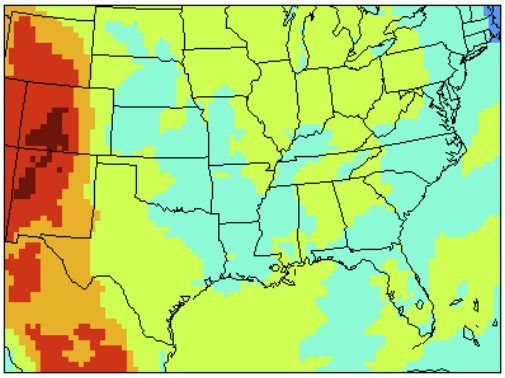
State of the Science of Air Quality in Texas:

Summary of Scientific Projects and Findings from the Texas Air Quality Research Program (AQRP) 2010-2017



Prepared by:
David Allen, Elena McDonald-Buller, and Gary McGaughey
The University of Texas at Austin

Reviewers:
Mark Estes, Liaison
Texas Commission on Environmental Quality

Members of the Air Quality Division
Texas Commission on Environmental Quality

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Program and Report Overview

Since its inception in 2010, the Texas Air Quality Research Program (AQRP) has had three primary objectives:

(1) to support scientific research related to Texas air quality including field measurement campaigns, ambient air quality and meteorological data analyses, controlled environmental chamber studies aimed at improving the understanding of atmospheric chemical processes, emissions inventory development and assessment, and meteorological and air quality modeling studies;

(2) to integrate AQRP research with the work of other organizations;

(3) to communicate the findings of sponsored research to air quality planning and management stakeholders and the scientific research community.

The AQRP is administered by the University of Texas at Austin under contract to the Texas Commission on Environmental Quality (TCEQ). The program has completed four funding cycles to date that have included the 2010-2011, 2012-2013, 2014-2015, and 2016-2017 biennia. The AQRP has sponsored more than 60 projects from researchers around the world. Projects have involved collaborations between academic institutions, state and national government agencies, and the private sector. The program has contributed directly to the understanding of specific and sometimes unique emissions and atmospheric physical and chemical processes that lead to air pollution in Texas and to the identification of effective, efficient approaches for air quality improvement and management.

This report summarizes the scientific findings from projects addressed by the AQRP during the current 2016-2017 project cycle as well as more briefly from previous AQRP funding cycles between 2010 and 2015. It is the third such summary, with the first report released in 2013 and the second in 2015. Within this report, findings are divided into sections corresponding to the areas where the AQRP performs research: emissions inventory development and assessment, tropospheric chemistry, and atmospheric physical processes and long-range transport of pollutants. Each section summarizes major findings by project topic areas. A complete list of projects by funding cycle as well as publications and presentations resulting from the program are also included.

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1. Introduction

1.1 Texas Air Quality

Exposure to air pollutants is a significant global public health issue. Within Texas, several of the largest urban areas exceed the National Ambient Air Quality Standard (NAAQS) for ozone, and concentrations of particulate matter and air toxics remain a health concern in many communities. Reducing emissions and improving air quality while supporting economic growth and an increasing population is challenging, yet substantial improvements in air quality have been made in Texas over the past several decades. From 2000 to 2016, ozone design values (i.e., the three-year average of the maximum fourth-highest 8-hour ozone concentrations) at regulatory monitors declined by 30% in Texas (Figure 1.1), ranking 6th overall among states and substantially above the national average decrease of 18% (TCEQ, 2017).

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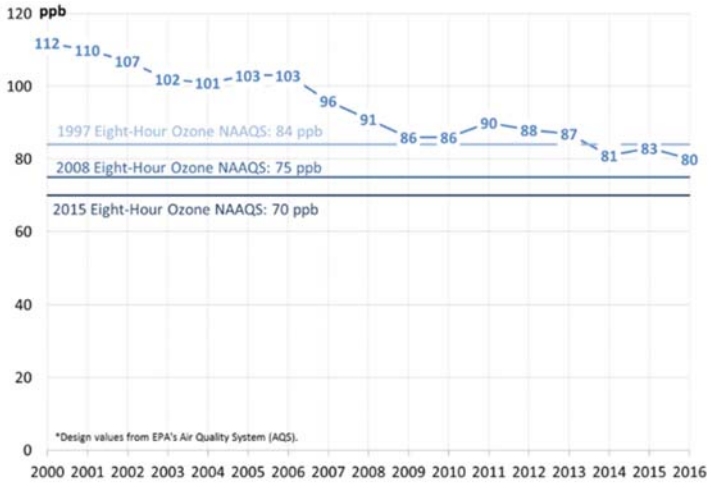

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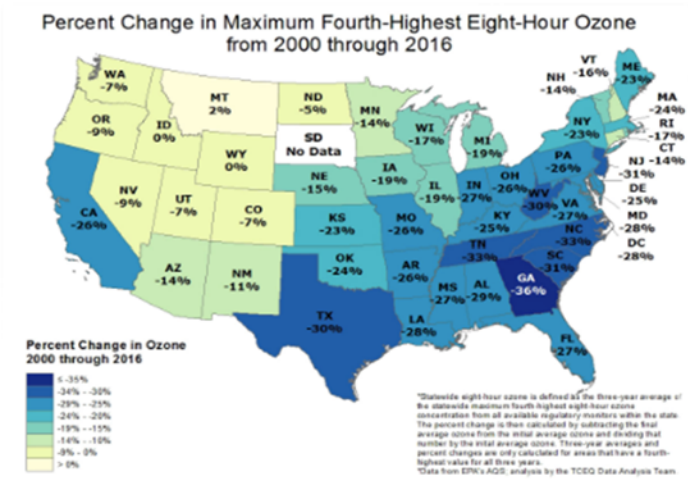


Figure 1.1. (a) Time series of maximum fourth-highest 8-hour averaged ozone concentrations in Texas and (b) percent change in statewide design values from 2000-2016. Source: https://www.tceq.texas.gov/airquality/airsuccess/airSuccessTXcompared.

Two of the most populated core based statistical areas (CBSAs) in the United States, Houston-The Woodlands-Sugarland and Dallas-Fort Worth, are located in Texas. Decreases in ozone design values in these areas were 29% and 22% from 2000 through 2016, ranking second and third, respectively, among improvements in air quality in the top five CBSAs (TCEQ, 2017). Figure 1.2 shows changes in 1-hour and 8-hour ozone design values from 2000 through 2016 for four metropolitan areas in eastern Texas. Although there is a continuing need for progress towards attainment with the 8-hour NAAQS for ozone, Figure 1.2 also demonstrates the substantial improvements over time even with the growth in population that has occurred in Texas cities. Reductions in concentrations of other criteria pollutants in addition to ozone also demonstrate progress towards improved air quality in Texas (Figure 1.3).

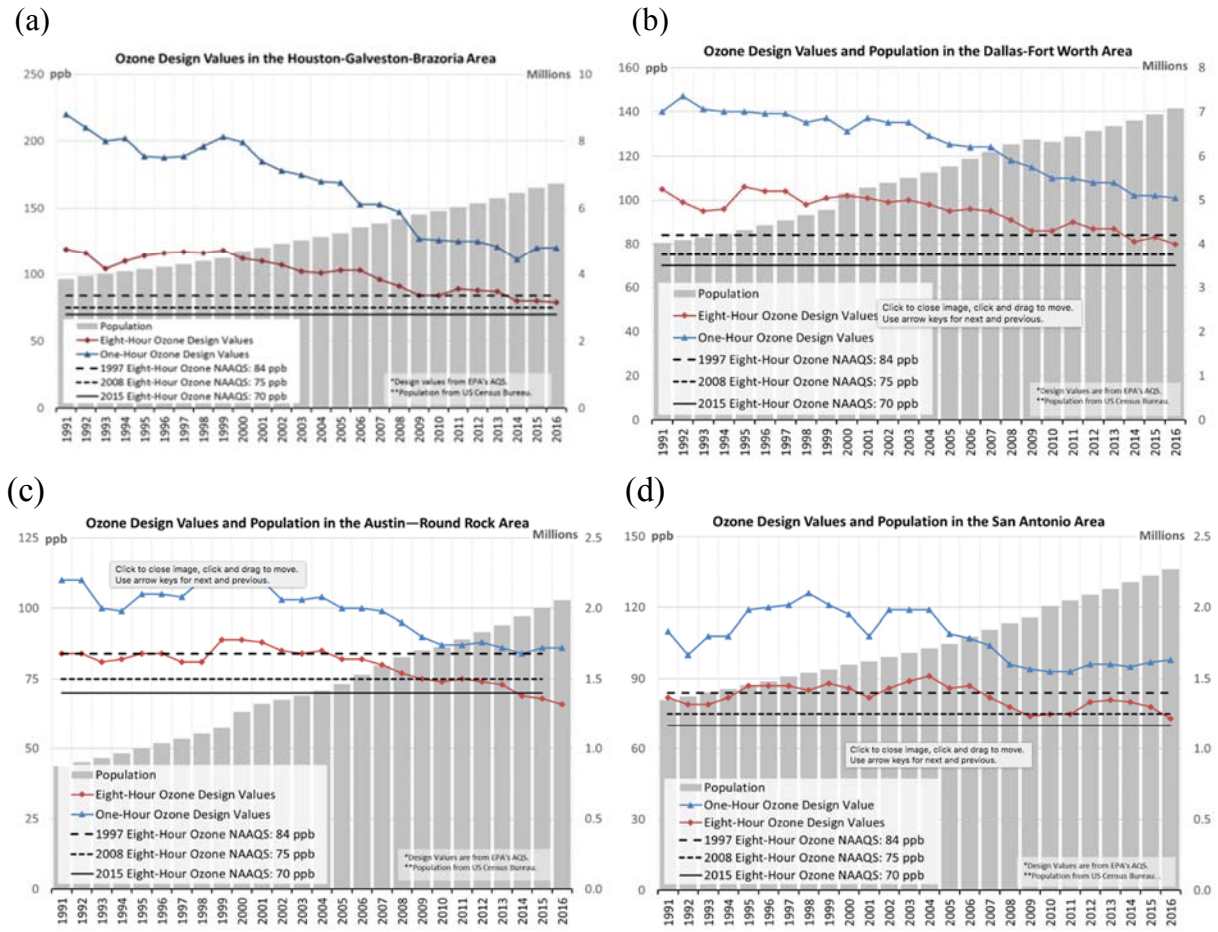
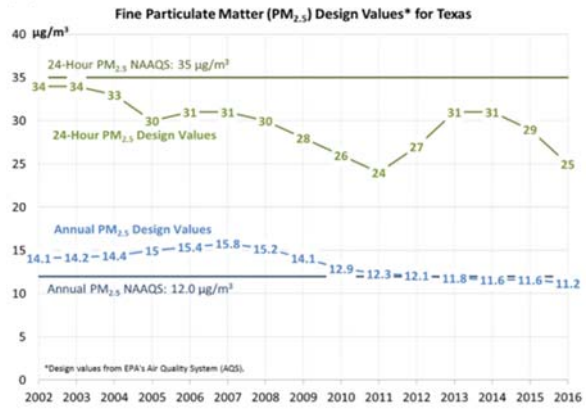


Figure 1.2. Time series of 1-hour and 8-hour averaged ozone design values and population growth for four eastern Texas metropolitan areas: (a) Houston-Galveston-Brazoria, (b) Dallas-Fort Worth, (c) Austin-Round Rock, and (d) San Antonio. Source: https://www.tceq.texas.gov/airquality/airsuccess/airSuccessTXcompared.

Identifying effective, efficient approaches to improve air quality has come from understanding the specific and sometimes unique emissions and atmospheric physical and chemical processes that lead to air pollution in Texas. Investments in air quality research have been instrumental in the success demonstrated by changes in the air quality metrics shown in Figures 1.1-1.3. These investments have helped to design emission reduction strategies to be most effective for conditions in Texas.

(a)



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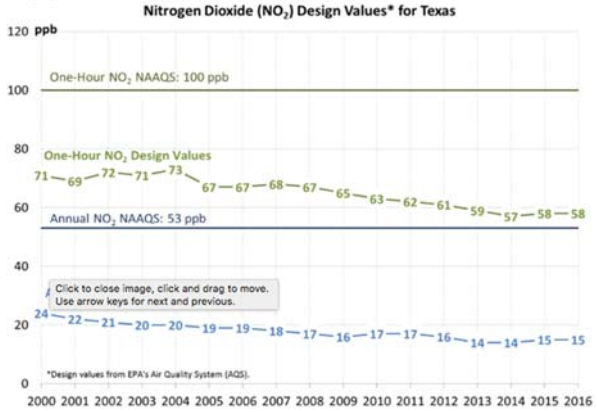

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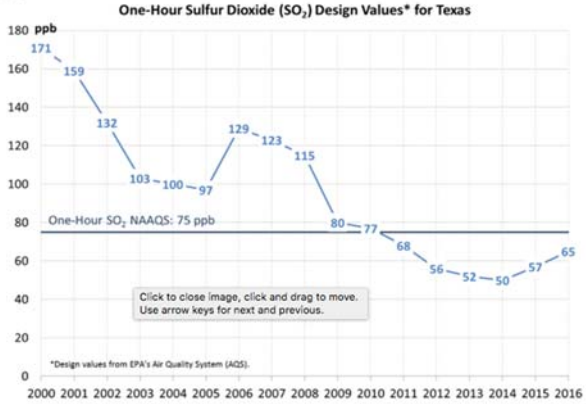

Figure 1.3. Time series of design values for (a) fine particulate matter, (b) nitrogen dioxide, and (c) sulfur dioxide concentrations in Texas from 2000-2016. Source: https://www.tceq.texas.gov/airquality/airsuccess/airSuccessTXcompared.

The synergy and information flow between intensive field measurement campaigns, data analysis studies, emissions inventory development and assessment, controlled laboratory experiments, and multi-scale chemical transport modeling that have occurred over time in Texas have been important to the overall accomplishments. Since 2000, multiple field measurement campaigns, of varying size and scope, have served as focal points for multi-faceted research efforts to advance the scientific understanding of air quality in the state. These studies have had direct policy relevance. For example, the Texas Air Quality Study (TexAQS) field campaign in 2000 involved approximately 300 researchers drawn from around the world and led to the identification of the role of Highly Reactive Volatile Organic Compounds (HRVOCs: ethene, propene, butenes, and 1,3-butadiene) in ozone formation in southeast Texas. Based on the findings of TexAQS 2000, the TCEQ revised the State Implementation Plan (SIP) for the Houston-Galveston-Brazoria region. TexAQS II in 2005 and 2006 documented substantial reductions in HRVOC concentrations relative to the measurements made in 2000, identified new mechanisms for activation of chlorine in sea salt particles, and quantified the intercity transport of ozone. Smaller measurement campaigns conducted since have focused on issues associated with HRVOCs initially raised during the 2000 TexAQS campaign. For example, two campaigns in 2009 (the Study of Houston Atmospheric Radical Precursors or SHARP and Formaldehyde and Olefin from Large Industrial Sources or FLAIR) sought better characterization of

olefin, formaldehyde, and free radical sources in southeast Texas. The 2010 Flare Study conducted controlled, full-scale flare tests at an industrial research facility in Tulsa, Oklahoma, that examined HRVOC emissions from flares operating at low flow rates and with low heating values. The effort ultimately guided the development of new operational performance recommendations for industrial flares.

Since its inception in 2010, the Texas Air Quality Research Program (AQRP) has contributed to the support of field measurements campaigns. These have included studies in 2011 to investigate the atmospheric chemistry, meteorology, and transport of ozone and precursor compounds in and around oil and gas production activities of the Barnett Shale and the Dallas-Fort Worth urban area. In 2013, the DISCOVER-AQ (Deriving Information on Surface Conditions from Column and Vertically Resolved Observations Relevant to Air Quality) campaign, under the leadership of the National Aeronautics and Space Administration (NASA), used southeast Texas as a test bed for the application of satellite measurements in characterizing air quality. Augmentations of the measurements, funded by the TCEQ and AQRP, leveraged the extensive investments made by NASA, and provided additional insights into the factors that control air quality in southeast Texas. More recently, the AQRP sponsored the logistical and infrastructure support and collection of mobile measurements for the San Antonio Field Study (SAFS) in 2017 that had the overall aim of investigating the regional conditions leading to ozone formation within and around San Antonio.

The AQRP has also contributed extensive support for ambient air quality and meteorological data analyses, controlled environmental chamber studies aimed at improving the understanding of atmospheric chemical processes, emissions inventory development and assessment, and meteorological and air quality modeling studies. Among the many results of these studies are new modeling approaches for estimating biogenic emissions and emissions from wildfires, new mechanistic representations of the atmospheric chemistry contributing to ozone and secondary organic aerosol formation, and new understanding of the contributions of the long-range transport of ozone and its precursors to air quality in Texas. To date, the AQRP program has sponsored more than 60 projects from researchers around the world.

1.2 Report Objectives

An essential component of the Texas Air Quality Research Program has been to communicate the findings of sponsored research to the air quality planning and management and research communities. This report summarizes the scientific understanding of key issues addressed by the AQRP during the current 2016-2017 project cycle as well as more briefly from previous AQRP funding cycles between 2010 and 2015. It builds on similar previous science syntheses (Allen et al., 2004; Allen et al., 2012; Allen et al., 2015). It characterizes, as applicable, uncertainties that exist, which can be important in guiding continued progress in the scientific understanding of air quality and evaluating the likelihood of the effectiveness of regulatory policies.

