

Scope of Work For

AQRP Project 17-053

Identifying and Apportioning Ozone Producing Volatile Organic Compounds in Central Texas

Prepared for

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

By

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Aerodyne Research, Inc.

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Version 2

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

Approvals

This Scope of Work was approved electronically on **11/18/2016** by Gary McGaughey, The University of Texas at Austin

Gary McGaughey
Project Manager, Texas Air Quality Research Program

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1.0 Abstract

Aerodyne Research, Inc. will conduct measurements using a mobile laboratory as a portable photochemistry super site to study ozone production and the emission sources that ultimately impact air quality in central Texas. We envision working at locations upwind, downwind and lateral to San Antonio. The suite of instrumentation has been selected to quantify key oxygenated volatile organic carbon species (OVOC) and nitrogen containing species (e.g. alkyl nitrates) to pinpoint and apportion ozone within broad categories of VOC emission sectors. The instrument payload will also directly quantify the instantaneous production rate of ozone to determine whether the chemical regime is NO_x limited or VOC limited. An additional component of this research project will be to characterize emission sources associated with oil and natural gas production in the Eagle Ford Shale play, including active medium to large processing flares, as well as oil and condensate tanks at wellpads.

The project will provide scientific insight into the VOCs that are contributing to the ozone in central Texas. The effectiveness of mitigation strategies will be informed by these results. This work will isolate ozone production due to VOC oxidation from biogenic sources, refinery emissions, emissions from oil producing well pads and emissions from natural gas production. The dataset will inherently contain regional transport of emissions and processed air. The project will quantify local ozone production rates and evaluate the ozone sensitivity regime.

This research project directly responds to two of the ten research priorities identified in the AQRP Strategic Research Plan FY 16-17: 1. Improving the understanding of ozone and particulate matter formation (in central Texas), and 2. Quantifying the local ozone production that impacts the design value (DV) monitors that exceed the NAAQS in central Texas. These research priorities will be addressed by the analysis of data generated by the planned air quality field study in central Texas.

2.0 Background

The Environmental Protection Agency (EPA) designates ozone as a criteria pollutant, with new 2015 standards set at 70 ppb (3-year average of the annual 4th maximum 8-hour daily maximum). The ozone monitor network in San Antonio indicates that the city is on the verge of being out of compliance for federal standards. The EPA monitor at Camp Bullis (C58), shows 14 maximum daily 8-hour averages exceeding 70 ppb since 2015. These exceed the 70 ppb EPA standard that came into effect in 2015, with enforcement of the standard expected to begin soon. The mitigation

strategy is likely to involve curtailing emissions of ozone-producing volatile organic compounds (VOCs) emitted either in the city (for those VOCs that are oxidized rapidly) or further upwind in regions such as the Eagle Ford or in the refineries at Corpus Christi.

Aerodyne Research, Inc. proposes to study emission sources that

influence air quality in central Texas. We will conduct measurements to track and quantify photochemistry with the mobile laboratory operating as a portable *super site*, upwind and downwind of San Antonio. Ultimately, this work will quantify and apportion which emission sources are producing ozone.

Ozone is produced from sunlight, NO_x and VOCs. VOCs are emitted from many different sources. They can be biogenic in origin, like isoprene and other terpenes; they can be oil & gas associated such as propane or various aromatic compounds. Numerous other anthropogenic compounds participate in ozone production chemistry. VOC intermediates can associate with NO_x and leave signature compounds that still retain information about the source. Although parent VOC measurements are very useful, they do not directly indicate the history of ozone formation or its sensitivity to NO_x and VOC emissions. Quantification of unique markers of oxidation, such as speciated oxygenated VOCs and alkyl nitrates, is an intriguing way to

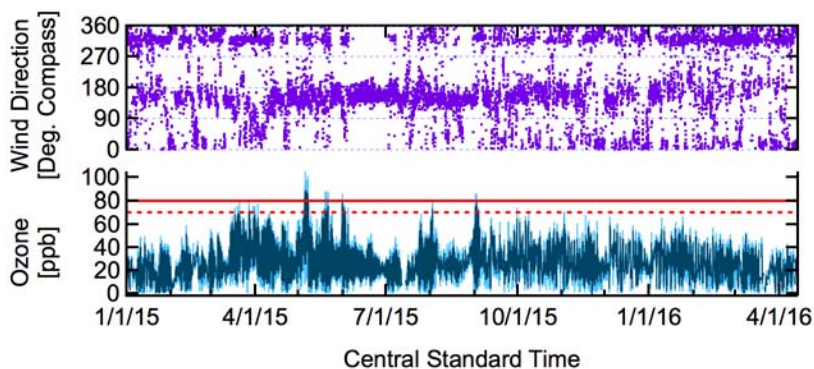


Figure 1. 1-hour ozone measurements from the Camp Bullis monitoring station are shown (pale blue) alongside 8-hour averages (dark blue) and wind direction (purple). EPA ozone limits (red) are shown at 80 ppb (solid, current standard) and 70 ppb (dotted, 2015 standard, yet to be enforced).

