed gas-phase mechanism. For example, in Parikh et al., 2011 we evaluated for implementation both the Odum-type and volatility basis set (VBS)

yield parameterization. As part of this work we will update our software to be consistent with the official CMAQ version 5.1 aerosol algorithms called aero6i that includes parameterizations for SOA production from isoprene oxidation products. This aero6i is compatible only with the SAPRC07tic that includes EPA's latest isoprene oxidation chemistry. We already have integrated that mechanism into our Morpho system. Using our software we will update aerosol parameters based on the results from our AQRP funded work. All evaluations of our aerosol updates will be evaluated by simulating archived and new UNC chamber experiments (Task 4.2). Comparisons will be made with predictions made by using the CMAQ aerosol algorithm aero6i.

Task 1 Deliverables

The parameters produced by this work will be optimized based on our UNC observational set and will substantially reduce uncertainty in those parameters needed for modeling in a regulatory air quality model like those described in Task 3. The schedule for Task 1 deliverables is shown in Section 7.

Task 2 Chamber Experiments: Interplay of Particle-Phase Composition, Phase, and Viscosity on IEPOX Multiphase Chemistry

Due to the importance of reactive uptake (or multiphase chemistry) of IEPOX into fine particles and the prevalence of organic aerosols in the total $PM_{2.5}$ mass, the study of reactive uptake of IEPOX on organic particles and mixed acidic sulfate/organic aerosol needs to be urgently addressed to provide a comprehensive understanding of the formation of isoprene SOA. As stated above, the multiphase chemistry of IEPOX has only been previously studied on pure sulfate aerosols of varying acidities.

There are two major goals of the new experiments proposed here: (1) Determine values of *trans-* -IEPOX (the predominant IEPOX isomer) on (i) pure submicron organic aerosol particles and (ii) submicron organic and inorganic mixed aerosol particles as a function of acidity and particle composition and (2) Identify the molecular composition of the products from the particle phase and any potential differences in composition at various starting aerosols. It should be noted that we will use real-time aerosol mass spectrometry (AMS), specifically our Aerodyne Aerosol Chemical Speciation Monitor (ACSM)[6,10,46,47], to measure the oxygen-to-carbon (O:C) elemental and organic-to-sulfate ($OA:SO_4^{2-}$) ratios. It is important to measure O:C and $OA:SO_4^{2-}$ using the ACSM, as liquid-liquid phase separations within aerosol is highly impacted by the oxidation state (O:C) and $OA:SO_4^{2-}$ ratios of aerosol components[48,49]. In general, previous work has showed that phase separation occurs for O:C < 0.5-0.6 and not for

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O:C ratios above 0.8[49]. In the intermediate regime (0.6-0.8), liquid-phase separation depends on composition and organic functional groups[49].

Synthesis of IEPOX and its Respective SOA Constituents

Required syntheses will be conducted by Prof. Gold and Dr. Zhang from our research team. Our group has published detailed synthetic routes to *trans-* -IEPOX and SOA constituents such as *cis-* and *trans*-3-MeTHF-3,4-diols[50]. Furthermore, other IEPOX-derived SOA constituents have now been synthesized, including the 2-methyltetrols and the IEPOX-derived organosulfates (OS)[10]. All reported syntheses yield products in high purity (> 99%), which be confirmed in this new work by ^{1}H and ^{13}C nuclear magnetic resonance (NMR) spectroscopy as well as by gas chromatography/mass spectrometry equipped with electron ionization (GC/EI-MS) and ultra performance liquid chromatography interfaced to high-resolution quadrupole time-of-flight mass spectrometry equipped with electrospray ionization (UPLC/ESI-HR-QTOFMS).