While progress in air quality has been impressive, it is evident that challenges remain. For example, the Dallas-Fort Worth and Houston-Galveston-Brazoria area are currently classified as nonattainment areas under the 2008 NAAQS for 8-hour averaged ozone concentrations. Regional, continental and even global factors can have important influences on air quality in many parts of Texas, which requires consideration of the effective and efficient balance between local, regional and national air quality improvement actions. In addition, growth in important economic sectors, such as energy development, coupled with expected population growth, will also continue to be important considerations for achieving and maintaining improvements in air quality.

Initial drafts were written by AQRP staff, including Dr. David Allen, Dr. Elena McDonald-Buller, and Mr. Gary McGaughey of the University of Texas at Austin. The report was revised based on reviews by both the TCEQ and the AQRP's Independent Technical Advisory Committee. Findings are divided into sections corresponding to the areas where the AQRP performs research: emissions inventory development and assessment, tropospheric chemistry, and atmospheric physical processes and long-range transport of pollutants. Each section has a summary of major findings by project topic areas; citations to the scientific literature provide additional details.

1.3 References

Allen, D.T., E. Olaguer, J. Nielsen-Gammon, M. Estes, G. Carmichael, G., W. Carter, M. Sattler, J. Scire, (2004), State of the Science of Air Quality in Eastern Texas: Major Scientific Findings and Recommendations.

Allen, D., E. McDonald-Buller, G. McGaughey, (2012), State of the Science of Air Quality in Texas: Scientific Findings from the Air Quality Research Program (AQRP) and Recommendations for Future Research.

Allen, D., E. McDonald-Buller, G. McGaughey, (2015), State of the Science of Air Quality in Texas: Scientific Findings from the Air Quality Research Program (AQRP) and Recommendations for Future Research.

Texas Commission on Environmental Quality, (2017), Air Quality Successes, available at: http://www.tceq.texas.gov/airquality/airsuccess/air-success-criteria.

For Further Information Regarding Intensive Field Campaigns:

TexAQS 2000:

Daum, P., J. Meagher, D. Allen, and C. Durrenberger. 2002. Accelerated Science Evaluation of Ozone Formation in the Houston-Galveston Area: http://www.utexas.edu/research/ceer/texaqsarchive/accelerated.htm

A web site describing TexAQS and its principal findings has been maintained by the University of Texas: www.utexas.edu/research/ceer/texaqs www.utexas.edu/research/ceer/texaqsarchive.

TexAQS II (TexAQS 2005-2006):

Parrish, D.D., D. Allen, T. Bates, M. Estes, F. Fehsenfeld, G. Feingold, R. Ferrare, R. Hardesty, J. Meagher, J. Nielsen-Gammon, R. Pierce, T. Ryerson, J. Seinfeld, E. Williams, (2009), Overview of the Second Texas Air Quality Study (TexAQS II) and the Gulf of Mexico Atmospheric Composition and Climate Study (GoMACCS)", *Journal of Geophysical Research - Atmospheres*, 114, D00F13.

AQRP Sponsored Campaigns:

AQRP Project 17-SAFS: Sullivan, D., (2017), San Antonio study logistics project, Submitted to the Texas Air Quality Research Program, http://aqrp.ceer.utexas.edu/.

Contributions of AQRP projects to the SHARP, FLAIR, Controlled Industrial Flare, Barnett Shale, and DISCOVER-AQ measurement programs are available at the AQRP web site: http://aqrp.ceer.utexas.edu/projects.cfm. See also overviews at:

Olaguer, E., C. Kolb, B. Lefer, B. Rappenglück, R. Zhang, J. Pinto, (2014), Overview of the SHARP campaign: Motivation, design and major outcomes, JGR Atmospheres, Introduction to a Special Collection, 119, 5, 2597–2610.

Torres, V., S. Herndon, Z. Kodesh, and D. Allen, D., (2012), Industrial flare performance at low flow conditions: Part 1. Study Overview, Industrial & Engineering Chemistry Research 51, 12559-12568.

The DISCOVER-AQ program is described at the NASA web site: .http://discover-aq.larc.nasa.gov/

2. Emissions Inventory Development and Assessment

Emission inventories are developed at varying spatial and temporal scales in support of air quality planning and management efforts. Applications include, for example, assessments of annual state or national air quality trends and as essential inputs to regional or global-scale chemical transport models. To date, the AQRP program has primarily focused on emission inventory development and analysis to support air quality management plans for ozone in Texas. This section summarizes findings from the 2016-2017 AQRP program related to emissions inventories as well as those from previous AQRP project cycles (2010-2015).

2.1 AQRP Projects during 2016-2017 and Related Previous Projects

2.1.1. Wildland Fires and Open Burning (AQRP Projects 16-008, 17-024, 12-018, 14-011)

Wildland fires and open burning can be substantial sources of ozone precursors and particulate matter. The influence of fire events on air quality in Texas and other parts of the southern United States has been well documented by observational and modeling studies (e.g., Junquera et al., 2005; Morris et al., 2006; Wang et al., 2006; Villanueva-Fierro et al., 2009; McMillan et al., 2010; Kemball-Cook et al., 2014). AQRP Project 16-008 (Wang et al., 2017) found average ozone enhancements of approximately 6-9 ppb in the Houston-Galveston-Brazoria area associated with the long-range transport of Central American fire plumes during the spring months of 2000-2015. The transport of Central American fire emissions into Texas is largely steered by the Bermuda High (Wang et al., 2009), and both MOPITT (or Measurements of Pollution In The Troposphere) and MODIS (Moderate Resolution Imaging Spectroradiometer) satellite instruments have detected significant enhancements of CO column densities and Aerosol Optical Depth (AOD), respectively, along the transport route from Central America fire regions to the Houston-Galveston-Brazoria area. AQRP projects have focused on the development and improvement of models for estimating emissions from fire events and the representation of the physical transport and chemical processing of emitted trace gases and particulate matter in chemical transport models.

The Fire INventory from NCAR (FINN) is a global fire emissions model that estimates daily emissions of trace gases and particles from open biomass burning (Wiedinmyer et al., 2011). FINN v.1 was released in 2010 and updated in 2011, and v.1.5 was released in 2014. AQRP Project 12-018 (McDonald-Buller et al., 2013) evaluated the sensitivity of FINN v.1 emissions estimates to variability in input parameters, including land cover, emission factors, fire detection, burned area, and fuel loading and investigated the effects on air quality using the Comprehensive Air Quality Model with extensions (CAMx). Variability in fire emissions is season- and region- dependent in the United States, and differences in emissions estimates due to varying input data resources can exceed a factor of two. The use of the different estimates of fire emissions had substantial impacts on predictions of ozone and fine particulate matter concentrations in Texas and other regions of the United States.

AQRP Project 14-011 (McDonald-Buller et al., 2015) made targeted improvements to FINN to benefit global and regional air quality management and research communities, with a special focus on needs for Texas. A new approach for estimating burned area from satellite-derived fire detections was incorporated into FINN to address a known under-prediction bias. Other improvements included better spatial resolution of land cover and fuel loadings in the United States and new satellite-based estimates of barren land and vegetative cover. Crop-specific emission factors and fuel

loadings were added as an option for users with land cover data that distinguishes major crop types typically found in the United States. FINN v.2 includes options to use different land cover data resources as an alternative to the default MODIS Land Cover Type (LCT) product. New global, U.S. national, and Texas regional products were compared, including the United Nations Global Land Cover (GLC-SHARE) and European Space Agency (ESA) Climate Change Initiative global products, U.S. Forest Service Fuel Characteristic Classification System (FCCS), U.S. Department of Agriculture National Agricultural Statistical Service Cropland Data Layer (CDL), and a Texas regional land cover product developed by Popescu et al. (2011). These modifications formed the basis of the next generation of the model, FINN v.2. The development of FINN v.2 for global applications is ongoing.

FINN v.2 emissions estimates were generated for 2012 and provided to the TCEQ to support air quality modeling efforts. AQRP Project 14-011 recommended use of the Texas regional land cover product with the Cropland Data Layer, the U.S. Forest Service FCCS in the continental U.S., and the MODIS LCT product elsewhere. These products provided the greatest spatial resolution and specificity in land cover and fuel loadings for the Texas regional domain and continental U.S.

Representation of the physical and chemical processing of trace gas and particulate matter emissions associated with biomass burning plumes in chemical transport models has been evolving through AQRP projects. The immediate dilution of fresh fire emissions into large grid volumes and poor representation of chemical processing may be factors that contribute to discrepancies between modeled and observed ozone impacts. AQRP Project 14-011 applied a diurnally varying, fuel-dependent technique to partition NO_x emissions into aged NO_z forms in fire plumes for CAMx simulations based on a subset of the parameterizations of Lonsdale et al. (2014). AQRP Project 17-024 (Lonsdale et al., 2017) began the development of a coupled plume-scale process model (i.e., Atmospheric and Environmental Research's large eddy simulation System for Atmospheric Modeling-Aerosol Simulation Program or SAM-ASP model) and parameterization for regional and global scale chemical transport models. Application of the full parameterizations of Lonsdale et al. (2014, 2015) into the Plume-in-Grid (PiG) module of CAMx was found to reduce the predicted impacts of fires on near source ozone by approximately 30%, indicating that sub-grid parameterization may help to mitigate the overestimation of fire impacts near the source seen in many Eulerian grid models.

AQRP Project 17-024 also constructed a trajectory-based modeling tool, known as STILT-ASP v.2.0 (i.e, Stochastic Time Inverted Lagrangian Transport model with an integrated Aerosol Simulation Program) to assess the effects of wildfire events on ozone or particulate matter at specific locations. STILT-ASP was used to estimate the impacts of out-of-domain and in-domain fires on air quality in Texas. Application of STILT-ASP showed fine structure in the impacts of fires on carbon monoxide concentrations along the southern boundary of the TCEQ CAMx modeling domain that was not evident in boundary conditions from the GEOS-Chem model. Thus, Lagrangian models, such as STILT-ASP, may be useful for evaluating boundary conditions for regional photochemical modeling during periods when remote biomass burning may affect air quality as well as for examining impacts at ambient monitoring sites and other critical locations.

2.1.2 Biogenic Hydrocarbons (AQRP projects 16-011, 14-008, 14-016, 14-017, 14-030)

Biogenic volatile organic compounds (BVOCs), particularly isoprene and monoterpenes, have been widely recognized for their key roles in atmospheric chemistry, including contributions as

precursors for tropospheric ozone (Atkinson, 2000) and secondary organic aerosol (SOA) formation (Tsigaridis and Kanakidou, 2003; Claeys et al., 2004; Xu et al., 2015). Li et al. (2007) found changes in modeled ozone concentrations of ±5-25 ppb over the Houston urban area and ±5-10 ppb over the Houston Ship Channel in response to changes in isoprene emissions locally or from regions to the north of Houston during TexAQS 2000. Recently, Bean et al. (2016) characterized the strong influence of the interaction of biogenic hydrocarbons and anthropogenic oxidants on organic aerosol formation in southeastern Texas during the DISCOVER-AQ field campaign in 2013.

Average Texas statewide biogenic VOC emissions reported in the EPA 2011 National Emission Inventory (NEI version 1) ranked first within the continental United States (EPA, 2014). Emissions of biogenic VOCs exhibit strong diurnal variability with temperature and sunlight and spatial gradients due to differences in land use/land cover. Interannual variability in isoprene and monoterpene emissions estimates can exceed 20% in eastern Texas climate regions associated with changes in meteorological and ecosystem conditions (Huang et al., 2014).

Characterization of land use/land cover has been a research priority in Texas since the late 1990s (e.g., Wiedinmyer et al., 2001; Feldman et al., 2010; Popescu et al., 2011; AQRP Project 14-016: Yu et al., 2015, Yu et al., 2017). Land cover in Texas is highly diverse, varying from dense forest in East Texas to grasses and croplands towards the central regions. Recent efforts (Yu et al., 2017; AQRP Project 16-011: Guenther et al., 2017) have applied land cover data at high spatial resolution (30m) for Texas and other regions of the United States drawing on ground survey, remote sensing and land surface model data products. Uncertainties remain in data representation, validation, harmonization, and synthesis globally across land cover types (Song et al., 2014). Huang et al. (2015) found that misclassification of land cover can lead to large differences in biogenic emissions estimates and predicted ozone concentrations in eastern Texas.

Several biogenic emissions models have been developed in the United States, including versions of the Biogenic Emission Inventory System (BEIS) and Model of Emissions of Gases and Aerosols from Nature (MEGAN) (AQRP Project 16-011: Guenther et al., 2017). Comparisons conducted using a similar framework and base data have often differed by more than a factor of two (Warneke et al. 2010; AQRP Project 16-011: Guenther et al., 2017). Johnson et al. (2016) found that isoprene emissions estimates were approximately 20% greater with MEGAN than BEIS, but terpene and soil NO_x emissions were 100% and 400% lower in the Houston-Galveston-Beaumont-Port Arthur domain during early summer and fall periods of 2016. In the eastern United States, use of MEGAN emissions resulted in a higher ozone response to future projected anthropogenic NO_x emission reductions relative to BEIS (Hogrefe et al., 2011).

The TCEQ formerly relied on the Global Biosphere Emissions and Interactions System (GloBEIS) for estimating biogenic emissions but transitioned within the last several years to evaluation of current versions of MEGAN and BEIS in support of regulatory modeling applications (e.g., Boyer, 2016; TCEQ, 2016). AQRP and other recent projects have provided information about the uncertainties and sensitivities associated with MEGAN. For example, AQRP Project 14-008 (McGaughey et al., 2008) demonstrated that MEGAN estimates of isoprene emissions were highly sensitive to the specific soil moisture and wilting point databases employed in the parameterization of water stress on plants during drought. AQRP Project 14-030 (Ying et al., 2015) evaluated the default drought parameterization scheme in MEGAN through comparisons with isoprene field measurements. Other AQRP efforts have investigated the use of different emission factors fields in MEGAN (AQRP Project 14-030: Ying et al., 2015; AQRP Project 14-016: Yu et al., 2015) or other

requisite input parameters such as Photosynthetically Active Radiation (PAR) (AQRP Project 14-017: Pour Biazar et al., 2015).

Studies over different global regions have evaluated MEGAN (primarily version 2.1) estimates of isoprene emissions using ground, aloft, and aircraft measurements as well as satellite remote sensing products (Müller et al., 2008; Langford et al., 2010; Geng et al., 2011; Song et al., 2008; Warneke et al., 2010; Carlton et al., 2011; Palmer et al., 2006; Millet et al., 2008) and indicated both high and low biases relative to observational data. Within Texas, MEGAN estimates of isoprene and monoterpene emissions have demonstrated a persistent high bias compared with aircraft flux data (e.g. Warneke et al., 2010). Predictions from CAMx and the Community Multiscale Air Quality (CMAQ) modeling system that have used MEGAN for biogenic emissions estimates have generally demonstrated a high bias in isoprene and ozone concentrations relative to aircraft and/or ground observations. For example, Kota et al. (2015) found that predicted daytime isoprene concentrations at nine surface sites in the Houston area from MEGAN v.2.1 were significantly higher than local observations when biogenic emissions dominated total isoprene concentrations, with mean normalized bias between 2.0 and 7.7 ppb and mean normalized error between 2.2 and 7.7 ppb.

AQRP projects have guided future improvements to the MEGAN model. AQRP Project 14-030 (Ying et al., 2015) for example, indicated that the use of emission factor fields from BEIS v3.61 and its input data (BELD4) could significantly improve MEGAN's capabilities in reproducing the observed isoprene concentrations in Texas. AQRP Project 14-017 (Pour Biazar et al., 2015) found that use of satellite-derived PAR in MEGAN resulted in lower isoprene emissions estimates (by ~15-29%) relative to PAR fields derived from WRF over Texas climate regions during August and September of 2013.

AQRP Project 16-011 (Guenther et al., 2017) incorporated results from previous Texas AQRP projects and other studies in the development of MEGAN3, a new version of the model. An objective was to improve the transparency, flexibility, and quality assessment of the diverse measurement data used to develop BVOC emission factors. The new MEGAN-Emissions Factor Processor (MEGAN-EFP) synthesizes leaf-level plant trait data, including BVOC emission factors, specific leaf area (SLA), and emission light dependence factor (LDF), with land cover data (ecotype and growth-form fractions) and other information such as canopy vertical variation and vegetation types. Differences in isoprene emissions estimates between BEIS3 and MEGAN 2.1 were found to be largely associated with estimates of SLA (the leaf area to leaf mass ratio), which are required for converting emissions measurements reported on a per-mass to a canopy scale (per-area) basis. MEGAN3 addresses the effects of canopy heterogeneity and stress responses on emissions. These include the addition of BVOC emissions induced by extreme weather and air pollution stress. MEGAN3 is exhibiting improved performance in simulating aircraft isoprene and monoterpene flux measurements relative to MEGAN v2.1. CAMx surface ozone in Texas tends to be lower with MEGAN3 in comparison to MEGAN2.1 (e.g., up to 20 ppb at Houston-Galveston-Brazoria area CAMS sites) in better agreement with observations at CAMS and CASTNET sites.