apportion ozone formation since they are created at the same time as the ozone is being produced. Additionally, these measurements will be used to ascertain the production rate of ozone, $P(O_3)$, and determine whether it is VOC-limited or NO_x-limited, which provides scientific underpinnings to possible abatement strategies.

In addition to deploying the Aerodyne mobile laboratory as a portable super site with comprehensive gas and particle measurements, we will engage in some focused direct source characterization particular to central Texas. We are actively negotiating with an industry stakeholder to look at *in-use* emissions from a medium to large plant flare. The 2010 TCEQ Flare study [Torres *et al.*, 2012] demonstrated that flares can operate at low destruction and removal efficiencies at “ordinary” levels of air or steam assist. Only a few in-use flares have been characterized [Ezra C. Wood *et al.*, 2012]. The TCEQ flare results, these limited measurements of in-use flares, and related modeling studies [Al-Fadhli *et al.*, 2012] have all indicated that HCHO emissions from flares are not nearly as important as the unburned hydrocarbons, in contrast to studies that have implicated HCHO as a major driver of ozone chemistry in flare plumes [Olaguer, 2012].

Additionally, we will characterize emissions from oil and produced water tanks while in the region. The project will collect a small number of site data to compare with the ambient VOC measurements and what is forecast from current inventory datasets.

3.0 Objectives

The overall objectives of this project are to elucidate the cause of high ozone concentrations in San Antonio and to inform regulatory decisions regarding mitigation procedures using analysis of data from an air quality study in and around San Antonio during May and June of 2017. More detailed objectives are to answer the following science questions:

The work plan describes a field deployment to central Texas in May/June of 2017. The instrument manifest, described elsewhere, has been selected to allow the comprehensive suite to address the following scientific questions:

Individual VOC emission sources (for example, oil production vs biogenic emissions) all participate in ozone production in central Texas. Can examination of the oxidation products and radical termination species (e.g. butanone and alkyl nitrates) that still retain specific parent VOC information be used to apportion the VOC component of regional ozone production?

What is the instantaneous rate of ozone production in central Texas and is it occurring under NO_x-limited or VOC-limited conditions? Coupled with question one, how does this answer and inform potential mitigation strategies?

Can improved characterization of specific industry sector emissions offer insight into the ozone and air quality impact? Do flares, specifically medium- to large-volume process flares in the Eagle Ford, constitute an emission source type not well represented in emission inventories?

3.1 General measurement strategy

We will operate the mobile laboratory at various sites between Corpus Christi and San Antonio. The strategy will be to move the portable supersite to a location that is forecast (based on meteorology) to have needed characteristics to meet the science objectives for 1-3 days into the future. Though forecast conditions will always be changing, the idea is to fully characterize the incoming Gulf air:

through the refinery complex, as it passes through the Eagle Ford, into, and out of San Antonio. The mobile laboratory has the capacity and capability to address the science questions with this strategy. With the assistance of collaborators and the TCEQ, specific locations and logistics will be chosen during the planning stages. It is anticipated, however that some sites with high scientific value, identified either during planning or during the course of the study will not have plug-in power or security available. The mobile laboratory can operate for 48-72 hours using its generators for electrical power.

