State of the Science of Air Quality in Texas

Scientific Findings from the Texas Air Quality Research Program (AQRP): 2016-2021

Prepared by:
David Allen
The University of Texas at Austin

Mark Estes, Independent Consultant

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Executive Summary

Since its inception in 2010, the Texas Air Quality Research Program (AQRP), administered by the University of Texas under contract to the Texas Commission on Environmental Quality (TCEQ), has had three primary objectives:

- 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;

- to integrate AQRP research with the work of other organizations;

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

During this grant cycle (2016 through 2021), the program has completed three funding cycles that have included the 2016-2017, 2018-2019, and 2020-21 biennia. The AQRP has sponsored 29 projects from researchers throughout the United States (U.S.) during this period. Projects have involved collaborations between academic institutions, national laboratories, 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 synthesizes the scientific understanding of key issues addressed by the AQRP during the 2016-2021 project cycles. Findings are divided into sections corresponding to the areas where the AQRP performs research:

- emissions inventory development and assessment,
- tropospheric chemistry,
- atmospheric physical processes and long-range transport of pollutants,
- chemical transport modeling, and
- field studies.

Among the results, in these areas, that have emerged from studies conducted during the 2016-2021 funding period are:

- Emissions Inventory Development and Assessment: Inventories for various emissions sources have been improved by adjusting inputs and conducting performance evaluations for relevant models. AQRP work during this project cycle included the following biogenic sources, biomass burning, mobile sources, dust, and other categories.
- Tropospheric Chemistry: 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 atmospheric pollutants, including alkyl nitrates (AN) and secondary organic aerosols (SOA) formed from isoprene oxidation.

- Atmospheric physical processes and long-range transport of pollutants: AQRP projects found that high regional background pollutants, stagnation and certain meteorologic patterns (e.g., recirculation) are associated with increased ozone levels in the Houston-Galveston- Brazoria (HGB) area. Biomass burning was found to continue to have large and variable impacts on air quality in Texas. Modeling tools in addition to remote and targeted monitoring efforts can provide important information on days when smoke influences air quality in Texas.
- Chemical transport modeling: Three-dimensional (3-D) chemical transport models, used in the development and evaluation of air quality management plans, require numerous inputs and parameters. Focused chemical mechanism development and evaluation tools were developed that may improve the degree of confidence in chemical transport models.
- Field studies:
    - San Antonio: Daytime ozone production rates were typically between five and ten parts per billion per hour (ppb/hr) and rarely exceeded 15 ppb/hr; analysis of the radicals containing hydrogen and oxygen (HO_X) destruction rates suggested that conditions were almost always nitrogen oxides (NO_x)-limited. Biogenic volatile organic compounds (BVOC) were found to play a significant role in net ozone production in San Antonio. Initial analyses suggested that oil and gas emissions (e.g., methane, ethane, propane), while elevated, were not competitive with BVOCs during the May 2017 field campaign.
    - Ozone measurements over Galveston Bay and the Gulf of Mexico: Modeling data tended to over-predict ozone, particularly on low ozone days. Possible reasons for this include an under-prediction of boundary layer height over the water.

The sections of the full report provide additional detail on 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. More information about these projects is available at http://aqrp.ceer.utexas.edu/ projects.cfm.

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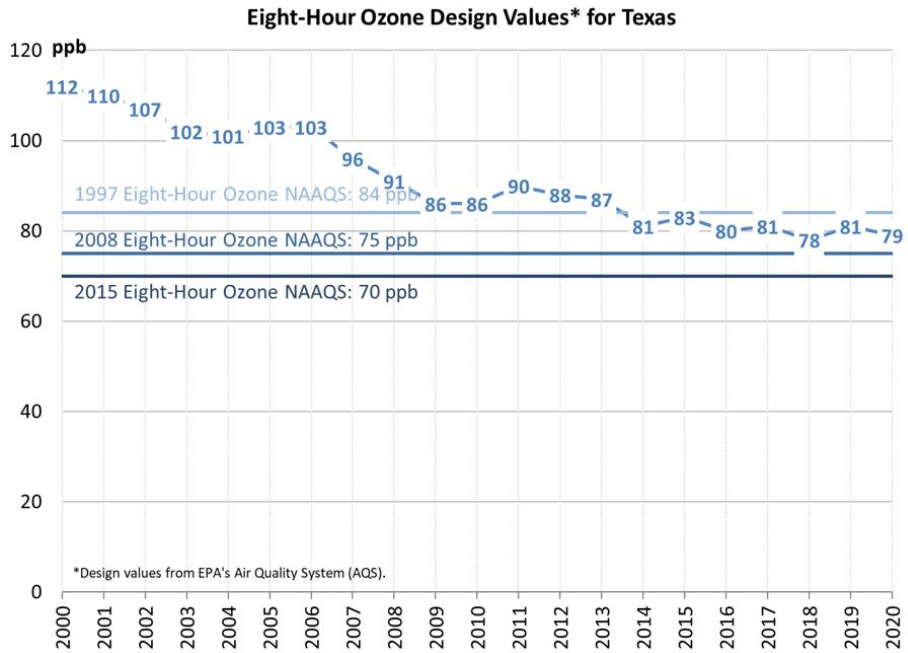
1. Introduction

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 some 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 2020, ozone design values (i.e., the three-year average of the maximum fourth-highest eight-hour ozone concentrations) at regulatory monitors declined by 32% in Texas (Figure 1.1), ranking 10th overall among states and substantially better than the national average decrease of 19% (TCEQ, 2021).