2.1.3 Evaluation of MOVES NO_x Emissions (AQRP Projects 16-010, 14-014)

Recent chemical transport modeling studies that apply EPA's National Emissions Inventory (NEI) have indicated that NO_x emissions are overestimated. Comparisons with ambient monitoring data, aircraft measurements, and/or satellite-based observations show generally improved agreement with model predictions when NO_x emissions (typically from the mobile source sector) are reduced by

factors ranging between 50% to 100% (Brioude et al., 2013; Anderson et al., 2014; Kota et al., 2014; Canty et al., 2015; Travis et al., 2016). For example, AQRP Project 14-014 (Choi and Li, 2015) used an inverse modeling approach and OMI (Ozone Monitoring Instrument) NO_2 satellite data to constrain NO_x emissions over Southeast Texas. Based on predicted ozone concentrations using a DISCOVER-AQ photochemical modeling episode for September 2013, Choi and Li (2015) estimated that NO_x emissions from Houston mobile sources in the 2011 NEI should be reduced by a factor of two.

Mobile source emissions are primarily estimated using EPA's Motor Vehicle Emission Simulator (MOVES) model, which predicts emissions and energy consumption at the national, state, county, or project level. Bai et al. (2016) note that tunnel studies and direct estimates of mobile source emissions have smaller biases relative to chemical transport modeling but suggest that NO_x emissions from MOVES are overestimated by 40−70% (Fujita et al., 2012, Anderson et al., 2014). Using MOVES predictions based on U.S. default inputs, AQRP Project 16-010 (Bai et al., 2017) performed a CO and NO_x emissions reconciliation analysis representative of morning commute conditions during 2015 at three urban near-road monitoring locations in Texas: El Paso, Houston, and Fort Worth. The study indicated that observed CO/NO_x ratios were consistently underpredicted by MOVES, implying that CO emissions were underestimated and/or NO_x emissions were overestimated. This finding is directionally consistent with studies for other U.S. (e.g. Fujita et al., 2012; Kota et al., 2014) and Texas (e.g., Rappenglück et al., 2013; Souri et al., 2016) areas. Bai et al. (2016) note that the overestimation of NO_x emissions by MOVES has commonly been attributed to emissions from light-duty passenger vehicles (Fujita et al., 2012; Rappenglück et al., 2013; May et al., 2014).

The majority of the previous studies relied on aggregated county-level estimates of mobile source emissions. Various recent studies suggest that the use of national default input data to MOVES causes overestimation of on-road mobile source NO_x emissions reported to the NEI; using local activity data improves county-level NO_x emissions (Koupal et al., 2014). In support of Texas air quality modeling applications, the TCEQ (Kite, 2017) and EPA (2015a) recommend that, where possible, local data inputs to MOVES, such as vehicle miles traveled (VMT), VMT distributions by vehicle type, vehicle fleet age distributions, meteorological data, and fuel specifications be used. Additionally, Kite (2017) emphasizes the importance of using hourly-specific datasets for doing emissions reconciliation analyses because pollutant ratios (e.g., CO/NO_x) are especially sensitive to the fleet mix of light-duty passenger and heavy-duty vehicles that can vary substantially by location, time-of-day, day-of-week and season.

Significantly, employing the best available local data for MOVES in the recent AQRP Project 16-010 analysis (Bai et al., 2017) improved agreement (within 30% but with variability among locations and seasons) between ambient- and emissions-derived CO/NO_x ratios at the El Paso, Houston, and Fort Worth near-road locations. Suggesting a priority for local data collection activities, MOVES analyses demonstrated that the predicted changes in emissions were sensitive to vehicle fleet mix and age distribution but relatively insensitive to vehicle speed distribution and meteorological data.

In support of photochemical modeling applications (such as those used in SIP development for the Dallas and Houston ozone nonattainment areas), TCEQ typically develops emissions inventories for on-road mobile sources that incorporate fine resolution temporally- and spatially-resolved link-based emissions for Texas areas. Recently, Yarwood et al., (2017) used a DISCOVER-AQ

photochemical modeling episode for September 2013 to assess the accuracy of TCEQ's NO_x emissions inventory with respect to NO_x concentrations in the Houston area. A sensitivity simulation that reduced NO_x emissions by a factor of two from Texas on-road mobile sources resulted in diurnal profiles that showed decreased morning peak NO_x concentrations at urban locations relative to observations (and base case predictions). Comparisons to available observed vertical profiles of NO_x also showed overall slight degradation suggesting that on-road NO_x emissions were better represented in the base case compared to the sensitivity scenario. Because predicted concentrations were relatively insensitive to NO_x emissions from non-Texas mobile source emissions, no determination could be made on whether on-road emissions outside of Texas were overstated.

2.1.4 Emissions from Heavy Refining Liquid Storage Tanks (AQRP Projects 17-007)

There has been an increased focus by EPA on VOC emissions from storage tanks associated with crude oil and natural gas production and petroleum refinery operations (EPA, 2011a; EPA, 2011b; EPA, 2015b; EPA, 2015c). There is particular uncertainty associated with emissions of heavy refinery liquids (e.g., fuel oil no. 6, liquid asphalt), which are non-uniform and complex mixtures of many chemical species with vapor pressures that are not known with certainty (Rosselot et al, 2014; US EPA 1988). For example, a study of four storage tanks holding heavy refinery liquids in Maine indicated that reported emissions of VOCs were substantially lower than measured (US EPA, 2015d). TCEQ recently sponsored two projects (Rosselot and Torres, 2014; Rosselot and Allen, 2015) to better understand the composition and properties of heavy refinery liquids and the most appropriate method for determining their vapor pressures. Illustrating the importance of even small uncertainties in vapor pressure on emissions estimates, Rosselot and Allen (2015) demonstrated that applying a vapor pressure value of 0.4 psi instead of 0.5 psi for a fixed-roof storage tank reduced the predicted tank emissions by 35%, while applying a vapor pressure value of 0.6 psi instead of 0.5 psi increased estimated emissions by 60%.

The purpose of AQRP Project 17-007 (Torres et al., 2017) was specifically to identify a reliable means of measuring the vapor pressure of heavy refinery liquids. The study materials for laboratory testing included a known recipe whose modeled vapor pressure could reasonably be expected to be correct within 10%, a hydraulic fluid with manufacturer-provided detailed vapor pressure data, and three field-sourced fuel oil no. 6 samples. The materials were distributed to multiple commercial laboratories for vapor pressure testing using three standard laboratory methods: ASTM D2879 (2010a, isoteniscope), ASTM E1719 (2012, ebulliometry), and ASTM D323 Procedure A (2015, Reid Vapor Pressure). Additionally, staff at The University of Texas operated two automated minimethod instruments: Grabner MINIVAP VP Visions (ASTM D6378, triple expansion method) and Eralytics Eravap EV 10 (ASTM D6378 with modifications designed to accommodate measuring the vapor pressure of heavy refinery liquids).

The results from Torres et al. (2017) found that the minimethod instruments could process samples of heavy refinery liquids with differences often an order of magnitude in measured vapor pressures compared to ASTM D2879 (isoteniscope). Analyses of commercial results and/or in-house testing demonstrated the importance of accounting for or removing dissolved air (and/or water) from the materials being analyzed. Although the vapor pressure results for ASTM E1719 (ebulliometry) agreed with estimates for the "known" material, the results had a relatively flat slope as a function of temperature and the results were obtained at higher temperatures than typical of heated storage tank conditions. ASTM D2879 consistently provided vapor pressures that were below those estimated for

the "known" material, suggesting that the results provided a lower bound on vapor pressure. Results from ASTM D323, which measures the air- and water-saturated vapor pressure of a material at 100°F, were in general agreement but higher than those provided by the other methods likely representative of an upper bound on vapor pressure.

2.1.5 2017 San Antonio Field Study (SAFS) (AQRP Projects 17-SAFS, 17-032, 17-053)

The San Antonio area is one of the most rapidly growing metropolitan regions in the United States. During recent years, ground-level monitoring stations in and around San Antonio have continued to measure maximum daily averaged 8-hour (MDA8) ozone concentrations greater than 70 ppbv. As of November 2017, the MDA8 ozone design value (2015-2017) at the Northwest San Antonio Continuous Ambient Monitoring Station (CAMS) was 74 ppbv (https://www.tceq.texas.gov/cgi-bin/compliance/monops/8hr_attainment.pl), just below the 2008 ozone NAAQS of 75 ppbv. During 2017, the TCEQ and AQRP sponsored the 2017 San Antonio Field Study (SAFS), an intensive measurement period during May 2017. In contrast to Houston and Dallas, San Antonio had not been the focus of previous intensive field campaigns. The objective of the 2017 SAFS was to collect an integrated dataset that could be used to investigate the meteorological, emissions, and atmospheric chemical conditions leading to ozone formation specifically within and around San Antonio.

Three primary components of the 2017 SAFS were supported through AQRP. AQRP Project 17-SAFS provided logistical and infrastructure assistance for the field campaign (Sullivan, 2017). Two additional projects (AQRP Project 17-053: Yacovitch and Herndon, 2017; AQRP Project 17-032: Wood, 2017) supported the collection of measurements by the Aerodyne Research, Inc. (ARI) mobile laboratory. The suite of instruments aboard the mobile laboratory (Table 2.1) were selected by Yacovitch and Herndon (2017) to specifically address 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 monitors that exceed the ozone NAAQS in central Texas.

Table 2.1. ARI gas species and particulate matter composition measurements.

Measurement Species or Class	**Instrument**
Ozone, O_3	2B Tech, 205 (UV absorption)
Carbon monoxide, CO	TILDAS (tunable infrared laser direct absorption spectroscopy)
Carbon dioxide, CO_2	Licor 6262
Nitric oxide, NO	Thermo 42c (chemiluminescence)
Nitrogen dioxide, NO_2	ARI CAPS-NO_2 (cavity enhanced phase shift)
Sulfur dioxide, SO_2	Thermo 41
Formaldehyde, HCHO	TILDAS
Hydrogen peroxide, H_2O_2	TILDAS
Hydrogen cyanide, HCN	TILDAS
Ethyne, C_2H_2	TILDAS
Methane, CH_4	TILDAS
Ethane, C_2H_6	TILDAS
Propane	TILDAS

Measurement Species or Class	Instrument
Various VOCs	I-CIMS-HRTOF (Iodide chemical ionization mass spectrometry-high mass resolving time-of-flight)
Various VOCs	PTR-ToF (proton transfer reaction time-of-flight mass spectrometry)
Various VOCs	GC-EI-TOF-MS (gas chromatograph with electron-impact time-of-flight mass spectrometer)
PM 1.5 size and composition	SP-AMS (soot particle aerosol mass spectrometer)
HO_2 + RO_2 radicals	ECHAMP (Ethane Chemical AMPlifier)

During May 2017, the ARI mobile laboratory was sited at three locations (Figure 2.1) with the timing at each location determined in daily coordination with the TCEQ and AQRP. To complement the suite of ARI measurements, TCEQ sponsored a second mobile laboratory operated by The University of Houston, Rice University, and Baylor University that sampled at a monitoring location just to the south of the San Antonio urban core and at the University of Texas at San Antonio (UTSA). The measurement dataset included meteorological, organic and inorganic gas phase compounds, particle composition and size, and ambient VOC canister measurements. To provide information on meteorological conditions above the surface, TCEQ sponsored a joint effort by The University of Texas at Austin and Sonoma Technologies for the operation of a radar wind profiler and acoustic sounder at UTSA and a ceilometer at Calaveras Lake during May-October 2017. A third TCEQ project supported the collection of ozonesonde launches by St. Edward's University.

At the time of this report, the 2017 SAFS datasets sponsored by the AQRP have been quality assured and delivered to the AQRP database archive. Preliminary analyses highlighted by Wood (2017) have quantified the ozone production rate in the Greater San Antonio area using ECHAMP measurements of HO_2 and RO_2 along with NO mixing ratios. Daytime ozone production rates were typically between 5 and 10 ppb/hr and rarely exceeded 15 ppb/hr; analysis of the HO_x destruction rates suggest that conditions were almost always NO_x-limited. Yacovitch and Herndon (2017) note that isoprene and its photoproducts measured by the CIMS and the PTR instruments appear to be dominated by organic nitrates at UTSA, which suggests that biogenic VOCs play a significant role in net ozone production in San Antonio**.** Initial analyses suggested that oil and gas VOC compounds (e.g., methane, ethane, propane), while elevated, were not competitive with biogenic VOCs during May 2017, but additional work is needed to quantify formation of nitrogen-containing oxidation products.

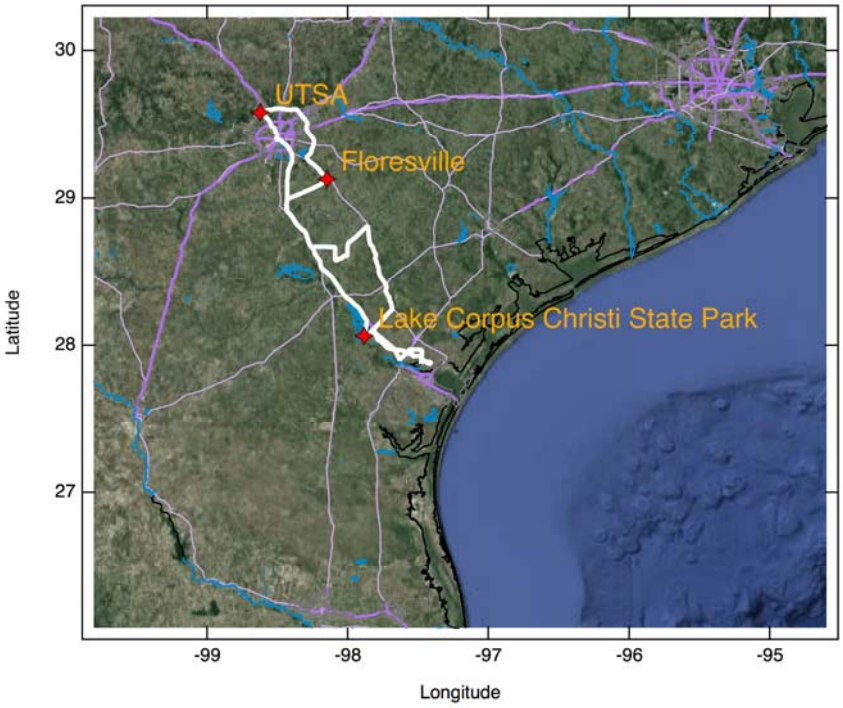

Figure 2.1. Measurement locations for AQRP Project 17-053 during May 2017. Red diamonds indicate the locations where the mobile laboratory was stationed. The white line indicates the route of the mobile laboratory.

2.2. AQRP Projects 2010-2015

2.2.1 Temporal Trends in HRVOC Emissions (AQRP Projects 10-006, 10-045, 13-005, 14-007)

Observational evidence indicated substantial reductions in emissions of ozone precursors in the Houston area between the TexAQS 2000 and TexAQS II field campaigns. Washenfelder et al. (2010) measured reductions of 29% ± 20% in NO_x emissions between August 2000 and September 2006 in the Houston industrial area. However, measurements during both campaigns also suggested that emission inventories significantly underestimated industrial VOC emissions in Houston (e.g., Ryerson et al., 2003; De Gouw et al., 2009; Parrish et al., 2009; Mellqvist et al., 2010; Washenfelder et al., 2010; Kim et al., 2011).

AQRP and other efforts supported continued investigation of trends in VOC and HRVOC emissions using a combination of mobile Differential Optical Absorption Spectroscopy (DOAS) and Solar Occultation Flux (SOF) during the 2009 SHARP campaign, (Lefer, 2010), 2011 (AQRP Project 10-006: Johansson et al., 2013) and DISCOVER-AQ campaign in 2013 (AQRP Project 13-005: Johansson et al., 2013; AQRP Project 14-007: Johansson et al., 2015). Alkane emissions were generally stable, but emissions of alkenes exhibited greater variations between 2006-2011 (Johanssen et al., 2014). For example, ethene and propene emissions measured from the Houston Ship Channel were 1,511 kg/h and 878 kg/h, respectively, in 2006, declining to approximately 600 kg/h for both species in 2009 and 2011. AQRP Project 14-007 (Johansson et al., 2015) reported decreases in alkene concentrations measured during the DISCOVER AQ campaign in 2013 relative to earlier campaigns in 2006, 2009 and 2011 but noted that measured VOC emissions were 5-15 times higher than those based on year-specific emission inventories, while for SO_2 and NO_2 the ratios were typically 0.5–2 (Johansson et al., 2014). These findings and others (e.g., AQRP project

10-045: Stutz et al., 2011) suggested the need for continued attention to the representation of alkenes within emissions inventories.

2.2.2 Barnett Shale 2011 Field Campaign (AQRP Project 10-006, 10-024, 10-034, 10-044)

Oil and gas production in the Barnett Shale experienced rapid expansion and economic growth between 2005 and 2010, with production continuing into the present day (e.g., Ethridge et al., 2015). An AQRP-sponsored field campaign conducted in 2011 sought to better understand the effects of Barnett Shale activity on air quality in the region. Aircraft airborne sampling data was used as a complement to ground based monitoring to investigate the atmospheric chemistry, meteorology, and transport of ozone and precursor compounds in and around the Dallas-Fort Worth area.