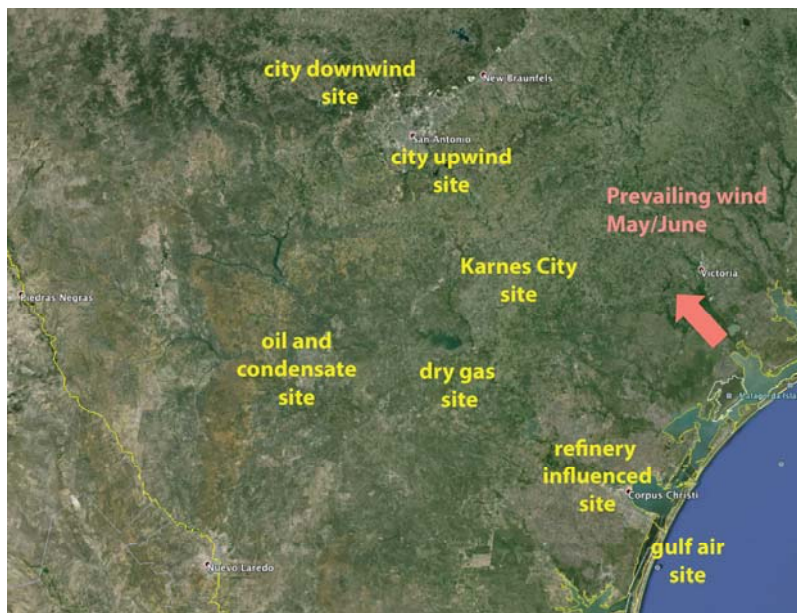


Figure 2. Map of notional sites for photochemical portion of the project.

3.2 Instrumentation

The Aerodyne Mobile Laboratory (AML) is a well-tested and extremely suitable measurement platform for the goals of the proposed study. Previous deployments have included measurements in urban polluted areas such as Mexico City during the 2006 MaxMEX/MILAGRO campaign [Scott C. Herndon et al., 2008; Ezra C Wood et al., 2009], the 2009 Queens, NY, study [P Massoli et al., 2012], or for more specific sources such as aircraft emissions [Santoni et al., 2011] or oil and gas extraction [Yacovitch et al., 2015]. Research and commercial instruments are installed into the AML to collect data while in motion for plume characterization, area mapping or portable deployment for photochemistry and transport experiments. Real-time monitoring of both gas-phase and particulate species is the key feature of the AML.

Most instruments proposed for this ozone study, including the TILDAS [McManus *et al.*, 2008; Nelson *et al.*, 2006] and the SP-AMS [Onasch *et al.*, 2012], have been successfully deployed by ARI researchers and others in numerous field campaigns. Further descriptions of the most novel (I-CIMS-HRTOF) and new additions to the analytical payload are described below. The instrument manifest includes all of the combustion tracers (CO₂, CO, NO, NO₂, SO₂) the light alkanes (CH₄, C₂H₆, C₃H₈) and alkenes (C₂H₄, C₃H₆), and oxygenated and aromatic VOCs. The comprehensive table of the instrument payload can be found at:

<https://www.dropbox.com/s/x2m2kk11388d3a9/AQRP-InstrumentManifest.pdf?dl=0>

3.3 Connecting science questions to work plan

Science Question One: *Individual VOC emission sources (for example, oil production vs biogenic emissions) all participate in ozone production in central Texas. Can examination of the oxidation products and radical termination species (e.g. butanone and alkyl nitrates) that still retain specific parent VOC information be used to apportion the VOC component of regional ozone production?*

Alkanes (e.g., propane, butane, isopentane, etc.) are the class of VOCs emissions from well pads in oil and gas production regions with a gradient in effective emission VOC profiles that is reflected in the geology of the region. Emissions from an oil-dominant well pad are different from emissions from a dry gas well that extracts little condensate. It is generally true though,

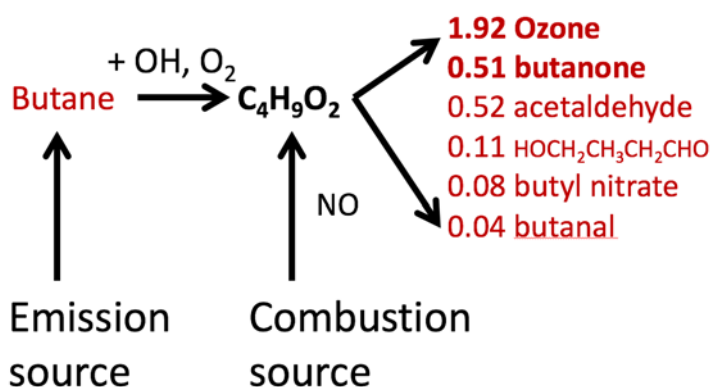


Figure 3 Apportionment of historical ozone production to responsible VOCs using indicator species. In this example, in the presence of plentiful NO_x, each molecule of butane oxidized will produce 1.92 molecules of ozone and 0.51 molecules of butanone. One ppb of butanone quantified by PTR-MS therefore indicates that 3.8 ppb of O₃ observed was from butane oxidation.