(a)



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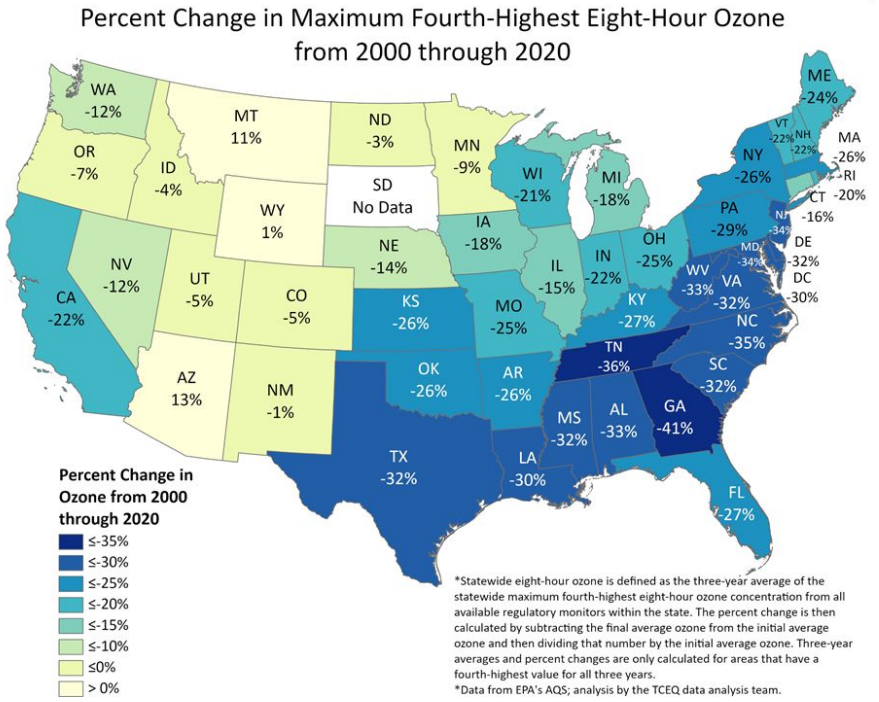
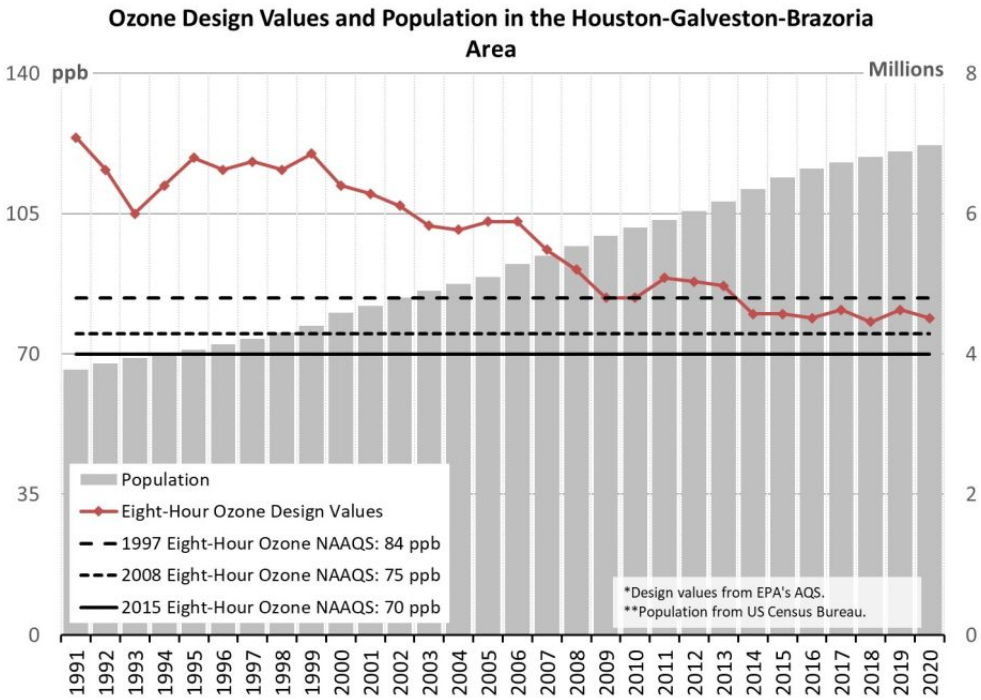


Figure 1.1 (a) Time series of maximum fourth-highest eight-hour averaged ozone concentrations in Texas and (b) percent change in statewide design values from 2000-2020. Source: https://www.tceq.texas.gov/airquality/airsuccess/airsuccesscriteria.

Two of the most populated combined statistical areas (CBSAs) in the U.S., Houston-Galveston-Brazoria (HGB) and Dallas-Fort Worth (DFW), are located in Texas. Decreases in ozone design values in these areas were 36% (HGB) and 28% (DFW) from 1991 through 2020 (TCEQ, 2021). Figure 1.2 shows changes in eight-hour ozone design values from 1991 through 2020 for four metropolitan areas in eastern Texas. Although there is a continuing need for progress towards attainment with the eight-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).