Aircraft measurements collected by AQRP Project 10-044 (Alvarez et al., 2011) over portions of the Barnett Shale did not find enhancements in ozone concentrations clearly associated with oil and gas emissions under the consistent meteorological conditions (i.e., sunny and hot with persistent near-surface southerly winds of approximately 10 mph) of the study period. Elevated concentrations of reactive alkenes and formaldehyde relative to background concentrations were measured on some occasions, such as immediately downwind of a large compressor station in the Eagle Mountain Lake area. Aircraft measurements within the photochemically aged plume downwind of Dallas-Fort Worth showed modest concentrations of NO, NO_2, and reactive alkenes and indicated enhancements in maximum ozone concentrations by factors of 1.5-2.5 relative to upwind concentrations that ranged between 30 and 50 ppb.

AQRP Project 10-006 (Johansson et al., 2011) used a surface mobile instrument platform to identify and quantify emissions from industrial activities. Significant rates of ethene emissions downwind of two gas treatment facilities with large compressor stations (up to 0.4 kg/hr) and from flash venting from a single condensate tank (2.0 kg/hr) were estimated, in contrast to other studies (e.g., Sullivan, 2010; TITAN, 2010; Zielinska et al., 2011).

AQRP Project 10-034 (Lefer and Brune, 2011) examined temporal and spatial variations of *in situ* net ozone production rates in the Dallas-Fort Worth area, as well as NO_x sensitivity, to determine of the fraction of ozone from background sources relative to that produced locally.
Ozone production rates suggested that that Meacham could be an ozone source region with higher rates than at Eagle Mountain Lake. Findings from AQRP Project 10-024 (Griffin et al., 2011) suggested that air masses transported to Eagle Mountain Lake were aged and originated over the Dallas-Fort Worth metropolitan area with only intermittent impacts of local sources.

More recent investigations focused on the Barnett Shale have estimated an overall significant contribution of light-molecular-weight alkanes (e.g., methane, ethane, propane, butanes, pentanes) from oil and gas production activities to regional VOCs (e.g., Zielinska et al., 2014; Zavala et al., 2014). Monitored concentrations of aromatics such as benzene in the Barnett Shale were consistently below the state and federal health-based exposure levels for acute risks (e.g., Bunch et al., 2014; Marrero et al., 2016). With respect to the potential impacts on ozone concentrations, an evaluation of measurement data collected during 2000-2006 and 2007-2013 found that although the overall trend in ozone concentrations was downward, monitoring sites in non-shale areas had an additional reduction of 4% in the annual numbers of ozone exceedance days compared to those located in the Barnett Shale (Ahmadi and Kuruvilla, 2016).

2.2.3 Industrial Flares
(AQRP Projects 10-009, 10-022, 10-045, 14-009)

Studies during TexAQS 2000 indicated that high temporal variability in emissions from industrial sources, particularly from sources of HRVOCs, were associated with rapid ozone formation in southeastern Texas (Murphy and Allen, 2005; Nam et al., 2006; Webster et al., 2007; Nam et al., 2008; Kleinman et al., 2003; Allen et al., 2004; Vizuete et al., 2008; Olaguer et al., 2009; Henderson et al., 2010). Emissions from industrial flares constituted 45% of all VOC and 77% of all HRVOC emissions in the 2006 Special Inventory that included hourly emissions data from 141 industrial locations (TCEQ, 2008). The temporal patterns of emissions from industrial flaring operations were found to consist of multiple components, including nearly constant, routinely variable, or episodic (Nam et al., 2006; Webster et al., 2007; Pavlovic et al., 2009; Pavlovic et al., 2012). AQRP projects sought to improve the understanding of emissions from flaring events to create improvements in flare operations and air quality in the region.

A key assumption had been that flares operating over the range of requirements stated in Title 40 Code of Federal Regulations (CFR) §60.18 achieved the assumed hydrocarbon destruction and removal efficiency (DRE) of 98-99% at varying vent gas flow rate turndown, assist ratios, and vent gas heat content. The TCEQ 2010 Flare Study (#2010-04) and AQRP Project 10-009 (Task 1: Allen and Torres, 2011) explored flare DRE performance through field tests at the John Zink Company, LLC flare test facility in Tulsa, Oklahoma. The results indicated that at low flow rates, and with low heating value gases, standard emission estimation methods understated emissions if excess steam or air-assist was used. The most efficient industrial flare operation was achieved at or near the incipient smoke point (Allen and Torres, 2011; Torres et al., 2012a; Torres et al., 2012b). Minimum levels of steam or air assist that complied with the flare manufacturer's recommendations should be used when possible.

Air quality modeling of theoretical scenarios with low flaring destruction efficiencies showed that the emission rates of unburned flare gases and chemical reactivity of unburned hydrocarbons explained much of the variability in ozone formation. In addition, unburned flare gases were found to potentially have a larger impact on ozone formation than the products of incomplete combustion (Al-Fadhli et al., 2011; Herndon et al., 2012). Field observations during the FLAIR campaign in 2009 supported these findings (Parrish et al., 2012; AQRP Project 10-045: Stutz et al., 2011). The development of remote sensing technologies (Allen and Torres, 2011) and modeling techniques (AQRP Project 10-009, Task 2: Rawlings et al., 2011; AQRP Project 10-022: Chen et al., 2011; Singh et al., 2012; Lou et al., 2012) offered approaches for improved detection, monitoring, and evaluation of flare operational conditions. Notably, the projects led to the development of a supplemental online flare operations training for plant personnel who monitor elevated, industrial-scale chemical and petrochemical flares (https://sfot.ceer.utexas.edu).

2.2.4 Satellite Observations of NO_2 Column Densities
(AQRP Project 13-TN2, 14-014)

Nitrogen oxides are precursors to both ozone and fine particulate matter. Anthropogenic NO_x emissions in the United States have declined substantially due, largely, to reductions from mobile and stationary point sources. Although emissions from point sources, such as electric generating units, are commonly measured directly using continuous emission monitors (CEMs), other spatially distributed NO_x sources and the sparseness of ground-level monitoring present challenges in tracking the spatial and temporal variations in emissions.

Satellite NO_2 column observations provide an effective proxy to infer NO_x emissions from surface-based sources (e.g., Boersma et al., 2008a; Lamsal et al., 2011; Lamsal et al., 2015; Streets et al., 2013; Tang et al., 2013; Vinken et al., 2014, Lin et al., 2010) and are widely used to estimate trends (e.g., Boersma et al., 2008b; Russell et al., 2012; Zhou et al., 2012; Schneider et al., 2015). For example, Kimura et al. (2012) found that NO_2 column densities in eastern Texas were highest over urban areas and highway corridors and decreased during 2005-2010 in reasonable agreement with changes in surface observations. More recent studies have also indicated declines in NO_2 column densities within various eastern Texas metropolitan areas (Lamsal et al., 2015; Tong et al., 2015). Lamsal et al. (2015) suggested that emissions reductions were greater during 2005-2010 relative to 2010-2013.

NO_2 column retrievals have been widely used to constrain emissions inventories for global and regional modeling (e.g., Boersma et al., 2008a; Kim et al., 2009; Lin et al., 2010; Tang et al. 2013; Tang et al., 2015; Vinken et al., 2014; Duncan et al., 2016), although differences in such top-down emissions estimates can arise between different operational products even if derived from the same satellite dataset (Kemball-Cook et al., 2015). AQRP Project 13-TN2 (Kim et al., 2013) developed techniques and software to more efficiently process and integrate geospatial datasets with air quality modeling predictions. AQRP Project 14-014 (Choi and Li, 2015) used a sector-based inversion methodology and NO_2 columns derived from the Ozone Monitoring Instrument (OMI) to downwardly adjust a National Emission Inventory (NEI) with a known high bias. The adjustments to the inventory, which reduced emissions from anthropogenic sectors and increased emissions associated with biogenic activity, showed improved agreement with available surface and aircraft observations. For example, the root mean square error and bias between simulated NO_x concentrations and aircraft NO_x measurements were reduced from 2.4 to 1.9 ppb and from 6.0 to 4.1 ppb, respectively.

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3. Tropospheric Chemistry

Since its inception, the AQRP program has supported projects focused on atmospheric chemistry in Texas. The unique combinations of industrial and urban emissions, and forested and coastal environments present features in chemical pathways that can be more significant in Texas than other regions. This section summarizes findings from the 2016-2017 AQRP program related to tropospheric chemistry as well as those from previous AQRP project cycles (2010-2015).

3.1 AQRP Projects during 2016-2017 and Related Previous Projects

3.1.1 Alkyl Nitrates from Anthropogenic and Biogenic Precursors (AQRP Projects 16-019, 10-042, and 12-012)

Alkyl nitrates (ANs) have the potential to influence tropospheric ozone and secondary organic aerosol formation over regional to global spatial scales. Primary pathways for the formation of ANs are OH-initiated oxidation of anthropogenic or biogenic VOC precursors in the presence of NO_x during the daytime and O_3 or NO_3-initiated oxidation of VOC precursors primarily at nighttime (Perring et al., 2013; AQRP Project 12-012: Hildebrandt Ruiz and Yarwood, 2013). VOC precursors to alkyl nitrates, including alkanes, alkenes, and aromatics, vary by location with anthropogenic or biogenic emission source regions (Day et al., 2010; Perring et al., 2013). Alkyl nitrates form in the presence of NO_x or NO_3, which are primarily of anthropogenic origin. Thus, the formation of ANs from biogenic hydrocarbon precursors is a main mechanism through which biogenic and anthropogenic emissions interact and affect air quality (Boyd et al., 2015). Advances in analytical techniques and their applications in laboratory studies and major field campaigns have led to new insights on the atmospheric chemistry and fate of alkyl nitrates (Perring et al., 2013; Fisher et al., 2016).

AN functionalities, yields, and fates are known to depend upon the size and structure of the organic backbone (R), as well as the location of the organic nitrate functional group on the backbone. Depending on their structure, ANs can be transported, chemically processed, removed by deposition to vegetation and other surfaces, or undergo partitioning into the aerosol phase where hydrolysis may serve as a loss mechanism (Bean and Hildebrandt Ruiz, 2016; Boyd et al., 2015; Liu et al., 2012). Chemical processing of ANs can result in loss of the nitrate group and release of nitrogen dioxide (NO_2) or retention of the nitrate group but changes in the level of functionality and vapor pressure of the product that influence its fate (Perring et al., 2013). Alkyl nitrates from large precursors (aromatics, terpenes, large alkanes) or chemically aged ANs from smaller precursors (anthropogenic alkenes, isoprene, and smaller alkanes) that have acquired additional functionalization and have lower vapor pressures are expected to partition into the aerosol phase and be subject to loss by hydrolysis or alternatively removed by deposition. Hydrolysis and deposition are processes that act as NO_x sinks. For water-soluble multifunctional organic nitrates, gas-phase dry deposition can be a significant loss process (Nguyen et al., 2015).

Informed by environmental chamber experiments and field measurements, modifications to the chemical mechanisms in CAMx and other photochemical grid models have improved the level of detail regarding the formation and fate of organic nitrates (AQRP Project 10-042: Yarwood et al., 2012; AQRP Project 12-012: Hildebrandt Ruiz and Yarwood, 2013; Fisher et al., 2016, Pye et al., 2015). AQRP Project 16-019 (McDonald-Buller et al., 2017) evaluated the individual and net effects of modifications to the Carbon Bond version 6 gas-phase mechanism (CB6r6d4) and SOA yields in CAMx. These included (1) a reduction in the lifetime of multifunctional organic nitrates against

hydrolysis from 6-hours to 1-hour reflecting recent findings that very short lifetimes are appropriate for acidic aerosols, (2) splitting of α-pinene and other terpenes to account for differences in SOA yields from nitrate radical (NO_3)-monoterpene chemistry, and (3) splitting of paraffinic carbon represented by PAR and PARH where PARH has much higher AN yield and contributes to SOA formation. More rapid alkyl nitrate hydrolysis increased total $PM_{2.5}$ mass concentrations due to an increase in particulate NO_3 primarily in terpene-rich areas of Texas and neighboring states but had negligible effect on regional ozone. Hourly total $PM_{2.5}$ mass concentrations increased by as much as 0.5 $\mu g/m^3$ on average due to an increase in particulate NO_3. Maximum increases in total $PM_{2.5}$ mass concentrations were approximately 6 $\mu g/m^3$ and occurred in areas where the sensitivity of multifunctional organic nitrates to biogenic emissions dominated anthropogenic emissions. Splitting terpenes was also important for $PM_{2.5}$ concentrations in these areas but had little impact on ozone. Differences in hourly total $PM_{2.5}$ mass and organic aerosol were within ± 0.5 $\mu g/m^3$ on average with maximum differences of -2 to +5 $\mu g/m^3$. Updating AN yields from alkanes using the PARH scheme resulted in small (1-2 ppb) widespread increases in ozone concentrations regionally, but increased ozone sensitivity to VOC emissions from the oil and gas sector and other anthropogenic sources

3.1.2 Chemical Pathways for Secondary Organic Aerosol from Isoprene (AQRP Projects 16-031 and 14-003)

The photochemical oxidation of isoprene has been shown to produce significant yields of gas-phase intermediates that contribute to SOA formation. In addition, gas phase oxidation pathways that form SOA precursors can impact ozone production. Predictions of isoprene-derived SOA formation have required fundamental improvements in the gas and aerosol-phase chemical mechanisms of regional and global scale chemical transport models and evaluation of revised mechanisms against controlled chamber experiments (Chen et al., 2015; AQRP Project 14-003: Vizuete and Surratt, 2015).

The production of isoprene-derived SOA is enhanced by anthropogenic emissions, including NO_x and SO_2 typical of urban areas (Budisulistiorini et al., 2015; Surratt et al., 2006, Kroll et al., 2006). Laboratory studies have demonstrated that the major pathway involving the formation of isoprene SOA is the reactive uptake of isoprene epoxydiols (IEPOX) onto acidic sulfate particles. This pathway accounts for more than 40% of the total organic aerosol mass during summer in the southeastern United States (Pye et al., 2013). Acidic sulfate particles are likely to be coated with existing SOA, which may impact the reactive uptake process of IEPOX into the acidic sulfate particles, depending on the phase state of the organic coating (Kroll et al., 2006; Liu et al., 2014).

AQRP Project 16-031 (Vizuete et al., 2017) examined the reactive uptake of IEPOX with varying relative humidity on three different SOA precursors, including SOA produced from the photochemical oxidaiton of toluene, from the photochemical oxidation of naphthalene, or from α-pinene ozonolysis (Hallquist et al; 2009). All types of coatings showed reductions in the reactive uptake process of IEPOX. The relationship between SOA coating thickness and reactive uptake coefficient was non-linear, exhibiting a negative correlation. The level of reduction in the reactive uptake coefficients of IEPOX depended on the SOA coating type (e.g., α-pinene SOA < naphthalene SOA) that was likely associated with differences in SOA viscosities.

A heterogeneous reaction parameterization algorithm was implemented in a 0-D model to account for the effects of organic SOA coatings as well as other parameters (i.e., relative humidity, diffusion in particle phase, particle reactivity) on uptake parameters of IEPOX. Microscopy data supported adoption of a core-shell morphology resistor coating approach for modeling the acid-catalyzed reactive uptake of IEPOX (Gaston et al., 2014). The 0-D model was used to predict 2-methyltetrols

(tetrols) and organosulfates (IEPOXOS) focusing on simulation of the field measurement period during the 2013 SOAS campaign at the Look Rock (LRK), Tennessee ground site. Overall, the modeling showed a 30% reduction in the reactive uptake coefficient of IEPOX across all modeling days when existing coatings were included. Tetrol and IEPOXOS concentrations were reduced on average by 20%-30%.

3.2 AQRP Projects 2010-2015

3.2.1 Sources and Concentrations of Ambient Formaldehyde (AQRP Projects 10-006, 13-005, 14-002, 14-045)

Formaldehyde originates from primary emissions sources, as well as secondary chemical production through the photochemical oxidation of biogenic and anthropogenic VOCs during the daytime and via ozone and nitrate radicals at night (Seinfeld and Pandis, 1998; Parrish et al., 2012; Olaguer et al., 2014). AQRP and other studies have characterized formaldehyde emissions and/or concentrations within Houston industrial areas during TexAQS II (Eom et al., 2008), DISCOVER-AQ (AQRP Project 14-002: Fried and Loughner, 2015), SHARP (Lefer, 2009), FLAIR (AQRP 10-045: Stutz et al., 2011) and other measurements campaigns (AQRP Project 10-006: Johansson et al., 2011; AQRP Project 13-005: Johansson et al., 2013). Assessments of the relative contribution of primary sources and secondary chemical production to ambient formaldehyde concentrations and fluxes in Houston have often been divergent (Olaguer et al., 2009; Rappenglück et al., 2010; Buzcu-Guven and Olaguer, 2011; Parrish et al., 2012; Olaguer, 2013; Zhang et al., 2013; Johansson et al., 2014). For example, Parrish et al. (2012) suggested that the major source of formaldehyde in the Houston area was secondary production from alkenes emitted by petrochemical facilities and on-road vehicles. This contrasted with earlier studies indicating a more significant influence of primary emissions (Rappenglück et al., 2010; Buzcu et al., 2011; Johansson et al., 2014). Olaguer et al. (2014) suggested that discrepancies may be due, in part, to differences in the assumed relationship between tracer combustion species and primary emissions, as well as in the spatial and temporal representations of the corresponding measurements. Understanding formaldehyde sources has been recognized as important to defining effective ozone control strategies in the Houston area.