that most of the volume of the emission is considered alkane, chemically. Though less reactive than alkenes like ethene and propene, both of which are commonly emitted by petrochemical facilities, at high enough concentrations alkanes can contribute to ozone production. Quantification of speciated VOCs is an important activity for tracing and identifying which VOCs contribute the most to ozone formation [Gilman *et al.*, 2013] [McDuffie *et al.*, 2016], but mainly reflects the local ozone production at the measurement site and not necessarily the ozone formation

integrated over the last day of the air mass' history. Alkyl nitrates (RONO_2) are formed by very similar reactions as those that form ozone from alkane oxidation, and therefore contain information about which VOCs contributed to ozone formation during the life of the air mass [Ben Hwan Lee et al., 2014a].

The use of such oxidation markers is most effective when their atmospheric lifetimes are comparable to that of ozone. For example, butanone, which is produced almost entirely from n-butane oxidation [Sommariva et al., 2011] has a lifetime due to photolysis and reaction with OH of several days (Figure 3). Some hydroxy alkyl nitrates appear to have shorter lifetimes [Yarwood et al., 2015] thus use of these indicators to apportion VOC contribution to ozone formation will be (still useful) lower limits.

Using alkyl-nitrates to attribute VOC emissions and ozone production has been demonstrated before [Gilman et al., 2013; Yarwood et al., 2015]. In this work, we will use this concept and collect data at several locations within a study area spanning from Corpus Christi to San Antonio. The table at the web-link above details several instrument systems all of which are required to perform the analysis. One of the newer instruments is a high resolution chemical ionization mass spectrometer (CIMS) [Huey, 2007] equipped with a time-of-flight (TOF) capable of obtaining time-resolved, sensitive, and selective measurements of a wide range of oxygenated volatile organic carbon (OVOC) present in ambient air [Bertram et al., 2011]. The selectivity of the CIMS depends on the particular reagent ion used. In this work we will utilize a CIMS instrument with the iodide (I^-) reagent ion, which has been demonstrated to be extremely effective for detecting a wide range of OVOCs [Berresheim et al., 2000]. While I^- has negligible sensitivity to non-oxygenated, or monoalcohol, monoketone, or monoaldehyde species, it can be effectively used to detect multifunctional species with polar moieties such as keto-, hydroxy-, peroxy, acid, and nitro groups that are capable of forming strong adducts with the I^- reagent [Ben H. Lee et al., 2014b]. A key aspect of the I^- adduct technique is that it provides measurements of highly functionalized VOCs that can be linked to precursors and that are not typically detected by other gas phase techniques such as Proton Transfer Mass Spectrometry [Ben H. Lee et al., 2016]. The range of OVOCs measured with this instrument will be leveraged to provide constraints on the influence of different VOC sources (Biogenic, Oil, Refinery, Dry Gas, Oil, and other) and the oxidation chemistry observed within the mixed ambient environment.

Previous field and laboratory work [Ben H. Lee et al., 2016] indicate that the suite of OVOCs detected by the I^- CIMS will be large enough to characterize and differentiate between the different sources and precursors and oxidation processes observed in central Texas. Lee and co-workers [Ben H. Lee et al., 2014b], deployed a high resolution I^- CIMS, aboard an aircraft, and detected a range of aliphatic and aromatic OVOCs as well as multifunctional alkyl nitrates that

were characteristic of their sources as well as of the oxidation conditions. In that work, the hydroxyl nitrate and hydroxy peroxides compounds exhibited strong differences between urban and other continental plumes. Similarly, biomass burning plumes were characterized by detection of high levels of phenolic species, which are known to be products of biomass burning [Mohr *et al.*, 2013], and power plant emissions depleted in VOCs were found to be rich in inorganic products such as ClNO₂ rather than organic nitrates.

Based on this previous work, it is expected that sources related to the Eagle Ford shale in oil producing regions (which largely emit C₄ to C₁₀ hydrocarbons) and refineries (which emit aromatics and light alkenes) will also form unique mixtures of hydroxy nitrates and multifunctional oxidized aromatic products that can be detected by iodide CIMS and used as unique signatures of these sources. While the sensitivity for iodide CIMS detection for small chain (C₁-C₄) oxidation products of emissions from dry gas sources is generally lower than that for longer chain products [Lopez-Hilfiker *et al.*, 2016] it is likely that C₁-C₄ species containing multiple functionalities (acid, nitrate, hydroxy) can be detected. In fact, iodide adducts of species such as glyoxylic acid (C₂H₂O₃) and propionic acid (C₃H₆O₂) have been observed during aircraft studies and have been shown to display different behavior inside and outside biomass burning plumes [Ben H. Lee *et al.*, 2014b].