(a)



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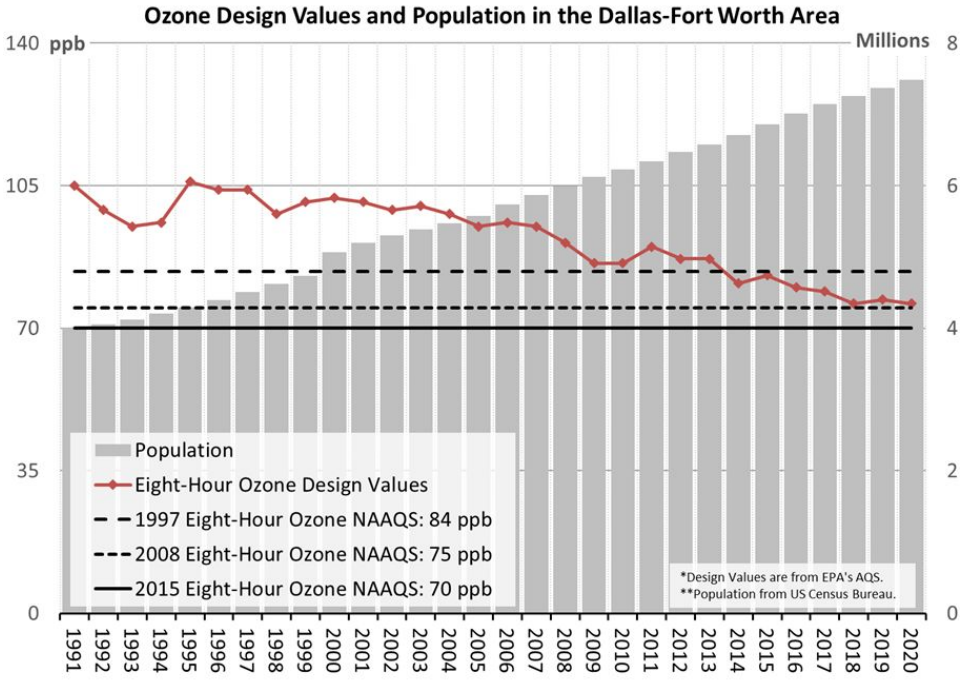
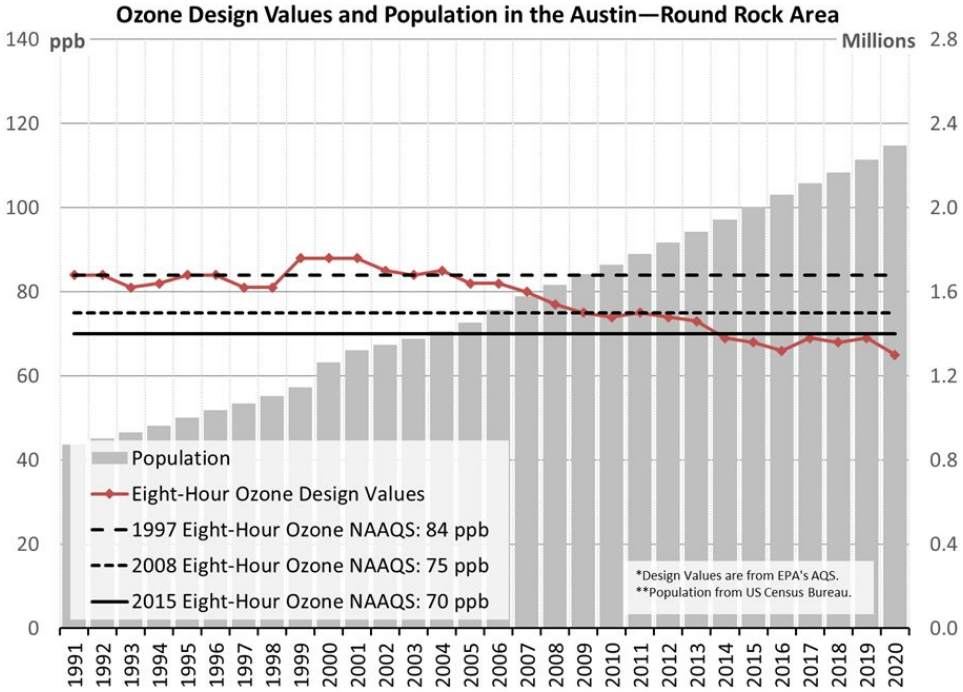

Ozone Design Values and Population in the Dallas-Fort Worth Area
ppb
Millions
140
105
70
35
0
8
6
4
2
0
Population
Eight-Hour Ozone Design Values
1997 Eight-Hour Ozone NAAQS: 84 ppb
2008 Eight-Hour Ozone NAAQS: 75 ppb
2015 Eight-Hour Ozone NAAQS: 70 ppb
*Design Values are from EPA's AQS.
**Population from US Census Bureau.
1991 1992 1993 1994 1995 1996 1997 1998 1999 2000 2001 2002 2003 2004 2005 2006 2007 2008 2009 2010 2011 2012 2013 2014 2015 2016 2017 2018 2019 2020

(c)


Ozone Design Values and Population in the Austin—Round Rock Area
ppb
Millions
140
120
100
80
60
40
20
0
2.8
2.4
2.0
1.6
1.2
0.8
0.4
0.0
Population
Eight-Hour Ozone Design Values
1997 Eight-Hour Ozone NAAQS: 84 ppb
2008 Eight-Hour Ozone NAAQS: 75 ppb
2015 Eight-Hour Ozone NAAQS: 70 ppb
*Design Values are from EPA's AQS.
**Population from US Census Bureau.
1991 1992 1993 1994 1995 1996 1997 1998 1999 2000 2001 2002 2003 2004 2005 2006 2007 2008 2009 2010 2011 2012 2013 2014 2015 2016 2017 2018 2019 2020

(d)