3.2.2 Ozone Production Efficiencies and Precursor Emissions Control Strategies (AQRP Projects 10-008, 10-032, 13-024, 14-020)

During TexAQS 2000, ozone production rates and ozone production efficiencies (OPE) in plumes originating from the Houston Ship Channel complex were found to be greater than those for the Houston urban core and other areas of the United States (Ryerson et al., 2003; Daum et al., 2003; Berkowitz et al., 2004; Kleinman et al., 2005). AQRP Project 13-024 (Ren and Luke, 2013) found OPEs of approximately 16 from observations during the summer of 2013 at a Galveston monitoring location. Zhou et al. (2014) indicated that large OPEs (8–15) occurred in diluted industrial plumes transported over the isoprene-rich northern rural areas, while lower OPEs (5-7) were found in urban and industrial plumes transported southward. AQRP Project 14-020 (Ren, 2015) calculated an average OPE of approximately eight from aircraft measurements during DISCOVER-AQ. Collectively these findings indicated the importance of highly reactive air masses to ozone formation in Houston, the contributions of both anthropogenic and biogenic emissions, and the variability in the locations of high ozone concentrations from highly reactive emissions due to Houston's complex meteorology.

Results from AQRP and other studies (e.g., Kleinman et al., 2005; Xiao et al., 2010; Sommariva et al., 2011) have indicated the importance of both HRVOC and NO_x emissions controls to reduce

ozone concentrations in Texas. In an investigation of the effects of structural and parametric uncertainties on predicted ozone and precursor concentrations, AQRP Project 10-008 (Cohan et al., 2011) identified the importance of emission rates, reaction rate constants, and boundary conditions on Dallas-Fort Worth area ozone concentrations under predominantly NO_x-limited conditions. AQRP Projects 10-032 (Lefer et al., 2011) and 14-020 (Ren, 2015) investigated ozone production sensitivity to NO_x and VOC emissions during field campaigns in southeastern Texas, including TexAQS 2000, TexAQS II Radical and Aerosol Measurement Program (TRAMP) in 2006, SHARP 2009, and DISCOVER-AQ in 2013. High rates of ozone production tended to be associated with VOC-sensitive conditions in the mornings throughout the Houston area, in contrast to the afternoon with primarily NO_x-sensitive conditions. Zhou et al. (2014) noted that periods with the most rapid ozone formation were VOC-sensitive while slow ozone formation was NO_x-limited. These findings have supported the development of strategies aimed at reducing NO_x and HRVOC in the State Implementation Plan (SIP) for Texas.

3.2.3 Nitryl Chloride Chemistry Effects on Tropospheric Oxidation Capacity and Ozone Formation
(AQRP Project 10-015)

Dinitrogen pentoxide (N_2O_5) is a nocturnal reservoir of NO_x formed from the reaction of nitrate radical (NO_3) and NO_2 (Simpson et al., 2015). Heterogeneous reaction of N_2O_5 can proceed via two pathways: hydrolysis to form soluble nitrate (Brown et al., 2009; Parrish et al., 2009) or reaction with chloride to form nitryl chloride ($ClNO_2$) and nitrate (Kercher et al., 2009; Osthoff et al., 2008; Thornton et al., 2010; Roberts et al., 2008). The photolysis of $ClNO_2$ at sunrise can affect oxidant cycling by providing a source of chlorine atoms that enhance VOC oxidation (Osthoff et al., 2008; Knipping and Dabdub, 2003; Tanaka et al., 2003). Chemical transport models have predicted increases in ozone of 1-6 nmol/mol due to $ClNO_2$ production in the Northern Hemisphere with seasonal and spatial variations (Simon et al., 2009; Sarwar et al., 2012; Sarwar et al., 2014).

The presence of nitryl chloride was characterized in the coastal environments of Houston during the 2006 TexAQS/Gulf of Mexico Atmospheric Composition and Climate Study (GoMACCS) (Osthoff et al., 2008). AQRP Project 10-015 (Koo et al., 2012) developed an initial parameterized mechanism for $ClNO_2$ chemistry. CAMx version 6.20 incorporated an extension of CB6r2 chemistry (CB6r2h) to address reactions involving ocean-borne halogen compounds. CB6r2h included updates to the chlorine (Cl) reaction mechanism of Koo et al. (2012) as well as reaction mechanisms for bromine and iodine (Yarwood et al., 2014).

3.2.4 Effects of Emissions Reductions on Nighttime Power Plant Plume Chemistry and Transport
(AQRP Project 10-020)

Plumes from coal-fired power plants are subject to nocturnal transport and chemical processing that may affect air quality downwind. AQRP Project 10-020 (Yarwood et al., 2012) and Brown et al. (2012) analyzed nighttime aircraft intercepts of plumes from two Texas power plants with different control technologies, low NO_x burner technology alone and coupled with selective catalytic reduction (SCR), to demonstrate the effect of NO_x emissions reductions on nighttime NO_x oxidation rates. The spatial extents of nighttime-emitted plumes were found to be limited, and mixing of highly concentrated plume NO_x with ambient ozone was a determining factor for its nighttime oxidation. Plume modeling showed that NO_x controls not only reduced emissions directly but also led to an additional overnight NO_x loss of 36% to 44% on average. The results implied that power plant NO_x emissions controls may produce a larger than linear reduction in next-day, downwind

ozone production following nighttime transport. The findings were also used to guide improvements in the Plume- in-Grid (PiG) formulation in CAMx.

3.2.5 Nighttime Nitrate Radical Chemistry in the Houston Urban Boundary Layer (AQRP Project 10-020)

Aircraft measurements during the second Texas air quality study provided unique insights on the nighttime chemistry and structure of the Houston urban boundary layer. AQRP Project 10-020 (Yarwood et al., 2012) found that production rates for NO_3 were generally higher within NO_x plumes of industrial origin than in rural plumes and plumes that originated from urban Houston and were transported downwind. Nitrate radical was the dominant nighttime oxidant, with net oxidation rates 3-5 times faster than those due to ozone (Brown et al., 2011; Brown and Stutz, 2012). Net VOC oxidation rates due to NO_3 and O_3 were primarily associated with highly reactive alkenes, including isoprene, isobutene, and 1,3-butadiene (Stutz et al., 2009; Brown et al., 2009; Brown et al., 2011; Brown and Stutz, 2012). Biogenic emissions were frequently observed at modest levels within the nocturnal boundary layer and underwent rapid oxidation mainly by NO_3 (Yarwood et al., 2012; Brown et al., 2011). These NO_3-VOC reactions were more significant as a NO_3 loss pathway than heterogeneous reactions of either NO_3 or N_2O_5 in the Houston urban boundary layer, in contrast to other urban locations (Stutz et al., 2009).

3.2.6 Mechanisms for HONO Formation (AQRP Projects 10-032 and 12-028)

Nitrous acid (HONO) is a precursor to the formation of hydroxyl radical (OH). Collectively known as HO_x, OH and hydroperoxyl radical (HO2) have important roles in the formation of ozone and fine particulate matter. Field campaigns, including TexAQS II, TRAMP, SHARP and FLAIR, sought to improve the characterization of HONO and its influence on radical budgets in the Houston area. AQRP Project 12-028 (Lefer et al., 2014; Karamchandani et al., 2015) indicated that photolysis of HONO in the early morning is an important radical production source in Houston. Sources of HONO include production by homogeneous gas-phase reactions, direct emissions from combustion sources, or production by heterogeneous reactions on ground or aerosol surfaces (Karamchandani et al., 2015). Measurements in the Houston area (Olaguer et al., 2009; Wong et al., 2012) and elsewhere (e.g., Wong et al., 2012; Acker et al., 2006a; Acker et al., 2006b, Zhou et al., 2007; Carter and Seinfeld, 2012; Spartaro et al., 2013) indicated that daytime observed HONO mixing ratios were often far larger than the expected photostationary state with OH and NO. Neither direct emissions of HONO nor homogeneous gas-phase reaction of OH with NO was sufficient to replicate observed nocturnal and daytime HONO formation.

Daytime gas-phase and heterogeneous mechanisms on aerosol surfaces were investigated for their contribution to enhanced HONO formation (Bejan et al., 2006; Li et al., 2008); Zhang et al., 2009; Lefer et al., 2010; Stemmler et al., 2006; Zhou et al., 2011; Ziemba et al., 2010). Wong et al. (2012) and AQRP Project 10-032 (Lefer et al., 2011) found that a likely source of daytime HONO could be photocatalytic conversion of gas-phase NO_2 on the ground. Karamchandani et al. (2015) implemented a surface model in CAMx that allowed heterogeneous production of HONO through a representation of the surface as a reservoir of deposited species that can sorb or penetrate soils and vegetation and undergo chemical processing and re-emission to ambient air. Couzo et al. (2015) found that this parameterization reduced the normalized mean error of modeled concentrations by 30-45% relative to SHARP measurements and had more significant effects than increases in direct HONO emissions.

3.2.7 NO_x Sink and Recycling Reactions and Gas-Particle Partitioning of Organic Nitrates (AQRP Projects 10-042 and 12-012)

Advances in the understanding the chemistry and gas-particle partitioning of organic nitrates from ambient and laboratory studies (e.g., Rollins et al., 2010; Liu et al., 2012; Rollins et al., 2013; Rindelaub et al., 2015; Bean and Hildebrandt Ruiz, 2015; Lee et al., 2015) have led to modifications in the chemical mechanisms of CAMx and other photochemical grid models. Environmental chamber experiments conducted as part of AQRP Project 10-042 (Yarwood et al., 2012) provided experimental evidence for NO_x production when organic nitrates degraded by OH reaction and photolysis and provided an initial foundation for modifications to the Carbon Bond mechanism in CAMx (CB6r1 mechanism). The CB6r2 mechanism was developed during AQRP Project 12-012 (Hildebrandt Ruiz and Yarwood, 2013) to improve the level of detail regarding the formation and fate of organic nitrates.

3.2.8 Representation of Alkene Chemistry in an Atmospheric Chemical Mechanism (AQRP Project 12-006)

Seven alkenes (ethene, propene, 1,3-butadiene, 1-butene, isobutene, trans-2-butene, and cis-2-butene) associated with industrial emissions have been classified as HRVOCs (Texas Administrative Code, Title 30, Part 1, Chapter 115; TCEQ, 2012) which contribute to ozone production. Condensed chemical mechanisms used for air quality modeling include versions of the Carbon Bond (CB) (Yarwood et al., 2005; Whitten et al., 2010; Yarwood et al., 2010) and Statewide Air Pollution Research Center (SAPRC) (Carter, 2000; Carter, 2010) mechanisms. These mechanisms were designed to model ozone formation from typical urban ambient VOC mixtures not under conditions influenced by HRVOC emissions. AQRP Project 12-006 (Heo and Carter, 2014) conducted environmental chamber experiments to evaluate the representation of alkene chemistry for HRVOCs and other VOCs in these mechanisms and implemented the SAPRC mechanism with varying levels of VOC lumping in CMAQ (Byun and Schere, 2006) to simulate ozone concentrations during the TexAQS II time period. The project indicated that an intermediate explicit representation of VOC species could yield benefits in performance as well as computational feasibility for routine air quality modeling applications. It also provided insights on the need for reliable emissions data as well as lumping methods for alkenes that could guide future chemical mechanism developments indicating as an example that explicit modeling of propene and 1,3-butadiene can potentially improve the accuracy of ozone predictions based on the spatial variability of their emissions in southeastern Texas.

3.2.9 Rate of Sulfur Dioxide to Sulfate Transformation in the Houston Ship Channel (AQRP Project 12-013)

The primary NAAQS for sulfur dioxide (SO_2) requires that the 99th percentile of 1-hour daily maximum concentrations averaged over 3 years not exceed 75 ppb. Fossil-fueled power plants and industrial facilities are the main sources of SO_2 emissions within the United States. The EPA (2010) recommended the use of the AERMOD steady-state Gaussian plume model for near-source 1-hour SO_2 modeling assuming no chemical transformation. Photochemical oxidants convert SO_2 to sulfate thereby reducing SO_2 concentrations. AERMOD does not treat photochemical oxidants and represents SO_2 transformation as a simple exponential decay process. This approach may not be appropriate for the reactive atmosphere of the Houston Ship Channel that may have more rapid SO_2 to sulfate conversion rates. Using aircraft measurements collected during TexAQS II in the Houston Ship Channel area, AQRP Project 12-013 (Koo and Morris, 2013) determined a representative SO_2 transformation rate of 0.04 hr^{-1} (half-life of 17 hours). This rate was higher than that reported for power plant plumes. This rate can be used with the AERMOD model to simulate 1-hour SO_2

concentrations within the Houston Ship Channel region.

3.2.10 Particulate Matter Sources and Composition in Southeastern Texas (AQRP Projects 12-032, 13-022, 14-005, 14-009,14-029)

Over the past 15 years, measurements during field campaigns have been made to better characterize particulate matter size, composition and concentrations in southeastern Texas and elsewhere (Zhang et al., 2015). TexAQS 2000 coincided with Gulf Coast Aerosol Research and Characterization Program (GC- ARCH) or the Houston Supersite, which improved the understanding of the concentrations, spatial and temporal variability, composition, and sources of fine particulate matter (i.e., particles with diameters less than or equal to 2.5 micrometers) in southeastern Texas (Russell et al., 2004). Measurements conducted during the SHARP, TexAQS/GoMACCS 2006, and DISCOVER-AQ campaigns continued to improve the understanding of the spatial and temporal characterization of fine particulate matter composition and sources and to develop new measurement approaches for characterizing aerosol concentration, size distribution, and optical properties (AQRP Project 14-005: Brooks and Yang, 2015). The Texas Air Quality Research Program supported several projects that collected measurements during the DISCOVER-AQ campaign.

AQRP Projects 13-022 (Griffin et al., 2014) and 14-009 (Griffin and Lefer, 2015) examined zonal-based spatial variations of submicron particulate matter composition across Houston during the DISCOVER-AQ campaign (Leong et al., 2017). Organic aerosol and sulfate were identified as important particulate matter species (Griffin and Lefer, 2015). Organic aerosol components, including hydrocarbon-like organic aerosol and forms of oxygenated organic aerosol representing less-aged fresh SOA or aged and oxidized regional SOA, were identified. Secondary organic aerosol represented more than 90% of organic aerosol in much of Houston except for the central core that exhibited a more primary character consistent with sources of primary aerosol such as motor vehicles. Higher levels of isoprene and monoterpenes that could contribute to SOA production were predicted in northwestern Houston than other zones. The relative importance of less-aged fresh SOA indicated the influence of anthropogenic and biogenic VOC emission sources and regional transport.

AQRP Projects 12-032 (Sheesley and Usenko, 2013) and 14-029 (Sheesley and Usenko, 2015) characterized sources of fossil and contemporary carbon in particulate matter at selected sites in the Houston area using radiocarbon analysis. For example, Moody Tower, an urban Houston site, had a consistent primary motor vehicle exhaust contribution of 18-27%, a fossil SOA contribution that varied from 5-33%, and biogenic SOA contribution of 40-75%. Conroe, a site north of Houston indicative of aged urban aerosol and biogenic emissions, had a lower contribution of motor vehicle exhaust (5-10%), a similarly variable fraction of fossil SOA (4-25%), and a biogenics contribution of 60-79%.

These findings were generally consistent with those of earlier studies. Measurements during TexAQS 2000 and GC-ARCH (Allen, 2005) indicated that fine particulate matter composition in southeast Texas was dominated by sulfate primarily from regional sources and organic carbon of regional and local origin. Fires can be an important event-based contributor to fine particulate matter mass. Secondary organic aerosol formation was associated with reactions of biogenic and anthropogenic precursors. Particle size distributions were not spatially homogeneous with higher concentrations of ultrafine particles in the industrial area than more residential sites. Yu et al. (2009) found that measured organic, elemental, and total carbon during the SHARP campaign were comparable to observations in the early 2000s (Allen, 2004, 2005). Bahreini et al. (2009) found greater organic aerosol mass downwind of the Houston industrial center relative to the urban area

during TexAQS 2006.

3.2.11 Contribution of Intermediate Volatile Organic Compounds (IVOCs) to Secondary Organic Aerosol Formation (AQRP 14-024)

Over half of fine particulate matter in the Houston region is composed of organic material, including primary organic aerosol (POA) and secondary organic aerosol (SOA), from sources such urban and industrial anthropogenic activity, fires, and biogenic VOCs. The importance of organics in understanding and controlling fine PM mass in the Houston region has been recognized in field campaigns such as TexAQS 2000 and DISCOVER-AQ in 2013. Gas-phase precursors of SOA are classified (in decreasing order of vapor pressure/volatility) as volatile organic compounds (VOC), intermediate volatility organic compounds (IVOC) or semivolatile organic compounds (SVOC). AQRP Project 14-024 (Hildebrandt Ruiz et al., 2015) identified potential IVOCs in a review of emissions inventories from point sources in Harris County. Five of six IVOCs examined in laboratory chamber experiments formed SOA.