Chamber Experiments

All experiments will be conducted under dark conditions in our indoor 10-m^3 Teflon smog chamber at the University of North Carolina at Chapel Hill (UNC), as previously described in publications resulting from our last AQRP grant[28,29]. Acidic ammonium sulfate seed aerosol will be injected into the chamber under dry conditions (RH< 5 %) using a custom-built atomizer with an atomizing solution of 0.06M $(NH_4)_2SO_4$ and 0.06M H_2SO_4 until the desired total aerosol mass concentration is achieved (typically 50-100 g m^{-3} in order to provide enough aerosol surface area to outcompete the chamber walls for IEPOX). After acidic sulfate aerosol injection, the chamber will be left static for at least 30 min to ensure that the seed aerosol concentration is stable and uniformly mixed. It is noted that the thermodynamic model, ISORROPIA-II[51-53], will be used to estimate aerosol pH. Inputs for the model include aerosol-phase sulfate, nitrate, and ammonium in µmol m^{-3}, measured by the ACSM as well as RH and temperature obtained from a commercial RH/temperature probe (OM-62, Omega Engineering Inc.). ISORROPIA-II predicted particle hydronium ion concentration per volume of air (H$^+_{air}$, g m^{-3}), aerosol water (LWC, g m^{-3}), and aerosol aqueous phase mass concentration (g m^{-3}). Our aerosol pHs typically range 0-2 in our chamber experiments, which is exactly consistent with recent field observations of aerosol pH[54].

To investigate the impact of organic coatings/mixtures on reactive uptake of IEPOX, stabilized acidified ammonium sulfate aerosol will then be coated by the condensation of oxidized products of either α-pinene (Sigma-Aldrich; > 99%) ozonolysis, OH-initated oxidation of toluene (Sigma-Aldrich; > 99%) (a model aromatic VOC typically most abundant in urban air)[5], or OH-initiated oxidation of dodecane (Sigma-Aldrich) (a model alkane VOC typically quite abundant in urban air) prior to IEPOX injection[55]. The oxidation of these VOCs were selected since they will lead to varying O:C ratios, resulting in varying viscosities of the aerosol mixtures[5]. Since organics

can affect the phase state (viscosity) of pre-existing aerosol, their presence within acidic sulfate aerosol could lower the diffusion rate of gaseous IEPOX and therefore determine whether if it is confined to the surface region of a particle or alternatively can proceed in the interior. As a result, the presence of organics within acidic sulfate aerosol could lower the γs previously measured on pure inorganic aerosols[28]. For α-pinene ozonolysis, approximately 300 ppb of ozone will be added after the acidic sulfate aerosol injection, then 2 or 5 0.15 μL injections of α-pinene will made. Nucleation of α-pinene ozonolysis products is prevented by multiple injections of α-pinene[56]. For OH-initiated oxidation of toluene and dodecane, OH radicals will be formed from the ozonolysis of tetramethylethylene (TME, Matheson) in darkness, as done in previous studies[57-59]; specifically, O_3 (1.4–1.6 ppm) will introduced into the chamber using an O_3 generator (Model L21, Pacific ozone) and followed by addition of a continuous flow of TME (1 $\times$ 10^9 molecule cm^{-3} s^{-1}). Under these conditions we can produce 3–4 $\times$ 10^6 molecule cm^{-3} of OH radicals in our chamber, which is an atmospherically relevant level.

After the acidic sulfate aerosol are coated/mixed with their respective SOA types described above and stabilized (well mixed), IEPOX will then be injected into the chamber for 2 h by passing 4 L min^{-1} of N_2(g) through a glass manifold heated at 60 ºC containing 50–300 μL of a 100 mg mL^{-1} ethyl acetate solution of *trans-* β-IEPOX, the predominant IEPOX isomer[60]. Chamber aerosol number distributions, which will be subsequently converted to total aerosol surface area and volume concentrations, will be measured by a scanning electrical mobility system (SEMS v5.0, Brechtel Manufacturing Inc.– BMI) containing a differential mobility analyzer (DMA, BMI) coupled to a mixing condensation particle counter (MCPC Model 1710, BMI). On completion of IEPOX injection and stabilization of aerosol size distribution, a filter sample will be collected for offline chemical analysis of the chamber-generated SOA. Aerosols will be collected onto 46.2mm Teflon filters (part no.: SF17471, Tisch Scientific) in a stainless-steel filter holder for 2 h at 15 L min^{-1} with a carbon strip denuder (Sunset Labs) upstream of the filter holder. Filters will be stored in 20 mL scintillation vials at -20 ºC prior to extraction and chemical analysis. An iodide-adduct high-resolution time-of-flight chemical ionization mass spectrometer (HR-TOF-CIMS, Aerodyne Research Inc.) will be used to continuously monitor IEPOX gas-phase concentrations as well as oxidation products of α-pinene, toluene, or dodecane[28,61]. Recently, we demonstrated that the Filter Inlet for Gases and AEROsol (FIGAERO) coupled to HR-TOF-CIMS can measure the volatility of IEPOX-derived SOA[62], which will also add in assessing the effect of organic coatings/mixtures on IEPOX uptake. As described in our previous studies[28], IEPOX-derived SOA components will be extracted from filters with high-purity methanol prior to chemical analysis by GC/EI-MS and UPLC/ESI-HR-QTOFMS.