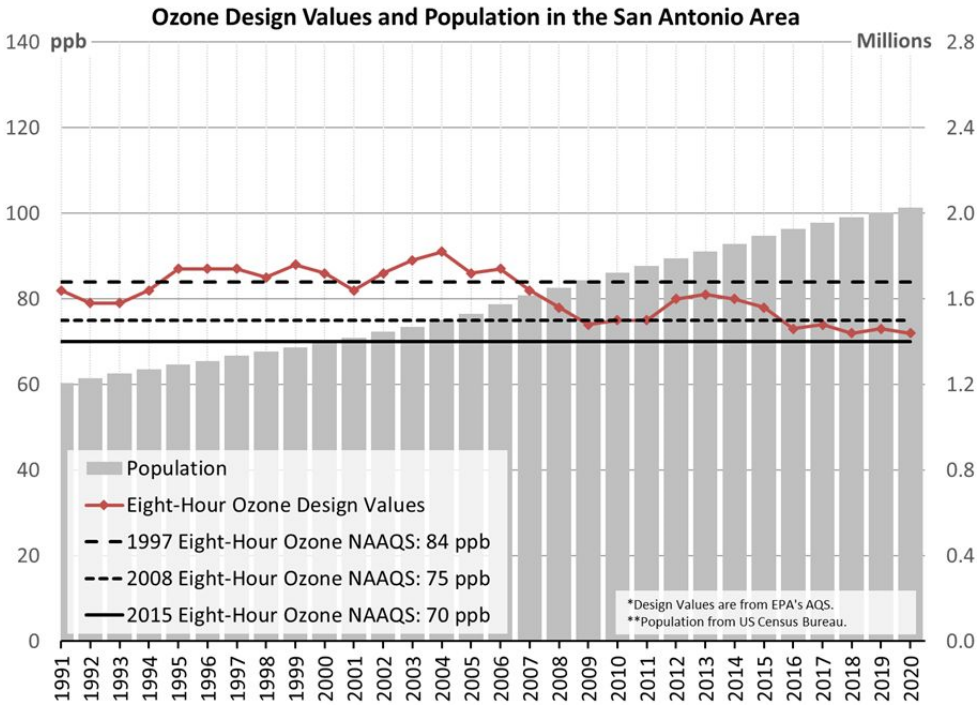
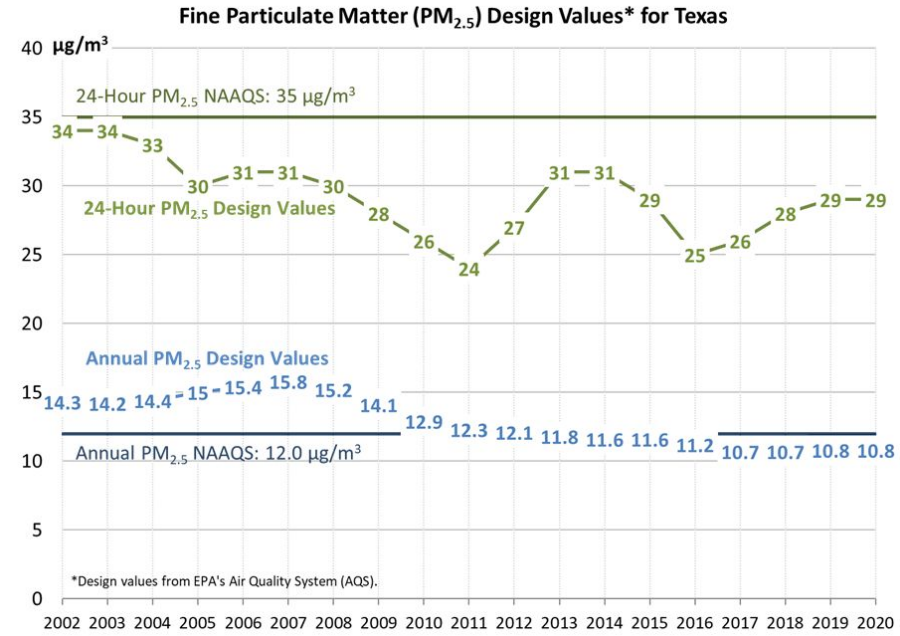
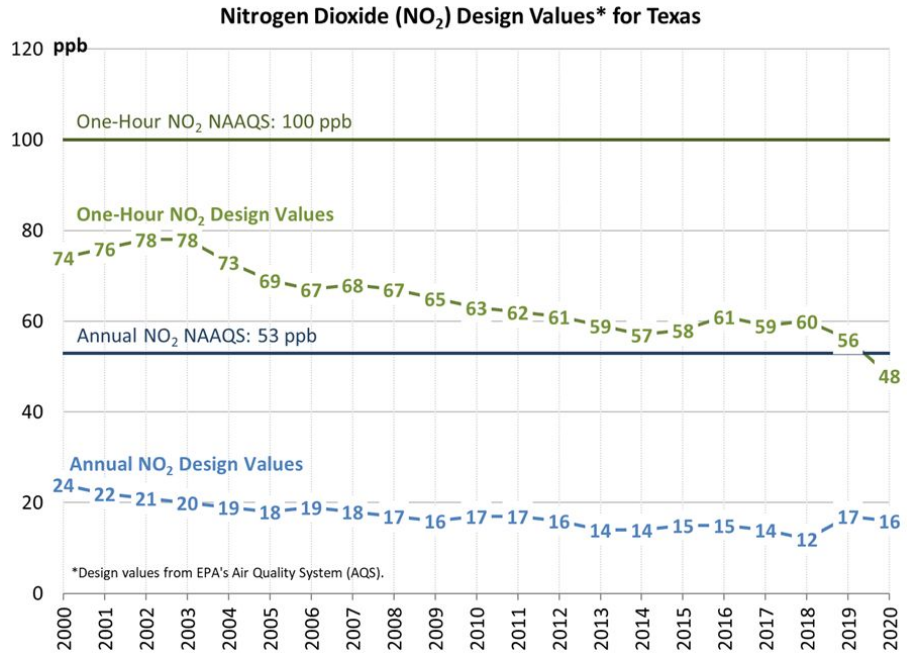


Figure 1.2 Time series of eight-hour averaged ozone design values and population growth for four eastern Texas metropolitan areas: (a) Houston-Galveston-Brazoria, (b) Dallas-Fort Worth, (c) Austin-Round Rock, and (d) San Antonio. Source: https://www.tceq.texas.gov/airquality/airsuccess/airsuccessmetro.