The project applied CAMx with the 1.5-dimensional volatility basis set (1.5-D VBS) to simulate organic aerosol formation in the Houston region during DISCOVER-AQ. Emissions of IVOCs from major combustion sources were added using IVOC fractions of total non-methane organic gas (NMOG) emissions estimated from laboratory studies. Ambient air quality data analyses during DISCOVER-AQ were used to guide model improvements. Biases in modeled versus observed organic carbon and chemically aged oxygenated OA (OOA: anthropogenic and biogenic) were generally within 30% at Houston area sites.

3.2.12 β-hydroxynitrates as Markers for Ozone Enhancements in Houston Industrial Plumes (AQRP 14-026)

β-hydroxynitrates (βHNs) are formed when HRVOCs or isoprene react in the presence of NO_x. AQRP Project 14-026 (Yarwood et al., 2015) developed a novel approach to link observed enhancements of ozone and formaldehyde to reactions of specific HRVOCs and isoprene in Houston Ship Channel plumes, leveraging aircraft measurements of C2-C5 hydroxynitrates collected during the Studies of Emissions and Atmospheric Composition, Clouds and Climate Coupling by Regional Surveys ($SEAC^4RS$) campaign in 2013. Ozone enhancements in plume intercepts ranged from 4 to 54 ppb with 6-24% directly attributable to HRVOC and isoprene emissions (as indicated by O_3/βHN ratios). Direct contributions of individual HRVOCs to the anthropogenic ozone enhancement ranked on average (in descending order) as ethene, propene, butenes, and butadiene and reflected in part differences in HRVOC reaction rates as plumes were photochemically processed downwind of release. Direct formation of ozone from the HRVOC emissions in the Houston Ship Channel explained 12-25% of the plume ozone increments; the remaining ozone was formed indirectly by the interaction of Houston Ship Channel emissions with emissions of other species such as isoprene. The project found that representing Houston Ship Channel emissions by multiple, narrower source plumes accelerated plume chemistry and improved the performance of the SCICHEM Lagrangian puff model. Plume chemistry was found to be sensitive to whether HRVOCs and NO_x were released together or segregated in separate plumes that interact as they disperse and overlap each other.

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4. Atmospheric Physical Processes and Long-Range Transport of Pollutants

Characterization of atmospheric physical processes and their effects on air quality are essential for air quality planning and management. AQRP projects have focused on improving modeling of physical pollutant loss mechanisms, cloud processes, and meteorological fields as well as understanding the contributions of air pollutants transported over varying spatial scales to air quality in Texas. This section summarizes findings from the 2016-2017 AQRP program as well as those from previous AQRP project cycles (2010-2015).

4.1 AQRP Projects during 2016-2017 and Related Previous Projects

4.1.1 Effects of Regional Background Ozone and Meteorological Events on Houston Area Air Quality (AQRP Project 16-008)

Air quality in the Houston-Galveston-Brazoria (HGB) area has improved substantially over the last 15 years driven by targeted emissions reductions implemented by the TCEQ as well as by the benefits of changes in regional background ozone concentrations (Berlin et al., 2013). In this context, Berlin et al., (2013) refer to regional background as ozone that would be present if none were produced from NO_x and VOC precursors emitted locally on a given day, or emitted on preceding days and recirculated locally by mesoscale circulations such as the land-sea breeze. Berlin et al. (2013) found that transported regional background contributed to more than half of the ozone in HGB on exceedance days (i.e., days when MDA8 ozone > 75 ppb) with a substantial but smaller local contribution. Regional background ozone transported into the HGB area declined by ~7-11 ppb between 1998 and 2012, contributing to reductions in measured surface ozone concentrations in the HGB area. Baseline ozone concentrations in air flowing into Texas from the Gulf of Mexico did not change significantly over this period.

AQRP Project 16-008 (Wang et al., 2017) found that high regional background ozone days often had high peak ozone concentrations in the HGB area during 2000-2015. For example, the 15% highest background ozone days in each single month had peak ozone concentrations that were 30 ppb greater than the other 85% of days and coincided with 55.5% of ozone exceedance days (i.e., when concentrations at two surface monitors in HGB exceeded 70 ppb). Mean peak ozone and regional background ozone over the HGB area declined over 2000-2015. Peak ozone decreased faster than background ozone indicating the key role of in-state emissions reductions. AQRP Project 16-008 estimated that about 62% of exceedance days would have been avoided if background ozone had been reduced by 30%. The same fractional reduction of local ozone would have avoided 40% of exceedance days.

AQRP Project 16-008 (Wang et al., 2017) investigated the effects of meteorological events on peak and regional background ozone concentrations in the HGB area. Stagnation was associated with an increase in the median peak ozone concentration of 26 ppb and background ozone by 16 ppb. The co-occurrence with ozone exceedances was 50% in the spring and 40% in the fall. Cold fronts and post-front events, transporting polluted air masses from the north and northeast, were interrelated and co-occurred with 15% of high ozone days. Post cold front conditions were associated with ozone increases during all seasons, with median enhancements in peak ozone of 11 ppb and in regional background ozone of 12 ppb. Cold fronts had a comparatively smaller effect. Peak ozone and background ozone exhibited a minimum in July, attributable to the strong maritime inflow

driven by the Bermuda High circulation.

4.1.2 Improved Representation of Atmospheric and Land Surface Processes for Meteorological Modeling (AQRP Projects 17-039, 14-004, 14-014, and 14-022)

AQRP and other recent projects have sought to improve the representation of physical processes in the Weather Research and Forecasting model (WRF) that is integral to Texas regional air quality modeling applications. A particular focus has been on Gulf of Mexico coastal areas where the effects of local-scale circulations such as land/sea breezes are often stronger than large-scale meteorological influences during conditions of poor air quality (Olaguer et al., 2009). Studies have evaluated treatments of vertical diffusion and convective mixing (Emery et al., 2009; ENVIRON, 2011; Tang et al., 2011; Li and Rappenglück, 2014; Haman et al., 2014), planetary boundary layer schemes (AQRP Project 12-TN1: Tong et al., 2013; Hu et al., 2010, 2013; Yerramilli et al., 2010; Kolling et al., 2013; Cuchiara et al., 2014; Wilmot et al., 2014) and/or land surface models (Cheng et al., 2008; Misenis and Zhang, 2010; Hegarty et al., 2015).

Meteorological models such as WRF typically incorporate data assimilation (i.e., "nudging") of observations or other analyses to improve near-surface meteorological predictions (e.g., Ngan et al., 2012, Li and Rappenglück, 2014; TCEQ, 2015; AQRP Project 14-014: Choi and Li, 2015). For example, assimilation of radar wind profiler data has reduced uncertainties in the simulation of daytime lower-tropospheric winds and planetary boundary layer heights (Nielsen- Gammon et al., 2007; Zhang et al., 2007; Stuart et al., 2007; TCEQ, 2015). AQRP Project 14-004 (Loughner and Follette-Cook, 2015) applied an iterative observational and data assimilation technique (Appel et al., 2014) to improve WRF simulations of sea/bay breezes that were critical to capturing the magnitude and spatial distribution of ozone concentrations in Houston.

AQRP Projects 14-022 (McNider et al., 2015) and 17-039 (McNider et al., 2017) have focused on the assimilation of satellite data to improve specifications of land surface parameters and WRF performance. The use of satellite observed skin temperatures or skin temperature tendencies for nudging of surface and deep soil moisture and thermal resistance was investigated as an alternative to the use of National Weather Surface (NWS) observations that have coarser spatial resolution. A Moderate Resolution Imaging Spectroradiometer (MODIS)-derived 1-km Green Vegetation Fraction (GVF) product (Case et al., 2014) for the continental United States was applied as an alternative to U.S. Geological Survey (USGS) data to capture seasonal and interannual variations in vegetation. Other evaluations included the use of Geostationary Operational Environmental (GOES) satellite-derived insolation and albedo as alternatives to WRF model-derived data. With the exception of data for albedo, the satellite data assimilation (i.e., insolation, vegetation fraction, skin temperature nudging of soil moisture and heat capacity) has in general improved WRF model performance with respect to 2-m temperature and humidity, wind speed, and skin temperatures statistics in much of Texas and the Eastern U.S. Performance relative to NWS observations in the Western U.S., including portions of Texas west of Amarillo, has indicated more mixed effectiveness. This may be associated with diurnal variations in skin temperature that are not captured by the satellite view angle during the assimilation period but remains a subject of investigation.

4.2 AQRP Projects 2010-2015

4.2.1 Dry Deposition (AQRP Project 10-021)

Dry deposition is estimated to account for 20-25% of total ozone removal from the troposphere globally (Lelieveld and Dentener, 2000; Wild, 2007). On a regional level in Texas, dry deposition represents the most important physical removal mechanism for ozone during the warm spring through early fall seasons (McDonald-Buller et al., 2001). Dry deposition models have been evaluated and inter-compared against observations (Zhang et al., 2002; Michou et al., 2005; Schwede et al., 2011; Park et al., 2014; Val Martin et al., 2014; Wu et al., 2011) yet significant uncertainties remain (Pleim and Ran, 2011). In many locations, including Texas, dry deposition measurements are extremely limited and remain uncharacterized for many compounds, land use/land cover classes, and climatic conditions (Huang et al., 2015).

In regional air quality models such as CAMx or CMAQ, dry deposition is often treated as a first-order removal mechanism with a characteristic dry deposition velocity V_d (ratio of deposition flux and concentration). Dry deposition algorithms (e.g. Wesely, 1989 and Zhang et al., 2003) within regional photochemical models typically employ a resistance approach to transport and surface uptake analogous to Ohm's law in electrical circuits. Estimates of component resistances require characterization of land use/land cover and meteorological parameters. A single land use/land cover category was typically used for urban environments, without representation of their heterogeneity. AQRP Project 10-021 (Corsi et al., 2011) conducted laboratory experiments to determine the surface resistances of fresh and weathered built environment materials. The project applied these resistance estimates with extensive geospatial data of the urban built environment and vegetative cover of Austin, Texas, to examine the modeled effects on the dry deposition of ozone. Changes in predicted daily maximum 8-hour average ozone concentrations were primarily attributed to deposition to urban vegetation and highlighted the importance of characterizing Texas urban landscapes undergoing rapid development.

4.2.2 Boundary Conditions for Regional Chemical Transport Models (AQRP Project 12-011)

Regional chemical transport models, such as CAMx and CMAQ require lateral and top boundary conditions that are routinely obtained from global-scale models (Giordano et al., 2015). Common global models employed for North American studies have included the Goddard Earth Observing System - Chemistry model (GEOS-Chem; Bey et al., 2001), the Model for OZone and Related Chemical Tracers (MOZART-4; Emmons et al., 2010), and AM3 (Donner et al., 2011). Representation of the contributions from the stratospheric-tropospheric exchange of ozone and transport of ozone or its precursors from anthropogenic or natural (e.g., wildfires, lightning, biogenic or oceanic) emission source regions in global models can have important influences on regional model performance. Evaluation of global model predictions at the outer boundaries of regional domains, frequently located over remote maritime or terrestrial areas, have utilized satellite datasets (Tang et al., 2009; Pfister et al., 2011; Henderson et al., 2014; McGaughey et al., 2014), observations at surface monitoring sites in remote U.S. regions (McDonald-Buller et al., 2011), ozonesondes (Pfister et al., 2011; Li and Rappenglück, 2014), or aircraft measurements (Tang et al., 2009; Pfister et al., 2011).

AQRP Project 12-011 (Emery et al., 2013) developed boundary condition inputs for CAMx utilizing output from three global models (GEOS-Chem, MOZART, and AM3) and evaluated surface ozone

predictions in the southwest, south central, and southeast regions surrounding Texas and the Gulf of Mexico. Performance of the models was generally comparable with differences associated with the representation of lightning NO_x and stratospheric intrusions. AM3 performance was superior in the southwest where the influence of higher ozone concentrations in the upper troposphere and lower stratosphere played a substantial role in the springtime regional surface ozone pattern.

4.2.3 Regional High Ozone Episodes and Synoptic-Scale Weather Patterns (AQRP Projects 13-016, 14-006, 14-010)

Continental-scale weather patterns establish the frequency of local meteorological conditions favorable for high ozone concentrations (Jacob and Winner, 2009; Ngan et al., 2011; Zhu et al., 2013). Synoptic weather conditions during high ozone episodes in eastern Texas often exhibit a ridge of high pressure in the lower atmosphere that extends south or southwest into the region (McGaughey et al., 2013). This large-scale circulation pattern often occurs in a post-frontal environment and is associated with the long-range transport of continental air with elevated concentrations of ozone and/or its precursors into Texas (Rappenglück et al., 2008; Ngan et al., 2011; 2012; AQRP Project 13-016: Morris and Lefer, 2013; AQPR Project 14-006: Alrick and Morris, 2015; McGaughey et al., 2015). Background ozone concentrations entering Texas vary by transport direction and season (Nielsen-Gammon et al., 2005; Berlin et al., 2013; Morris and Lefer, 2013) and are correlated, in part, to predominant continental-scale weather patterns. Using meteorological data from 1998-2013, AQRP Project 14-010 (Wang, 2015) found that variation in the westernmost extent of the Bermuda High was the most important predictor of monthly ozone concentrations in the Houston-Galveston- Brazoria area.

4.2.4 Simulation of Clouds and Precipitation (AQRP Projects 14-022 and 14-025)

Photochemistry and consequently ozone formation are strongly influenced by clouds, which can both attenuate and enhance the actinic flux of ultraviolet (UV) radiation (Emery et al., 2010; Byun et al., 2007; TCEQ, 2011). In addition, clouds affect the rate and depth of vertical mixing in the lower troposphere (Langford et al., 2010). The vertical depth and spatial and temporal distributions of clouds are among the most difficult meteorological phenomena to accurately simulate (Pour-Biazar et al., 2007; Emery et al., 2010).

AQRP and other studies have focused on improvements to the simulation of clouds and their effects in meteorological and air quality models. For example, assimilation of GOES satellite data in WRF (Pour-Biazar et al.; 2011) and application of GOES data to correct photolysis rates in CMAQ have improved performance of the models (Pour-Biazar et al., 2007). Surface ozone predictions in CAMx were found to be more responsive to the placement of sub-grid clouds than to the application of photolysis rates (ENVIRON, 2011; TCEQ, 2011). In order capture the effects of sub-grid clouds, AQRP Project 14-025 (Emery et al., 2015) developed a “Cloud-in-Grid” treatment for CAMx that simulated the impact of vertical convective transport for both in-cloud and ambient fractions of the grid column and demonstrated improvements in the simulation of boundary layer concentrations of ozone and NO_x.

AQRP Project 14-022 (McNider et al., 2015) found that large differences between WRF and satellite insolation at the surface was largely due to the placement of clouds. Application of a GOES-derived insolation product in WRF reduced model bias and error in 2-m temperatures within Texas. Performance across the entire continental U.S. was sensitive to the characterization of surface albedo, suggesting that application of satellite-derived albedo may be beneficial.

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5. Summary of Projects and Publications from the Texas Air Quality Research Program: 2010-2017

In total 63 research projects and three science synthesis projects have been funded by the AQRP between 2010 and 2017. The projects are listed by funding cycle in Table 5-1 through Table 5-4, with one or more topical areas shown in parentheses. Full project reports are available at the AQRP web site (http://aqrp.ceer.utexas.edu/reports.cfm).

5.1 AQRP Research Projects: 2016-2017

Table 5-1. AQRP Research Projects 2016-2017.

Project Number	Title
16-008	High Background Ozone Events in the Houston-Galveston-Brazoria Area: Causes, Effects, and Case Studies of Central American Fires *(Emission Inventory Development and Assessment; Atmospheric Physical Processes and Long-Range Transport of Pollutants)*
16-010	MOVES-Based NO_x Analyses for Urban Case Studies in Texas ((*Emission Inventory Development and Assessment)*
16-011	A Next Generation Modeling System for Estimating Texas Biogenic VOC Emissions (*Emission Inventory Development and Assessment)*
16-019	The Influence of Alkyl Nitrates from Anthropogenic and Biogenic Precursors on Regional Air Quality in Eastern Texas *(Tropospheric Chemistry)*
16-031	Condensed Chemical Mechanisms for Ozone and Particulate Matter Incorporating the Latest in Isoprene Chemistry *(Tropospheric Chemistry)*
17-007	Evaluating Methods for Determining the Vapor Pressure of Heavy Refinery Liquids *(Emission Inventory Development and Assessment)*
17-024	Improving the Modeling of Wildfire Impacts on Ozone and Particulate Matter for Texas Air Quality Planning (*Emission Inventory Development and Assessment)*
17-032	Spatial Mapping of Ozone Formation near San Antonio *(Tropospheric Chemistry)*
17-039	Use of Satellite Data to Improve Specifications of Land Surface Parameters (*Atmospheric Physical Processes and Long-Range Transport of Pollutants)*
17-053	Identifying and Apportioning Ozone Producing VOCs in Central Texas *(Tropospheric Chemistry)*
17-SAFS	San Antonio Study Logistics Project

5.2 AQRP Research Projects: 2010-2015

Table 5-2. AQRP Research Projects 2010-2011.