The data acquired with the CIMS can be analyzed with statistical techniques including several variants of principal component analysis and especially two and three dimensional Positive Matrix Factorization (PMF) [Ulbrich *et al.*, 2009], which the proposers have successfully adapted to analyze aerosol mass spectra. Component analysis techniques such as PMF deconvolve the signal in each spectrum among different *basis* components, and for this reason they are very applicable to data from mass spectrometry based techniques, where the total spectrum measured at a given time is a linear combination of spectra from different sources. A recent example of the power of this method for CIMS data was obtained at the Centreville site during the SOAS 2013 campaign [P. Massoli *et al.*, 2016]. A key result from the PMF analysis was the identification of 5 main different factors (i.e., mass spectral signatures) that could be linked to different oxidation processes of the two main biogenic precursors (isoprene and terpenes) and a factor that contained highly oxidized molecules that was associated with anthropogenic plumes with high SO₂ levels. Analogous analysis of data from central Texas is likely to yield several classes of oxidized organic species that differ according to precursors (Biogenic, Oil, Refinery, Dry Gas, Oil, and other) and oxidation conditions.

An additional prototype instrument to be deployed is a cryogenic-preconcentration – gas chromatograph – TOF-MS (CP-GC-MS) [Lerner *et al.*, 2016; Obersteiner *et al.*, 2016], which will allow for the speciation of C₅-C₁₀ hydrocarbon and organic volatile organic compounds with a single oxygen functional group (e.g. monoalcohol, monoketone, monoaldehyde), along with C₂-

C4 alkyl nitrates. This instrument allows for the quantification of the reported species to part-per-trillion (pptv) sensitivities, albeit at discrete integrated sampling times of several minutes collected and analyzed every 10 to 30 minutes. These measurements will serve as a compliment to the fast time resolution CIMS, providing both overlap of concurrently measured species at far greater precision [see instrument payload table] and separation and quantification of isomeric species (e.g. propanal and acetone [C₃H₆O]). Additionally, the CP-GC-MS will quantitate C₅-10 alkane and C₆-C₉ aromatic species, allowing for characterization of oil/gas emissions [Gilman *et al.*, 2013; Katzenstein *et al.*, 2003], and biogenic species such as isoprene and speciated monoterpenes.

Science Question Two: What is the instantaneous rate of ozone production in central Texas and is it occurring under NO_x-limited or VOC-limited conditions? Coupled with question one, how does this answer inform potential mitigation strategies?

In the sections above, we have outlined how we intend to apportion ozone formation to specific source VOC categories via measurement of alkyl nitrate end products. This approach relies on starting products (VOCs) and terminating products (alkyl nitrates). A second complimentary approach to this problem will target the intermediate species and their oxidation chemistry. Using the UMass peroxy radical measurements we will quantify the ozone production rate $P(O_3)$ throughout the region in order to better understand varying ozone production rates due, for example, to large local sources of VOCs. Knowledge of $P(O_3)$, when combined with measurements of NO and controlling for radical initiation rates and VOC reactivities, will reveal which NO_x regime dominates ozone chemistry in San Antonio (VOC-limited vs NO_x-limited). We will determine whether ozone production in air masses are NO_x-limited or VOC-limited in two main ways, first by examination of the HO_x radical budget and second through examination of indicator species.

A common way to assess the chemical regime is by quantifying the individual HO_x radical termination steps. These can be classified into two general groups of reactions: HO_x-HO_x reactions, such as the reaction of HO₂ with either HO₂ or RO₂ to form H₂O₂ and ROOH, respectively; and HO_x-NO_x reactions, e.g. the reaction of OH with NO₂ to form HNO₃. When ozone production is NO_x-limited, HO_x-HO_x reactions comprise the bulk of radical termination reactions, whereas under VOC-limited conditions HO_x-NO_x reactions dominate. Quantitatively, when the rate of HO_x radical termination by HO_x-NO_x reactions is greater than 50% of the total termination rate, $P(O_3)$ is VOC-limited. This quotient is usually written as " L_N/Q ", where L_N is the rate of HO_x-NO_x reactions, and Q is equal to both the total rate of radical termination rates and radical production rates since these are equal [Kleinman, 2005]. This method has been used to characterize $P(O_3)$ in several cities including Houston, Mexico City, New York City, Nashville,