(a)


Fine Particulate Matter ($PM_{2.5}$) Design Values* for Texas
µg/m³
24-Hour $PM_{2.5}$ NAAQS: 35 µg/m³
24-Hour $PM_{2.5}$ Design Values
34 34 33 30 31 31 30 28 26 24 27 31 31 29 25 26 28 29 29
Annual $PM_{2.5}$ Design Values
14.3 14.2 14.4 15 15.4 15.8 15.2 14.1 12.9 12.3 12.1 11.8 11.6 11.6 11.2 10.7 10.7 10.8 10.8
Annual $PM_{2.5}$ NAAQS: 12.0 µg/m³
*Design values from EPA's Air Quality System (AQS).
0 5 10 15 20 25 30 35 40
2002 2003 2004 2005 2006 2007 2008 2009 2010 2011 2012 2013 2014 2015 2016 2017 2018 2019 2020

(b)


Nitrogen Dioxide (NO_2) Design Values* for Texas
ppb
One-Hour NO_2 NAAQS: 100 ppb
One-Hour NO_2 Design Values
74 76 78 78 73 69 67 68 67 65 63 62 61 59 57 58 61 59 60 56 48
Annual NO_2 NAAQS: 53 ppb
Annual NO_2 Design Values
24 22 21 20 19 18 19 18 17 16 17 17 16 14 14 15 15 14 12 17 16
*Design values from EPA's Air Quality System (AQS).
0 20 40 60 80 100 120
2000 2001 2002 2003 2004 2005 2006 2007 2008 2009 2010 2011 2012 2013 2014 2015 2016 2017 2018 2019 2020

(c)

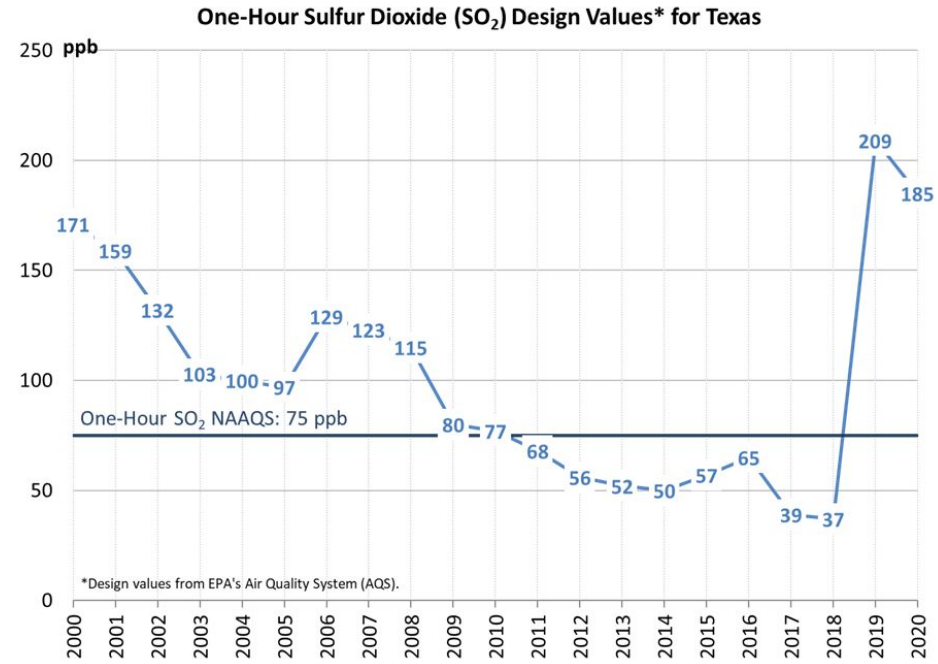
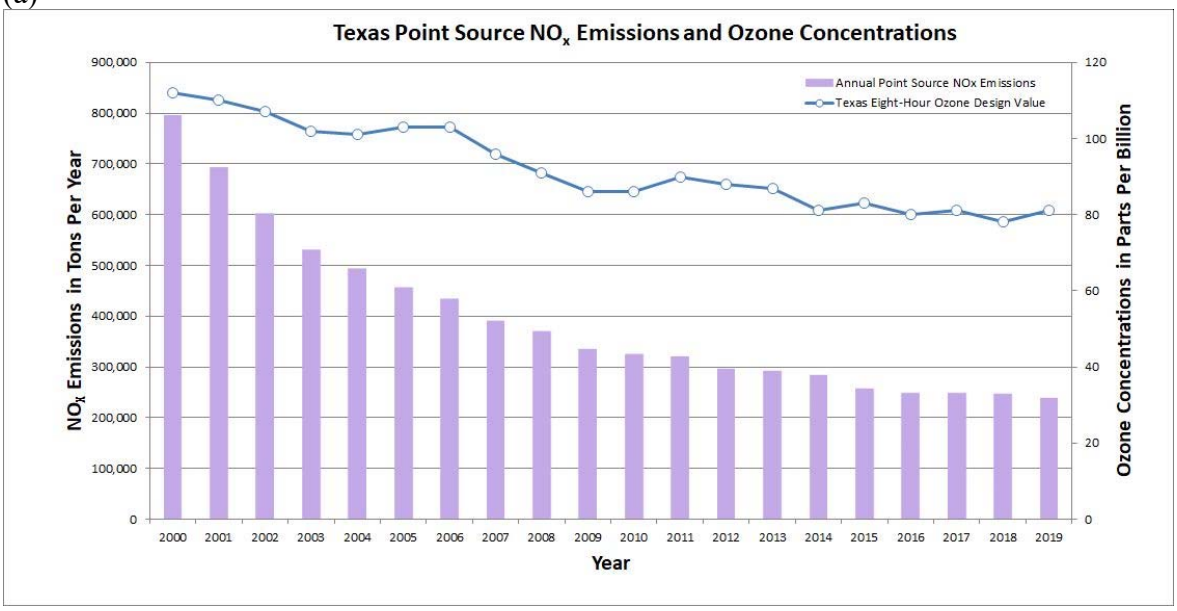