Control experiments will be conducted to determine wall losses of aerosol and of IEPOX. Further, we will conduct uptake experiments of IEPOX on pure organic aerosols derived from α-pinene ozonolysis and OH-initiated oxidations of toluene and dodecane. These experiments will

provide further insights into the affect of organics on IEPOX multiphase chemistry, especially when compared to our previous AQRP work on pure inorganic aerosols and on the newly proposed mixed organic/sulfate aerosol.

Model Simulations: Derive Multiphase Kinetics

Reaction kinetics of SOA generation will be investigated with a zero-dimensional time-dependent chemical box model incorporating explicit aqueous-phase SOA formation from IEPOX[28]. This model was developed with our previous AQRP grant. The model is initialized with the amount of *trans-* -IEPOX added to the injection manifold and the measured aerosol total surface area and mass concentration. By requiring the model output to match the SOA growth and SOA chemical composition due to reactive uptake (multiphase chemistry) of IEPOX onto mixed organic and acidic sulfate aerosol, this will allow us to directly derive the particle-phase reaction rates for individual SOA constituents as well as the overall particle-phase reaction rate for bulk IEPOX-derived SOA.

Task 2 Deliverables

Particle-phase rate constants for IEPOX-derived SOA will be derived for IEPOX uptake onto mixed organic and acidic sulfate aerosol of varying composition, phase, volatility, and viscosity. The schedule for Task 2 deliverables is shown in Section 7.

Task 3 Implementation in a regulatory air quality model

We have chosen a regulatory CMAQ modeling episode already developed by the Environmental Protection Agency (EPA) to explore isoprene oxidation chemistry[63]. EPA
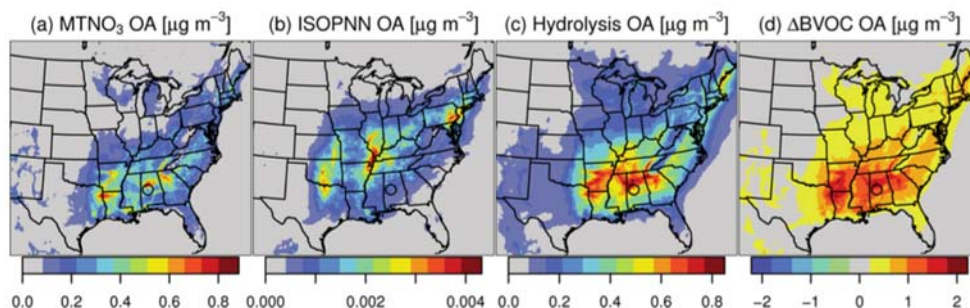

Figure 3. Predicted concentration (a) of monoterpene nitrate SOA, (b) of isoprene nitrate SOA, (c) of SOA from hydrolysis of nitrates, and (d) change in BVOC SOA compared to base CMAQ v5.0.2+ without explicit pON SOA. τ = 3 h pseudohydrolysis (Pye et al. 2015).

developed the CMAQ modeling episode for the horizontal domain shown in Figure 3. The simulation has a 12 km grid resolution over Houston and spans May through June 2013. This episode uses SAPRC07tic and aero6i to predict isoprene oxidation and SOA formation. Details of the implementation, model performance, meteorological inputs, and the emission inventory can be found in Pye et al., 2015. With this modeling platform it is our goal to quantify the changes from our proposed changes (Tasks 4.1-4.2) in the gas and aerosol algorithms relative to this base simulation. Our analysis will look at absolute changes in species concentration and PM

concentrations similar to what is shown in Figure 3. Since CMAQ is process analysis enabled, we will also use UNC process analysis software to quantify changes in radical and nitrogen budgets like those shown in Table 1.

Task 3 Deliverables

This task will produce modeling data quantifying the importance that new isoprene oxidation chemistry has to potentially alter ozone and PM predictions in Houston. The schedule for Task 3 deliverables is shown in Section 7.