Phoenix, and Philadelphia [Kleinman, 2005]. Q (or equivalently $P(\text{HOx})$) will be well quantified in San Antonio using direct measurements of O_3 , HONO (I⁻ CIMS), HCHO (QC), CH_3CHO and other OVOCs (PTR-MS), and alkenes (PTR-MS and GC-FID). OH and HO_2 concentrations will not be directly quantified, but the sum of $\text{RO}_2 + \text{HO}_2$ and alkyl- RO_2 will be measured. This will constrain the rates of $\text{HO}_2 + \text{HO}_2$ and $\text{RO}_2 + \text{HO}_2$ to within a factor of two. A potentially important loss process for both NO_x and HOx that was found to be dominant in an air mass downwind of evaporative emissions from the Deepwater Horizon spill of 2010 was alkyl nitrate formation ($\text{RO}_2 + \text{NO} \rightarrow \text{RONO}_2$) from C5 to C9 alkanes [Neuman et al., 2012]. The rate of RONO_2 formation will be constrained using the alkyl peroxy radical measurements and the effective branching ratio for this reaction which will be quantified by the correlation between O_3 and total alkyl nitrates.

The concentrations or ratios of concentrations of compounds that persist in the atmosphere following rapid HOx/ NO_x chemistry (i.e., O_3 , HCHO, organic nitrates) can also be used as an indicator of whether ozone formed in an air mass under NO_x - or VOC-limited conditions. These include $[\text{HCHO}]/[\text{NO}_2]$, $[\text{H}_2\text{O}_2]/[\text{HNO}_3]$, and the ratio of O_3 to NO_x oxidation products (e.g., $[\text{O}_3]/([\text{HNO}_3] + [\text{PAN}])$), [Sillman, 1995; Tonnesen and Dennis, 2000]. For example, values of $[\text{H}_2\text{O}_2]/[\text{HNO}_3]$ higher than 0.2 are associated with NO_x -limited ozone production. This technique has been used to assess the chemical nature of ozone formation in Nashville, Atlanta, Los Angeles, and other cities [Pollack et al., 2012; Sillman, 1995]. For example, ozone formation in Los Angeles is currently VOC-limited (NO_x -saturated) all day during the weekdays, but NO_x -limited during the weekend in the afternoon due to reduced NO_x emissions from diesel trucks. As a result, NO_x is more efficient in catalyzing O_3 formation during the weekend, evident by increased ratios of $\text{O}_3/(\text{PAN} + \text{HNO}_3)$ on the weekend (7.9 weekend, 5.3 weekday) [Griffith et al., 2016]. Most of these indicator species will be quantified by the AML instrumentation, and thus can be used to assess integrated ozone formation both upwind and downwind of San Antonio.

Science Question Three: *Can improved characterization of specific industry sector emissions offer insight into the ozone and air quality impact? Do medium-large process flares represent an emission source not well represented in emission inventories?*

This project is geared toward using the mobile lab suite as a rolling photochemistry supersite. We have, however, identified two potential oil and gas emission sources where additional information would be insightful. Site safety flares at gas processing plants are a potential source of emissions where an in-use data point would be significant. Prior work has found that operating large capacity flares with excess “flare assist” leads to an overestimate of the destruction and removal efficiency (DRE) of the vent gas [Torres et al., 2012]. Gas processing facilities handle and flare significantly larger volumes of gas at a single location than facilities in

other sectors [*Mitchell et al.*, 2015]. We propose to devote two days of this study to characterize the emissions from a processing plant in the Eagle Ford. If the in-use DRE of a flare is lower than the manufacturer's specified DRE (99%) by even a seemingly acceptable degradation in performance (say 95%), this would imply that emissions are five times greater than the inventory value. Observational top-down burden estimates [*de Gouw et al.*, 2009] are often greater than inventory bottom-up VOC and DRE discrepancy is a likely explanation [*S. C. Herndon et al.*, 2012]. We are currently negotiating with an operator to allow site access for this project.