Figure 1.3 Time series of design values in Texas for (a) fine particulate matter ($PM_{2.5}$) (annual average and maximum daily) (b) nitrogen dioxide (NO_2) (annual average and maximum one-hour), and (c) sulfur dioxide (SO_2) (increase in the last several years has been driven by new monitors located near sources). Source: https://www.tceq.texas.gov/airquality/airsuccess/airsuccesscriteria.

Identifying effective, efficient approaches to reduce emissions and 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 1.1-1.4. These investments have helped to design emission reduction strategies to be most effective for conditions in Texas.

(a)



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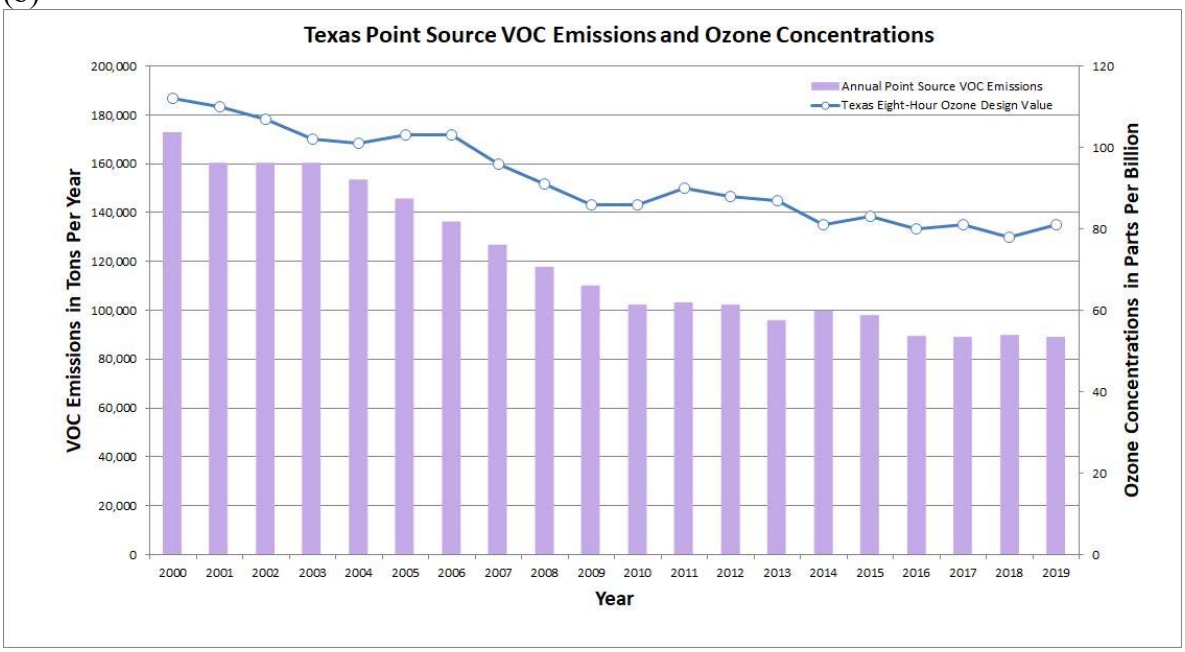

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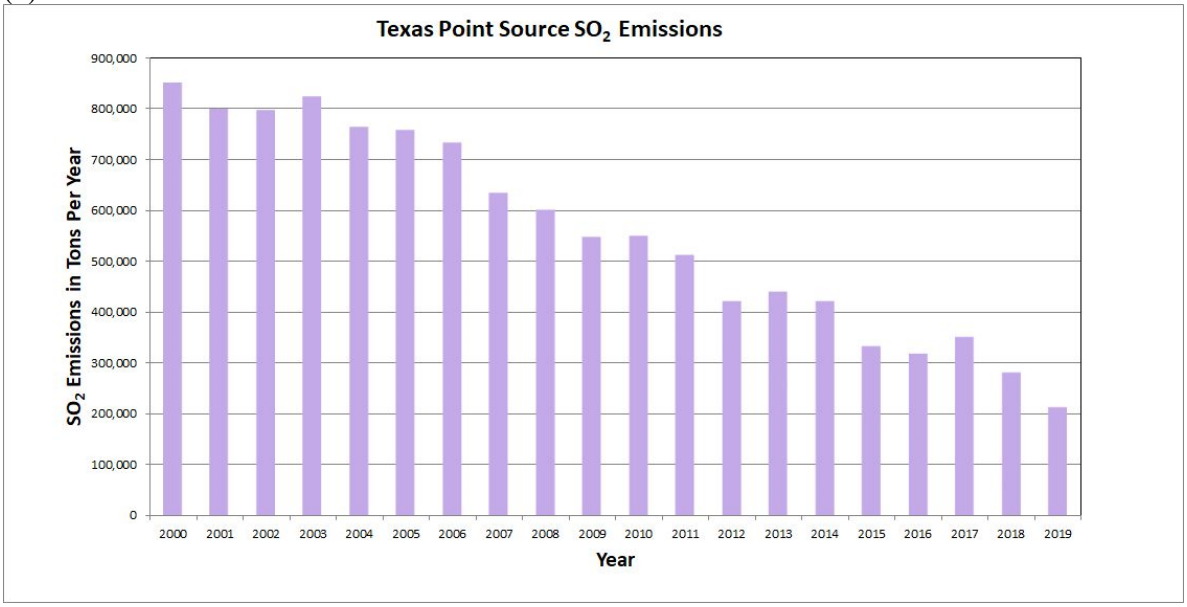