Task 4 Project Reporting and Presentation

As specified in Section 7.0 "Deliverables" of this Scope of Work, AQRP requires the regular and timely submission of monthly technical, monthly financial status and quarterly reports as well as an abstract at project initiation and, near the end of the project, submission of the draft final and final reports. Additionally, at least one member of the project team will attend and present at the AQRP data workshop. For each reporting deliverable, one report per project will be submitted (collaborators will not submit separate reports), with the exception of the Financial Status Reports (FSRs). The lead PI (or their designee) will electronically submit each report to both the AQRP and TCEQ liaisons and will follow the State of Texas accessibility requirements as set forth by the Texas State Department of Information Resources. The report templates and accessibility guidelines found on the AQRP website at http://aqrp.ceer.utexas.edu/ will be followed. ****Draft copies of any planned presentations (such as at technical conferences) or manuscripts to be submitted for publication resulting from this project will be provided to both the AQRP and TCEQ liaisons per the Publication/Publicity Guidelines included in Attachment G of the subaward.**** Finally, our team will prepare and submit our final project data and associated metadata to the AQRP archive.

Task 4 Deliverables

Abstract, monthly technical reports, monthly financial status reports, quarterly reports, draft final report, final report, attendance and presentation at AQRP data workshop, submissions of presentations and manuscripts, project data and associated metadata. The schedule for Task 4.4 Deliverables is shown in Section 7.

5.0 Project Participants and Responsibilities

This collaborative project will be conducted under a grant from the Texas Air Quality Research Program with UNC as the lead organization. Dr. William Vizuete of UNC is serving as Principal Investigator with overall responsibility for the research and associated quality assurance. The scientists working on this project and their specific responsibilities are listed in Table 2.

Table 2. Project participants and their responsibilities.

Participant	Project Responsibility
Dr. William Vizuete	Principal Investigator, air quality model guidance, data analysis and reporting; Mechanism development
Dr. Jason Surratt	Mechanism development; Manage smog chamber experiments, data analysis, and reporting
Dr. Avram Gold	Lead organic synthetic efforts, data analysis and reporting
Dr. Zhenfa Zhang	Conduct the synthetic chemical production
UNC Graduate Student	Conduct smog chamber experiments, simulation runs and data analysis

6.0 Timeline

Project Task	2016				2017							
	9	10	11	12	1	2	3	4	5	6	7	8
Submit Work Plan with detailed budget (including Quality Assurance Performance Plan) to AQRP	■											
Task 1- Update SAPRC-07 and Aerosol Module for Isoprene Oxidation	■	■	■	■	■	■						
Task 2- Chamber Experiments: Interplay of Particle-Phase Composition, Phase, and Viscosity on IEPOX Multiphase Chemistry	■	■	■	■	■	■						
Task 3- Implementation in a regulatory air quality model							■	■	■			
Task 4a- Draft Final Report										■		
Task 4b- Final Report acceptable to TX AQRP											■	■

7.0 Deliverables

AQRP requires certain reports to be submitted on a timely basis and at regular intervals. A description of the specific reports to be submitted and their due dates are outlined below. One report per project will be submitted (collaborators will not submit separate reports), with the

exception of the Financial Status Reports (FSRs). The lead PI will submit the reports, unless that responsibility is otherwise delegated with the approval of the Project Manager. All reports will be written in third person and will follow the State of Texas accessibility requirements as set forth by the Texas State Department of Information Resources. Report templates and accessibility guidelines found on the AQRP website at http://aqrp.ceer.utexas.edu/ will be followed.

Abstract: At the beginning of the project, an Abstract will be submitted to the Project Manager for use on the AQRP website. The Abstract will provide a brief description of the planned project activities, and will be written for a non-technical audience.

Abstract Due Date: Wednesday, August 31, 2016

Quarterly Reports: Each Quarterly Report will provide a summary of the project status for each reporting period. It will be submitted to the Project Manager as a Microsoft Word file. It will not exceed 2 pages and will be text only. No cover page is required. This document will be inserted into an AQRP compiled report to the TCEQ.

Quarterly Report Due Dates:

Report	Period Covered	Due Date
Aug2016 Quarterly Report	June, July, August 2016	Wednesday, August 31, 2016
Nov2016 Quarterly Report	September, October, November 2016	Wednesday, November 30, 2016
Feb2017 Quarterly Report	December 2016, January & February 2017	Tuesday, February 28, 2017
May2017 Quarterly Report	March, April, May 2017	Friday, May 31, 2017
Aug2017 Quarterly Report	June, July, August 2017	Thursday, August 31, 2017
Nov2017 Quarterly Report	September, October, November 2017	Thursday, November 30, 2017

Monthly Technical Reports (MTRs): Technical Reports will be submitted monthly to the Project Manager and TCEQ Liaison in Microsoft Word format using the AQRP FY16-17 MTR Template found on the AQRP website.