Project Number	Title
10-006	Quantification of Industrial Emissions of VOCs, NO_2 and SO_2 by SOF and Mobile DOAS *(Emission Inventory Development and Assessment)*
10-008	Factors Influencing Ozone-Precursor Response in Texas Attainment Modeling *(Tropospheric Chemistry)*
10-009	Additional Flare Test Days for TCEQ Comprehensive Flare Study *(Emission Inventory Development and Assessment)*
10-015	An Assessment of Nitryl Chloride Formation Chemistry and its Importance in Ozone Non-Attainment Areas in Texas *(Tropospheric Chemistry)*
10-020	NO_x Reactions and Transport in Nighttime Plumes and Impact on Next-Day Ozone *(Tropospheric Chemistry)*
10-021	Dry Deposition of Ozone to Built Environment Surfaces (*Atmospheric Physical Processes and Long-Range Transport of Pollutants)*
10-022	Development of Speciated Industrial Flare Emission Inventories for Air Quality Modeling in Texas *(Emissions Inventory Development and Assessment)*
10-024	Surface Measurements and One-Dimensional Modeling Related to Ozone Formation in the Suburban Dallas-Fort Worth Area *(Emissions Inventory Development and Assessment)*
10-029	Wind Modeling Improvements with the Ensemble Kalman Filter (*Atmospheric Physical Processes and Long-Range Transport of Pollutant)*
10-032	SHARP Data Analysis: Radical Budget and Ozone Production *(Tropospheric Chemistry)*
10-034	Dallas Measurements of Ozone Production *(Emission Inventory Development and Assessment)*
10-042	Environmental Chamber Experiments to Evaluate NO_x Sinks and Recycling in Atmospheric Chemical Mechanisms *(Tropospheric Chemistry)*
10-044	Airborne Measurements to Investigate Ozone Production and Transport in the Dallas/Fort Worth (DFW) Area During the 2011 Ozone Season *(Emission Inventory Development and Assessment)*
10-045	Quantification of Hydrocarbon, NO_x and SO_2 Emissions from Petrochemical Facilities in Houston: Interpretation of the 2009 FLAIR Dataset *(Emission Inventory Development and Assessment)*
10_11-DFW	Fort Worth (DFW) Field Study
10-SSA	State of the Science Assessment 2012

Table 5-3. AQRP Research Projects 2012-2013.

Project Number	Title
12-004	DISCOVER-AQ Ground Sites Infrastructure Support
12-006	Environmental Chamber Experiments and CMAQ Modeling to Improve Mechanisms to Model Ozone Formation from HRVOCs *(Tropospheric Chemistry)*
12-011	Investigation of Global Modeling and Lightning NO_x Emissions as Sources of Regional Background Ozone in Texas (*Atmospheric Physical Processes and Long-Range Transport of Pollutants)*
12-012	Interactions Between Organic Aerosol and NO_y: Influence on Oxidant Production *(Tropospheric Chemistry)*
12-013	Development of Transformation Rate of SO_2 to Sulfate for the Houston Ship Channel using the TexAQS 2006 Field Study Data (*Tropospheric Chemistry)*
12-018	The Effects of Uncertainties in Fire Emissions Estimates on Predictions of Texas Air Quality *(Emissions Inventory Development and Assessment)*
12-028	Implementation and Evaluation of New HONO Mechanisms in a 3-D Chemical Transport Model for Spring 2009 in Houston *(Tropospheric Chemistry)*
12-032	Collect, Analyze, and Archive Filters at two DISCOVER-AQ Houston Focus Areas: Initial Characterization of PM Formation and Emission *(Tropospheric Chemistry)*
12-TN1	Investigation of Surface Layer Parameterization of the WRF Model and Its Impact on the Observed Nocturnal Wind Speed Bias *(Atmospheric Physical Processes and Long-Range Transport of Pollutant)*
12-TN2	Development of IDL-based Geospatial Data Processing Framework for Meteorology and Air Quality Modeling *(Atmospheric Physical Processes and Long-Range Transport of Pollutant)*
13-005	Quantification of Industrial Emissions of VOCs, NO_2 and SO_2 by SOF and mobile DOAS during DISCOVER AQ *(Emission Inventory Development and Assessment)*
13-016	Ozonesonde Launches from the University of Houston and Smith Point, Texas in Support of DISCOVER AQ *(Atmospheric Physical Processes and Long-Range Transport of Pollutant)*
13-022	Surface Measurements of PM, VOCs, and Photochemically Relevant Gases in Support of DISCOVER-AQ (*Tropospheric Chemistry)*
13-024	Surface Measurement of Trace Gases in Support of DISCOVER-AQ in Houston in Summer 2013 *(Tropospheric Chemistry)*

Table 5-4. AQRP Research Projects 2014-2015.

Project Number	Title
14-002	Analysis of Airborne Formaldehyde Data Over Houston Texas Acquired During the 2013 DISCOVER-AQ and SEAC4RS Campaigns *(Tropospheric Chemistry)*
14-003	Update and Evaluation of Model Algorithms Needed to Predict Particulate Matter from Isoprene *(Tropospheric Chemistry)*
14-004	Emission Source Region Contributions to a High Surface Ozone Episode during DISCOVER-AQ (*Atmospheric Physical Processes and Long-Range Transport of Pollutants)*
14-005	Sources and Properties of Atmospheric Aerosol in Texas: DISCOVER-AQ Measurements and Validation *(Tropospheric Chemistry)*
14-006	Characterization of Boundary-Layer Meteorology during DISCOVER-AQ Using Radar Wind Profiler and Balloon Sounding Measurements *(Atmospheric Physical Processes and Long-Range Transport of Pollutant)*
14-007	Improved Analysis of VOC, NO_2, SO_2 and HCHO data from SOF, mobile DOAS and MW-DOAS during DISCOVER-AQ *(Emissions Inventory Development and Assessment)*
14-008	Investigation of Input Parameters for Biogenic Emissions Modeling in Texas during Drought Years *(Emissions Inventory Development and Assessment)*
14-009	Analysis of Surface Particulate Matter and Trace Gas Data Generated during the Houston Operations of DISCOVER-AQ *(Tropospheric Chemistry)*
14-010	Impact of Large-Scale Circulation Patterns on Surface Ozone Concentrations in Houston-Galveston-Brazoria *(Atmospheric Physical Processes and Long-Range Transport of Pollutant)*
14-011	Targeted Improvements in the Fire Inventory from NCAR (FINN) Model for Texas Air Quality Planning *(Emission Inventory Development and Assessment)*
14-014	Constraining NO_x Emissions Using Satellite NO_2 Column Measurements over the Southeast Texas *(Emission Inventory Development and Assessment)*
14-016	Improved Land Cover and Emission Factor Inputs for Estimating Biogenic Isoprene and Monoterpene Emissions for Texas Air Quality Simulations *(Emission Inventory Development and Assessment)*
14-017	Incorporating Space-borne Observations to Improve Biogenic Emission Estimates in Texas *(Emission Inventory Development and Assessment)*
14-020	Analysis of Ozone Formation Sensitivity in Houston Using the Data Collected during DISCOVER-AQ and SEAC^{4}RS *(Tropospheric Chemistry)*
14-022	Use of satellite data to improve specifications of land surface parameters *(Atmospheric Physical Processes and Long-Range Transport of Pollutant)*

14-023	Assessment of Two Remote Sensing Technologies to Control Flare Performance *(Emission Inventory Development and Assessment)*
14-024	Sources of Organic Particulate Matter in Houston: Evidence from DISCOVER-AQ Data, Modeling and Experiments *(Tropospheric Chemistry)*
14-025	Development and Evaluation of an Interactive Sub-Grid Cloud Framework for the CAMx Photochemical Model *(Atmospheric Physical Processes and Long-Range Transport of Pollutant)*
14-026	Quantifying Ozone Production from Light Alkenes using Novel Measurements of Hydroxynitrate Reaction Products in Houston during the NASA SEAC^{4}RS Project *(Tropospheric Chemistry)*
14-029	Spatial and Temporal Resolution of Primary and Secondary Particulate Matter in Houston during DISCOVER-AQ *(Tropospheric Chemistry)*
14-030	Improving Modeled Biogenic Isoprene Emissions under Drought Conditions and Evaluating Their Impact on Ozone Formation *(Emission Inventory Development and Assessment)*
	State of the Science Assessment 2015

5.3 Publications

FY10-11

10-006

Johansson, J., Johan Mellqvist, Jerker Samuelsson, Brian Offerle, Jana Moldanova, Bernhard Rappenglück, Barry Lefer, and James Flynn (2014), Formaldehyde Quantitative Measurements and Modeling of Industrial Formaldehyde Emissions in the Greater Houston Area during Campaigns in 2009 and 2011, Journal of Geophysical Research: Atmospheres, 119, DOI: 10.1002/2013JD020159

Johansson, J. K. E., J. Mellqvist, J. Samuelsson, B. Offerle, B. Lefer, B. Rappenglück, J. Flynn, and G. Yarwood (2014), Emission measurements of alkenes, alkanes, SO2, and NO_2 from stationary sources in Southeast Texas over a 5 year period using SOF and mobile DOAS, J. Geophys. Res. Atmos., 119, doi:10.1002/2013JD020485.

10-008

Digar, A., D.S. Cohan, X. Xiao, K.M. Foley, B. Koo, and G. Yarwood (2013). Constraining ozone-precursor responsiveness using ambient measurements. *Journal of Geophysical Research*, 118(2), 1005-1019, doi:10.1029/2012JD018100.

10-009

The following papers were published in the journal Industrial & Engineering Chemistry Research in a Special Issue on Industrial Flaring:

Torres, V.M., Herndon, S., Wood, E., Al-Fadhli, F.M., Allen, D.T., Emissions of Nitrogen Oxides from Flares Operating at Low Flow Conditions, *Industrial & Engineering Chemistry Research,* 51, 12600-12605, DOI: 10.1021/ie300179x (2012)

Pavlovic, R.T., Al-Fadhli, Kimura, Y., Allen, D.T., and McDonald-Buller, E.C. Impacts of Emission Variability and Flare Combustion Efficiency on Ozone Formation in the Houston-Galveston-Brazoria Area, *Industrial & Engineering Chemistry Research,* 51, 12593-12599, DOI: 10.1021/ie203052w (2012).

Knighton, W.B., Herndon, S.C., Franklin, J.F., Wood, E.C., Wormhoudt, J., Brooks, W., Fortner, E.C., and Allen, D.T. Direct measurement of volatile organic compound emissions from industrial flares using real-time on-line techniques: Proton Transfer Reaction Mass Spectrometry and Tunable Infrared Laser Differential Absorption Spectroscopy, *Industrial & Engineering Chemistry Research,* 51, 12674-12684, DOI: 10.1021/ie202695v (2012)

Torres, V.M., Herndon, S., Kodesh, Z., Nettles, R., and Allen, D.T. "Industrial flare performance at low flow conditions: Part 1. Study Overview" *Industrial & Engineering Chemistry Research,* 51, 12559-12568, DOI: 10.1021/ie202674t (2012).

Torres, V.M., Herndon, S. and Allen, D.T. "Industrial flare performance at low flow conditions: Part 2. Air and Steam assisted flares" *Industrial & Engineering Chemistry Research,* 51, 12569-12576, DOI: 10.1021/ie202675f (2012)

Herndon, S.C., Nelson, D.D., Wood, E.C., Knighton, W.B., Kolb, C.E., Kodesh, Z., Torres, V.M., and Allen, D.T., Application of the carbon balance method to flare emissions characteristics, *Industrial & Engineering Chemistry Research,* 51, 12577-12585, DOI: 10.1021/ie202676b (2012)

Al-Fadhli, F.M., Kimura, Y., McDonald-Buller, E.C., and Allen, D.T. Impact of flare destruction efficiency and products of incomplete combustion on ozone formation in Houston, Texas, *Industrial & Engineering Chemistry Research,* 51, 12663-12673, DOI: 10.1021/ie201400z (2012).

The following presentations were given at the Air& Waste Management Association June 2012 Conference, and papers were published in the Conference Proceedings:

Torres, V.M., Allen, D.T., Herndon, S. and Kodesh, Z., Overview of the Texas Commission on Environmental Quality 2010 Flare Study, Air and Waste Association Annual Meeting, Extended Abstract 2012-A-437-AWMA, San Antonio, June 2012.

Torres, V.M., Al-Fadhli, F.M., Allen, D.T., Herndon, S., and Wood, E., NO_x Emissions from Industrial Flaring, Air and Waste Association Annual Meeting, Extended Abstract 2012-A-315-AWMA, San Antonio, June 2012.

10-015
The following papers are currently under development:

Measurements of Nitryl Chloride in Several Metropolitan Areas and Comparison with Regional Models
J.M. Roberts, H. Osthoff, E.J. Williams, B. Lerner, J.A. Neuman, J.B. Nowak, S.B. Brown, W.P. Dube, N.L. Wagner, T.B. Ryerson, I.B. Pollack, J.S. Holloway, A. Middlebrook, R. Bahreini, B. Koo, G. Yarwood
In preparation for Journal of Geophysical Research

Hydrochloric acid at the Pasadena ground site during CalNex 2010 and its role as a source of aerosol chloride
J.M. Roberts, P.R. Veres, A.K. Cochran, C. Warneke, J. de Gouw, R. Weber, R. Ellis, T. Vandenboer, J. Murphy, B. Koo, G. Yarwood
In preparation for Journal of Geophysical Research

10-020
Brown, S. S. et al. (2012), Effects of NO_x control and plume mixing on nighttime chemical processing of plumes from coal-fired power plants, J. Geophys. Res., 117, D07304, doi:10.1029/2011JD016954.

Brown, S. S., Dubé, W. P., Bahreini, R., Middlebrook, A. M., Brock, C. A., Warneke, C., de Gouw, J. A., Washenfelder, R. A., Atlas, E., Peischl, J., Ryerson, T. B., Holloway, J. S., Schwarz, J. P., Spackman, R., Trainer, M., Parrish, D. D., Fehshenfeld, F. C., and Ravishankara, A. R.: Biogenic VOC oxidation and organic aerosol formation in an urban
nocturnal boundary layer: aircraft vertical profiles in Houston, TX, Atmos. Chem. Phys., 13, 11317-11337, doi:10.5194/acp-13-11317-2013, 2013.

In preparation for Atmosphere:
Reactive Plume Modeling to Investigate NO_x Reactions and Transport at Night
Prakash Karamchandani, Shu-Yun Chen, Greg Yarwood, Steven S. Brown, David Parrish

In preparation for Atmosphere:
Modeling Overnight Power Plant Plume Impacts on Next-Day Ozone Using a Plume-in-Grid Technique
Greg Yarwood, Chris Emery, Steven S. Brown, David Parrish

10-021
The Project Investigators presented findings from this project at the Air & Waste Management Association June 2012 Conference. The title of the submitted abstract was *Dry Deposition of Ozone to Built Environment Surfaces* and the authors are Yosuke Kimura, Dustin Poppendeck, Erin Darling, Elena McDonald-Buller, and Richard Corsi

10-022
Kanwar Devesh Singh, Tanaji Dabade, Hitesh Vaid, Preeti Gangadharan, Daniel Chen, Helen G. Lou, Xianchang Li, Kuyen Li, and Christopher B. Martin "Computational Fluid Dynamics Modeling of Industrial Flares Operated in Stand-By Model, "*Industrial & Engineering Chemistry Research* **2012** *51* (39), 12611-12620

Kanwar Devesh Singh, Preeti Gangadharan, Daniel Chen, Helen H. Lou, Xianchang Li, P. Richmond, " Parametric Study of Ethylene Flare Operations and Validation of a Reduced Combustion Mechanism," Engineering Applications of Computational Fluid Mechanics, Vol. 8, No. 2, pp. 211–228 (2014).

Hitesh S. Vaid, Kanwar Devesh Singh, Helen H. Lou, Daniel Chen, Peyton Richmond, "A Run Time Combustion Zoning Technique towards the EDC Approach in Large-Scale CFD Simulations," International Journal of Numerical Methods for Heat and Fluid Flow, Vol. 24 No. 1, 2014, pp. 21-35.

K. Singh, T. Dabade, H. Vaid, P. Gangadharan, D. Chen, H. Lou, X. Li, K. Li, C. Martin, "Computational Fluid Dynamics Modeling of Industrial Flares Operated in Stand-By Mode," Industrial Flares special issue, Ind. & Eng. Chem. Research, 51 (39), 12611-12620, October, 2012.

H. Lou, D. Chen, C. Martin, X. Li, K. Li, H. Vaid, K. Singh, P. Gangadharan, "Optimal Reduction of the C1-C3 Combustion Mechanism for the Simulation of Flaring, " Industrial & Engineering Chemistry Research, Industrial flares special issue, 51 (39), 12697-12705, October 2012.