Figure 1.4 Time series of point source emissions in Texas for (a) NO_x, (b) volatile organic compounds (VOC), and (c) SO_2 from 2000-2016. Ozone concentrations are shown along with point source emissions for nitrogen oxides and VOC, since these emissions react in the atmosphere to form ozone. Source: https://www.tceq.texas.gov/airquality/airsuccess/airsuccessemissions.

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 overall air quality improvement. 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, http://dept.ceer.utexas.edu/ceer/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 (HRVOC: 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. For further information please see TCEQ's webpage: Houston-Galveston-Brazoria: Ozone History, https://www.tceq.texas.gov/airquality/sip/hgb/hgb-ozone-history. TexAQS II in 2005 and 2006 (TexAQS II, https://www.tceq.texas.gov/airquality/research/texaqs) 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 HRVOC initially raised during the TexAQS 2000 campaign. For example, two campaigns in 2009 (the Study of Houston Atmospheric Radical Precursors or SHARP and Formaldehyde

and Olefin from Large Industrial Releases or FLAIR) sought better characterization of olefin, formaldehyde, and free radical sources in southeast Texas (Lefer et al., 2010; Stutz et al., 2010). 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 (Torres, 2010). The effort ultimately guided the development of new operational performance recommendations for industrial flares (U.S. EPA, 2012). Since 2010, the Texas Air Quality Research Program (AQRP) has continued to contribute to the support of field measurements campaigns. These have included studies in 2016-2021 to perform mobile measurements for the region from Corpus Christi to San Antonio, a region that had previously seen limited scientific field studies.

The AQRP has also contributed extensive support for ambient air quality and meteorological data analyses, 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, emissions from fires, and emissions of dust, and new understanding of the contributions of the long-range transport of ozone and its precursors to air quality in Texas. In the period covered by this report (2016-2021), the AQRP has sponsored 29 projects from researchers throughout the U.S.

1.2 Report Objectives

An essential component of the AQRP 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 2016-2021 project cycles. It builds on similar previous science summaries (Allen et al., 2004; Allen et al., 2012; Allen et al., 2015; Allen, et al., 2017). It characterizes uncertainties, which can be important in guiding progress in the scientific understanding of air quality and evaluating the expected effectiveness of regulatory policies.

While progress in air quality has been impressive, challenges remain. 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 of this report were written by AQRP staff and have followed frameworks established in previous State of the Science reports. The report was revised based on comments received from reviewers, including 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,
- atmospheric physical processes and long-range transport of pollutants,
- chemical transport modeling, and
- field studies.

Each section has a summary of major findings by project topic areas; citations to the scientific literature provide additional details.

1.3 References

AQPR Projects:
AQRP Project 10-009: Torres, V. (2010), Additional Flare Test Days for TCEQ Comprehensive Flare Study, Submitted to the Texas Air Quality Research Program, http://aqrp.ceer.utexas.edu/.

AQPR Project 10-032: Lefer, B., Brune, W., Dibb, J., Ren, X., and Stutz, J. (2010), SHARP Data Analysis: Radical Budget and Ozone Production, Submitted to the Texas Air Quality Research Program, http://aqrp.ceer.utexas.edu/.

AQRP Project 10-045: Stutz, J., Vizuete, W., Herndon, S., and Mount, G. (2010), Quantification of Hydrocarbon, NOx and SO2 Emissions from Petrochemical Facilities in Houston: Interpretation of the 2009 FLAIR Dataset, Submitted to the Texas Air Quality Research Program, http://aqrp.ceer.utexas.edu/.

Other:
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U.S. EPA Office of Air Quality Planning and Standards (OAQPS), (2012), Parameter for Properly Designed and Operated Flares, Report for Flare Review Panel, available at: https://www3.epa.gov/airtoxics/flare/2012flaretechreport.pdf.

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 essential inputs to regional or global-scale chemical transport models. The Texas Air Quality Research Program (AQRP) 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 2016-2021 AQRP related to emissions inventories as well as those from previous AQRP project cycles that put these findings into context.

2.1 AQRP Projects during 2016-2021 and Related Previous Projects

2.1.1. Wildland Fires and Open Burning (AQRP Projects 16-008, 18-022)

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 U.S. has been well documented by observational and modeling studies (e.g., Junquera et al., 2005; Morris et al., 2006; McMillan et al., 2010; Villanueva-Fierro et al., 2009; Wang et al., 2006; 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 carbon monoxide (CO) column densities and Aerosol Optical Depth (AOD), respectively, along the transport route from Central American 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 (described in Section 4 of this report).

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). AQRP projects have tracked the development of FINN over multiple biennia. FINN v1 was released in 2010 and updated in 2011, and v.1.5 was released in 2014. AQRP Project 12-018 evaluated the sensitivity of FINN v1 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 U.S., 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 U.S.

AQRP Project 14-011 made targeted improvements to FINN, 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 U.S. 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 U.S. FINN v2.2 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 generations of the model, FINN v2 and FINN v2.2.