MTR Due Dates:

Report	Period Covered	Due Date
Aug2016 MTR	Project Start - August 31, 2016	Thursday, September 8, 2016
Sep2016 MTR	September 1 - 30, 2016	Monday, October 10, 2016
Oct2016 MTR	October 1 - 31, 2016	Tuesday, November 8, 2016
Nov2016 MTR	November 1 - 30 2016	Thursday, December 8, 2016
Dec2016 MTR	December 1 - 31, 2016	Monday, January 9, 2017
Jan2017 MTR	January 1 - 31, 2017	Wednesday, February 8, 2017
Feb2017 MTR	February 1 - 28, 2017	Wednesday, March 8, 2017
Mar2017 MTR	March 1 - 31, 2017	Monday, April 10, 2017
Apr2017 MTR	April 1 - 28, 2017	Monday, May 8, 2017
May2017 MTR	May 1 - 31, 2017	Thursday, June 8, 2017
Jun2017 MTR	June 1 - 30, 2017	Monday, July 10, 2017
Jul2017 MTR	July 1 - 31, 2017	Tuesday, August 8, 2017

Financial Status Reports (FSRs): Financial Status Reports will be submitted monthly to the AQRP Grant Manager (Maria Stanzione) by each institution on the project using the AQRP FY16-17 FSR Template found on the AQRP website.

FSR Due Dates:

Report	Period Covered	Due Date
Aug2016 FSR	Project Start - August 31	Thursday, September 15, 2016
Sep2016 FSR	September 1 - 30, 2016	Monday, October 17, 2016
Oct2016 FSR	October 1 - 31, 2016	Tuesday, November 15, 2016
Nov2016 FSR	November 1 - 30 2016	Thursday, December 15, 2016
Dec2016 FSR	December 1 - 31, 2016	Tuesday, January 17, 2017
Jan2017 FSR	January 1 - 31, 2017	Wednesday, February 15, 2017
Feb2017 FSR	February 1 - 28, 2017	Wednesday, March 15, 2017
Mar2017 FSR	March 1 - 31, 2017	Monday, April 17, 2017
Apr2017 FSR	April 1 - 28, 2017	Monday, May 15, 2017
May2017 FSR	May 1 - 31, 2017	Thursday, June 15, 2017
Jun2017 FSR	June 1 - 30, 2017	Monday, July 17, 2017
Jul2017 FSR	July 1 - 31, 2017	Tuesday, August 15, 2017
Aug2017 FSR	August 1 - 31, 2017	Friday, September 15, 2017
FINAL FSR	Final FSR	Monday, October 16, 2017

Draft Final Report: A Draft Final Report will be submitted to the Project Manager and the TCEQ Liaison. It will include an Executive Summary. It will be written in third person and will follow the State of Texas accessibility requirements as set forth by the Texas State Department of Information Resources. It will also include a report of the QA findings.

Draft Final Report Due Date: Tuesday, August 1, 2017

Final Report: A Final Report incorporating comments from the AQRP and TCEQ review of the Draft Final Report will be submitted to the Project Manager and the TCEQ Liaison. It will be written in third person and will follow the State of Texas accessibility requirements as set forth by the Texas State Department of Information Resources.

Final Report Due Date: Thursday, August 31, 2017

Project Data: All project data including but not limited to QA/QC measurement data, metadata, databases, modeling inputs and outputs, etc., will be submitted to the AQRP Project Manager within 30 days of project completion (September 29, 2017). The data will be submitted in a format that will allow AQRP or TCEQ or other outside parties to utilize the information. It will also include a report of the QA findings.

AQRP Workshop: A representative from the project will present at the AQRP Workshop in the first half of August 2017.

Presentations and Publications/Posters: All data and other information developed under this project which is included in **published papers, symposia, presentations, press releases, websites and/or other publications** shall be submitted to the AQRP Project Manager and the TCEQ Liaison per the Publication/Publicity Guidelines included in Attachment G of the Subaward.

8.0 References

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