H. Lou, C. Martin, D. Chen, X. Li, K. Li, H. Vaid, A. Tula, K. Singh, "Validation of a Reduced Combustion Mechanism for Light Hydrocarbons," Clean Technologies and Environmental Policy, Volume 14, Issue 4, pp 737-748, August 2012, DOI 10.1007/s10098-011-0441-6.

Helen H. Lou, Christopher B. Martin, Daniel Chen, Xianchang Li, Kyuen Li, Hitesh Vaid, Anjan Tula Kumar, Kanwar Devesh Singh, & Doyle P. Bean, "A reduced reaction mechanism for the simulation in ethylene flare combustion," Clean Technologies and Environmental Policy, Volume 14, Issue 2, pp 229-239, April 2012, doi:10.1007/s10098-011-0394-9.

10-024

E.T. Gall, R.J. Griffin, A.M. Steiner, J.E. Dibb, E. Scheuer, L. Gong, A.P. Rutter, B.K. Cevik, S. Kim, B. (2016) Lefer, and J. Flynn, Evaluation of nitrous acid sources and sinks in urban outflow, *Atmos. Environ.*, *127*, 272-282.

B. Karakurt Cevik, A.P. Rutter, L. Gong, R.J. Griffin, J.H. Flynn, B.L. Lefer, and S. Kim (2016), Estimates of airmass aging using particle and other measurements near Fort Worth, *Atmos. Environ.*, *126*, 45-54.

A.P. Rutter, R.J. Griffin, B. Karakurt Cevik, K.M. Shakya, L. Gong, S. Kim, J.H. Flynn, and B.L. Lefer (2015), Sources of air pollution in a region of oil and gas development downwind of a large city, *Atmos. Environ.*, *120*, 89-99.

S. Kim, A.B. Guenther, B. Lefer, J. Flynn, R. Griffin, A.P. Rutter, L. Gong, and B. Karakurt Cevik (2015), Field observations of the role of stabilized Criegee radicals in sulfuric acid production in a high biogenic VOC environment, *Environ. Sci. Technol.*, *49*, 3383-3391.

L. Gong, R. Lewicki, R.J. Griffin, A. Rutter, F.K. Tittel, B.L. Lefer, J.H. Flynn, J.E. Dibb, and E. Scheuer (2012), Gas-particle partitioning of ammonia in the Fort Worth, TX area, *American Association for Aerosol Research Annual Conference*, Minneapolis, MN, October 2012. (poster)

B. Karakurt Cevik, L. Gong, R. Lewicki, R.J. Griffin, A. Rutter, F.K. Tittel, B.L. Lefer, J.H. Flynn, J.E. Dibb, and E. Scheuer 2012), Comparison of estimates of airmass aging using particle and other measurements near Fort Worth, TX, *American Association for Aerosol Research Annual Conference*, Minneapolis, MN.

A. P. Rutter, B. Karakurt Cevik, K.M. Shakya, L. Gong, C. Gutierrez, M. Calzada, S. Kim, R.J. Griffin, J.H. Flynn, and B.L. Lefer, Source apportionment of organic aerosols and VOCs near Fort Worth, TX (2012), *American Association for Aerosol Research Annual Conference*, Minneapolis, MN.

S. Kim, A.B. Guenther, T. Karl, B.L. Lefer, J.H. Flynn, R.J. Griffin, and A.P. Rutter, Sub-urban OH response to isoprene chemistry: A case study in the Dallas Fort-Worth area (2012), *American Geophysical Union Winter Meeting,* San Francisco, CA, December 2012. (poster)

10-032

Ren, X., D. van Duin, M. Cazorla, S. Chen, J. Mao, L. Zhan, W. H. Brune, J. H. Flynn, N. Grossberg, B. L. Lefer, B. Rappenglück, K. W. Wong. C. Tsai, J. Stutz, J. E. Dibb, B. T. Jobson, W. T. Luke and P. Kelley (2013), Atmospheric oxidation chemistry and ozone production: Results from SHARP 2009 in Houston, Texas, *Journal of Geophysical Research- Atmospheres,118*,5770-5780,doi: 10.1002/jgrd.50342.

10-042

Heo, G., McDonald-Buller, E.C., Carter, W.P.L., Yarwood, G., Whitten, G.Z. and Allen, D.T. "Modeling Ozone Formation from Alkene Reactions using the Carbon Bond Chemical Mechanism, *Atmospheric Environment*, 59, 141-150, DOI: 10.1016/j.atmosenv.2012.05.042 (2012).

Heo, G. Y. Kimura, E. McDonald-Buller, D. T. Allen, G. Yarwood, G. Z. Whitten Evaluation of a New Toluene Mechanism for Carbon Bond 05 Using Environmental Chamber Data and Ambient Data, Air and Waste Management Association Annual Meeting, Paper #154, Detroit, June 2009

In preparation for Atmospheric Environment: *Environmental chamber experiments to evaluate* NO_x *removal and recycling represented in atmospheric mechanisms for air quality modeling*
Gookyoung Heo, William Carter, Greg Yarwood, Gary Z. Whitten, David T. Allen

In preparation for Atmospheric Environment: *Evaluation of mechanisms for modeling ozone formation from isoprene in SAPRC-07 and CB6 using environmental chamber data with low initial* NO_x
Gookyoung Heo, William Carter, Greg Yarwood

10-045

Olga Pikelnaya, James H. Flynn, Catalina Tsai, and Jochen Stutz (2013), Imaging DOAS detection of primary formaldehyde and sulfur dioxide emissions from petrochemical flares, Journal of Geophysical Research, Volume 118, Issue 15, pages 8716–8728, 16 August 2013, DOI: 10.1002/jgrd.50643

The following papers were published in Industrial & Engineering Chemistry Research Special Issue on Industrial Flaring. The paper edition of this special edition came out in Fall 2012.

W. Berk Knighton, Scott C. Herndon, Ezra C. Wood, Edward C. Fortner, Timothy B. Onasch, Joda Wormhoudt, Charles E. Kolb, Ben H. Lee, Miguel Zavala, Luisa Molina, and Marvin Jones. "Detecting Fugitive Emissions of 1,3-Butadiene and Styrene from a Petrochemical Facility: An Application of a Mobile Laboratory and a Modified Proton Transfer Reaction Mass Spectrometer," *Industrial & Engineering Chemistry Research* 2012 *51* (39), 12706-12711
Ezra C. Wood, Scott C. Herndon, Ed C. Fortner, Timothy B. Onasch, Joda Wormhoudt, Charles E. Kolb, W. Berk Knighton, Ben H. Lee, Miguel Zavala, Luisa Molina, and Marvin Jones. "Combustion and Destruction/Removal Efficiencies of In-Use Chemical Flares in the

Greater Houston Area," *Industrial & Engineering Chemistry Research* 2012 *51* (39), 12685-12696
Pikelnaya, O., J. H. Flynn, C. Tsai, and J. Stutz (2013), Imaging DOAS detection of primary formaldehyde and sulfur dioxide emissions from petrochemical flares, J. Geophys. Res. Atmos., 118,8716–8728, doi:10.1002/jgrd.50643.

This project has also resulted in the following publications:
Olga Pikelnaya, Jochen Stutz, Scott Herndon, Ezra Wood, Oluwayemisi Oluwole, George Mount, Elena Spinei, William Vizuete, Evan Couzo, "*Formaldehyde and Olefin from Large Industrial Sources (FLAIR) in Houston, TX – Campaign Overview",* in preparation for Journal of Geophysical Research

Olga Pikelnaya, Scott Herndon, Ezra Wood, and Jochen Stutz, "*Observations of emissions from ships in the Houston Ship Channel during 2009 FLAIR campaign,"* under development.

FY12-13 12-006

Journal Papers:

Gookyoung Heo, Peng Wang, Qi Ying, Ron Thomas, William P.L. Carter. Using chemically detailed emissions data to test assumptions used in developing chemical mechanisms: a case study for southeast Texas, USA. [To be submitted to Atmospheric Environment in Summer 2014]

Peng Wang, Gookyoung Heo, William P.L. Carter, Qi Ying. Comparison of a detailed and a lumped version of SAPRC-11 photochemical mechanism during a summer ozone episode. [To be submitted to Atmospheric Environment in Summer 2014]

Gookyoung Heo, Chia-Li Chen, Ping Tang, William P.L. Carter. Evaluation of mechanisms for major terminal and internal alkenes with environmental chamber data. [To be submitted to Atmospheric Environment in Summer 2014]

Gookyoung Heo, Shunsuke Nakao, William P.L. Carter. Evaluation of mechanisms for 1,3-butadiene with environmental chamber data. [To be submitted to Atmospheric Environment in Summer 2014]

Conference Paper:

Heo, G., Carter, W.P.L., Wang, P., Ying, Q., Thomas, R. (2013). Evaluating and improving atmospheric chemical mechanisms used for modeling ozone formation from alkenes. Presented at the 12th Annual CMAS Conference, Chapel Hill, NC, October 28-30, 2013.

12-012

Conference presentations:

C. Faxon, J. Bean, L. Hildebrandt Ruiz. Evidence of atmospheric chlorine chemistry in Conroe, TX: Regional implications. American Chemical Society Southwest Regional Meeting, November 2013, Waco, TX.

J. Bean, C. Faxon, L. Hildebrandt Ruiz. Atmospheric processing of pollutants in the Houston Region: First insights from DISCOVER-AQ. American Chemical Society Southwest Regional Meeting, November 2013, Waco, TX.

L. Hildebrandt Ruiz, J. Bean, G. Yarwood, B. Koo, U. Nopmongcol. Formation and Gas-Particle Partitioning of Organic Nitrates: Influence on Ozone Production. American Association for Aerosol Research Annual Meeting, October 2013, Portland, OR.

Planned publications:
C. Faxon, J. Bean and L. Hildebrandt Ruiz. Preliminary title "Significant Inland Concentrations of $ClNO_2$ Detected in Conroe TX during DISCOVER-AQ 2013". Submission planned for August 2014.
J. Bean, C. Faxon and L. Hildebrandt Ruiz. Manuscript summarizing particle-phase measurements from DISCOVER-AQ. Submission planned for late 2014.

13-016
Gary Morris presented a poster entitled "Tropospheric Ozone Pollution Project (TOPP) Overview: A Context for DISCOVER-AQ Houston 2013" at the DISCOVER-AQ Science Team Meeting on February 27, 2014.

13-022
A. Bui, Y.J. Leong, N. Sanchez, H.W. Wallace, and R. Griffin, Distribution, influential factors, and sources of aerosol liquid water during the DISCOVER-AQ 2013 campaign in Houston, TX, *American Association for Aerosol Research Annual Meeting*, Minneapolis, MN, October 2015. (poster)

Y.J. Leong, N. Sanchez, H.W. Wallace, B. Karakurt Cevik, J. Flynn, Y. Han, P. Massoli, C. Floerchinger, E. Fortner, S. Herndon, B. Lefer, and R. Griffin, Overview of surface measurements of submicron particulate matter in the greater Houston area during the DISCOVER-AQ 2013 field campaign, *American Association for Aerosol Research Annual Meeting*, Minneapolis, MN, October 2015.

B. Lefer, J. Flynn, L. Judd, X. Ren, M. Estes, and R. Griffin, The spatial and temporal variability of ozone in the Houston metropolitan area during DISCOVER-AQ and its relation to meteorological conditions, *American Geophysical Union Winter Meeting*, San Francisco, CA, December 2014.

R. Sheesley, T. Barrett, S. Yoon, A. Clark, L. Hildebrandt-Ruiz, R. Griffin, B. Karakurt Cevik, R. Long, R. Duvall, and S. Usenko, Spatial trends in surface-based carbonaceous aerosol, including organic, water-soluble, and elemental carbon, during DISCOVER-AQ in Houston, TX, *American Geophysical Union Winter Meeting*, San Francisco, CA, December 2014. (poster)

H.W. Wallace, Y.J. Leong, B.K. Cevik, M.G. Camp, J.H. Flynn, B.L. Lefer, and R.J. Griffin, Characterization of nocturnal aerosol formation in Houston during DISCOVER-AQ, *American Association for Aerosol Research Annual Meeting*, Orlando, FL, October 2014.

R. Ferrare, J. Crawford, R. Griffin, C. Hostetler, B. Anderson, B. Holben, R. Hoff, A. Beyersdorf, and L. Ziemba, DISCOVER-AQ investigation of aerosol impacts on air quality over Houston, *American Association for Aerosol Research Annual Meeting*, Orlando, FL, October 2014.

H.W. Wallace, Y.J. Leong, B.K. Cevik, M.G. Camp, J.H. Flynn, B.L. Lefer, and R.J. Griffin, Characterization of nocturnal aerosol formation in Houston during DISCOVER-AQ, *International Global Atmospheric Chemistry Quadrennial Meeting*, Natal, Brazil, September 2014. (poster)

H.W. Wallace, Y.J. Leong, B. Lefer, B.K. Cevik, J.H. Flynn, R.W. Talbot, P.L. Laine, B.C. Sive, X. Lan, D. Anderson, Y. Zhou, M. Camp, and R.J. Griffin, Characterization of aerosol organic nitrate in the outflow from Houston, TX, during the DISCOVER-AQ campaign, *American Chemical Society Annual Meeting*, San Francisco, CA, August 2014.

Y.J. Leong, H.W. Wallace, B. Lefer, B.K. Cevik, J.H. Flynn, R.W. Talbot, P.L. Laine, B.C. Sive, X. Lan, D. Anderson, Y. Zhou, M. Camp, R.J. Griffin, Chemical characterization of submicron aerosol emissions in the greater Houston area using an aerosol mass spectrometer on a mobile platform, *American Geophysical Union Winter Meeting,* San Francisco, CA, December 2013. (poster)

13-024

NASA AQAST meeting at Rice University in Houston, TX (Jan. 14-16, 2014), where Xinrong Ren gave a talk titled: "Measurements of trace gases at the Manvel Croix and Galveston sites during DISCOVER-AQ."

NASA DISCOVER-AQ science meeting at NASA Langley in Hampton, VA, where Winston Luke gave a talk titled: "NOAA/Air Resources Laboratory Surface Observations at Galveston and Manvel-Croix: Summary and Comparison with Aircraft Data."

A paper is in preparation with the intent to submit to Atmospheric Chemistry and Physics within about 3 months.

12-028

Implementation and Refinement of a Surface Model for HONO formation in a 3-D Chemical Transport Model. Prakash Karamchandani[1], Chris Emery[1], Greg Yarwood[1], Barry Lefer[2], Jochen Stutz[3], Evan Couzo[4], and William Vizuete[5]. ([1]ENVIRON, [2]University of Houston, [3]University of California-Los Angeles, [4]Massachusetts Institute of Technology, and [5]University of North Carolina.)

Impacts of heterogeneous HONO formation on radical sources and ozone chemistry in Houston, Texas. Evan Couzo[1], Barry Lefer[2], Jochen Stutz[3], Greg Yarwood[4], Prakash Karamchandani[4], Barron Henderson[5], and William Vizuete[1]. ([1]University of North Carolina (now at MIT), [2]University of Houston, [3]University of California-Los Angeles, [4]ENVIRON, [5]University of Florida.)

12-032
Poster at the American Geophysical Union national meeting (Dec 2013) *Initial characterization of surface-based carbonaceous aerosol during DISCOVER-AQ in Houston, TX* Rebecca J. Sheesley, Tate E. Barrett, Subin Yoon, Adelaide Clark and Sascha Usenko

Poster at the DISCOVER-AQ Science Working Group meeting (Feb 2014) *Initial characterization of surface-based carbonaceous aerosol during DISCOVER-AQ in Houston, TX* Rebecca J. Sheesley, Tate E. Barrett, Subin Yoon, Adelaide Clark and Sascha Usenko

Manuscript in preparation. Submission planned to Atmospheric Environment in summer 2014. Draft title: "*Initial characterization of surface-based carbonaceous aerosol during DISCOVER-AQ in Houston, TX*."

12-TN1
Presentation:
"A regional chemical reanalysis prototype" Pius Lee, Greg Carmichael, Tianfeng Chai, Rick Saylor, Li Pan, Hyuncheol Kim, Daniel Tong, and Ariel Stein

Poster:
"Preliminary analyses of flight measurements and CMAQ simulation during Southeast Nexus (SENEX) field experiment" Li Pan, Pius Lee, Hyun Cheol Kim, Daniel Tong, Rick Saylor and Tianfeng Chai

Publication:
Pius Lee, Fantine Ngan, Hang Lei, Barry Baker, Bright Dornblaser, Gary McGaughey, and Daniel Tong. An Application for Improving Air Quality: a Houston Case Study, Earthzine 2014 [available at: http://www.earthzine.org/2014/03/29/an-application-for-improving-air-quality-a-houston-case-study/?shareadraft=baba698217_53330c8eab882]

12-TN2
The project team presented at the Community Modeling and Analysis System (CMAS) Conference in October 2013.

Presentations:
"HCHO and NO_2 column comparisons between OMI, GOME-2 and CMAQ during 2013 SENEX campaign (21 slides)" Hyun Cheol Kim, Li Pan, Pius Lee, Rick Saylor, and Daniel Tong

Posters:
Fine-scale comparison of GOME-2, OMI and CMAQ NO_2 columns over Southern California in 2008" Hyun Cheol Kim, Sang-Mi Lee, Fong Ngan, and Pius Lee