In addition to the specific emissions from the process flare, we will look at the VOC emission profile from in-use tank emissions in oil producing and in wet-gas producing areas. This emission source is distributed throughout the entire region but it will be important to connect this source to the regional VOC emissions profile. We will use this exercise to check that the VOC emission profile from a few oil/condensate tanks can be connected plausibly to VOC emissions in the area. We seek to look at this specific emission vector with the suite of instruments on the AML, with results to inform a feasibility analysis of a more comprehensive study in the future.

4.0 Task Descriptions

Task 4.1: Project Design and site selection (November 2016 – January 2017)

The PI and measurement team will work with TCEQ to select sites in the region. We seek to select locations from Corpus Christi to Carrizo Springs to San Antonio that will enable the observation of emissions signatures and photochemically processed air. The outcome of this task will be a power point file with sites, goals and action items associated with the logistic preparation tasks.

Task 4.2: Mobile Laboratory preparation (January 2017 – April 2017)

The GC-MS will be prepared for integration into the Aerodyne mobile laboratory. The instrument designs and operation will be modified as needed due to space constraints. Instrumentation for the measurement of alkyl nitrates and other photochemical products will be adapted for mobile applications taking into account both mounting, and inlet considerations. Finally, the analytical instrumentation will be integrated into the Aerodyne Mobile laboratory. The outcome of this task will be successful integration of field-ready instruments into the Aerodyne mobile laboratory.

Task 4.3: Field deployment (May 2017 – June 2017)

The three-week field project is planned for May and June in the greater San Antonio area. Measurements of photo-oxidants, NO_x, selected hydrocarbons, aerosol size and composition will be made on board the Aerodyne mobile laboratory in central Texas. This includes the Gulf Coast (e.g., Corpus Christi), northwest of San Antonio (usually a downwind high O₃ site), and in between in locations with suspected biogenic, oil and gas producing areas in both the 'wet' and 'dry' gas regions. This task will be conducted by the Aerodyne Research, Inc team in conjunction with collaborators (Drexel University, Montana State University and others). The outcome of this task will be the raw data collected during the field deployment.

Task 4.4: Follow-up laboratory work (June 2017 – August 2017)

Following the completion of the field measurements, additional laboratory work will be conducted if necessary as part of the data quality assurance procedure. This would likely involve additional instrumental calibrations and diagnostic tests to ensure the accuracy of the data collected. This task will be conducted by the research team. The outcome of this task is a fuller understanding of the performance of the instruments during the field deployment.

Task 4.5: Data work-up and analysis (August 2017)

The raw data collected during the field deployment will be processed to produce the final time series data set as well as photochemical production rates as a function of location. Apportionment of the ozone formation based on likely VOC emission sources and intra-urban sources will be analyzed. The deliverable resulting from this task will be the quality-assured dataset and the project final report which summarizes the preliminary analysis performed.

Task 4.6. Project Reporting and Presentation (September 2016 – August 2017)

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, members of the research 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.

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

Schedule: The schedule for Task 4.6 “Deliverables” is shown in Section 7.

5.0 Project Participants and Responsibilities

Name	Title/Affiliation	Responsibilities
Scott Herndon	PI, Director of Field Measurement Research, ARI	The PI will oversee, manage, and be directly involved in all tasks.
Tara Yacovitch	Principal Scientist, ARI	Quality assurance of the field measurements, and contribute to the data analysis.
Manjula Canagaratna	Principal Scientist, ARI	Operation and analysis of the aerosol and gas phase CIMS measurements
Rob Rosicoli	Principal Scientist, ARI	Operation and analysis of the Infrared spectroscopy measurements
Brian Lerner	Senior Scientist, ARI	Construction, operation and analysis of the gas chromatographic measurements
Conner Daube	Research Associate, ARI	Mobile lab foreman, operation and analysis of the chemiluminescence instruments
W. Berk Knighton	Associate Professor, MSU	Operation and analysis of the proton transfer reaction mass spectrometer

6.0 Timeline

The tasks described in section 4 will be executed following the following timeline:

- *Task 4.1: Project Plan (November 2016 – January 2017)*
- *Task 4.2: Mobile Laboratory preparation (February 2017 – April 2017)*
- *Task 4.3: Field deployment (May 2017 – June 2017)*
- *Task 4.4: Follow-up laboratory work (June 2017 – August 2017)*
- *Task 4.5: Data work-up and analysis (August 2017)*
- *Task 4.6. Project Reporting and Presentation (September 2016 – August 2017)*

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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