AQRP Project 18-022 applied FINN v2.2 to Texas. Overall model changes led to increases in predicted emissions of particulate matter with diameters less than 2.5 microns ($PM_{2.5}$), NO_x and non-methane hydrocarbons. It is difficult to capture the full complexity of the interactions between model parameters that contribute to variations in emissions estimates for any given fire event or between different fire events. However, results of performance evaluations conducted in AQRP Project 18-022 indicate that the modifications to FINN made between versions 1.5 and 2.2 have improved representation of wildfire smoke in photochemical modeling results. Overall statistics for the CAMx model Aerosol Optical Depth (AOD) comparison with satellite data indicate similar performance with the two versions of the emissions model. However, when smoke-dominated events were identified, the relationship between modeled and observed AOD improved. Case studies of smoke events show that model runs conducted with FINN v2.2 frequently showed better agreement with satellite observations of AOD relative to model runs conducted with FINN v1.5. Project 18-022 also applied FINN v2.2 to fires in Texas for the period for 2012-2018. As shown in Figure 2.1, annual emissions due to fires in Texas continue to be large in magnitude and highly variable. Emissions from fires outside the state, transported into Texas can also be large and variable.

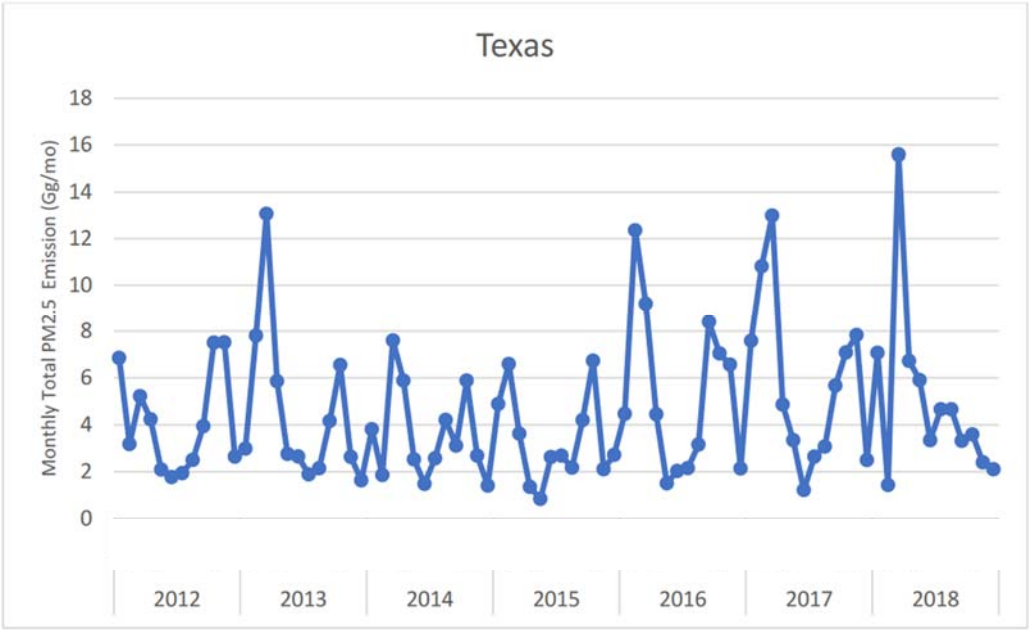

Figure 2.1 Annual trends in monthly total $PM_{2.5}$ emissions in gigagrams per month (Gg/mo) from FINN v2.2 during 2012 through 2018 in Texas with active fire detections from the Visible Infrared Imaging Radiometer Suite (VIIRS) and Moderate Resolution Spectroradiometer (MODIS).

2.1.2 Biogenic Hydrocarbons
(AQRP projects 16-011, 18-005, 20-007)

BVOCs, in particular, isoprene and monoterpenes, have been widely recognized for their key roles in atmospheric chemistry, including contributions as precursors for tropospheric ozone (Atkinson, 2000) and SOA formation (Tsigaridis and Kanakidou, 2003; Claeys et al., 2004). Li et al. (2007) found changes in modeled ozone concentrations of ±5-25 parts per billion (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 a Houston field campaign in 2013.

Emissions of BVOCs exhibit strong diurnal variability with temperature and sunlight and spatial gradients due to differences in land use/land cover. Inter-annual 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., 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 (30 meters)

for Texas and other regions of the U.S. drawing on ground survey, remote sensing and land surface model data products. Uncertainties still 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 U.S., 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 exhibited much larger differences in the Houston-Galveston-Beaumont-Port Arthur domain during early summer and fall periods of 2016. In the eastern U.S., 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 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 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; AQRP Project 14-016) or other requisite input parameters such as Photosynthetically Active Radiation (PAR) (AQRP Project 14-017).

Studies over different global regions have evaluated MEGAN 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 (Kota et al., 2015).

AQRP Project 16-011 (Guenther et al., 2017) incorporated results from previous Texas AQRP projects and other studies in the development of MEGAN v3, 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 v2.1 were found to be largely associated with estimates of SLA (the leaf area to leaf dry mass ratio), which are required for converting emissions measurements reported on a per-mass to a canopy scale (per-area) basis. MEGAN v3 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. MEGAN v3 exhibited 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 MEGAN v3 in comparison to MEGAN v2.1, making MEGAN v3 in better agreement with observations at Continuous Air Monitoring Stations (CAMS) and Clean Air Status and Trends Network (CASTNET) sites.

Biogenic emission estimates are also strongly influenced by the emission factors used for specific tree species. AQRP Project 18-005 performed measurements of isoprene, monoterpene and sesquiterpene emission factors for dominant urban and native Texas tree and crop species. These emission factors, with emission factors from other studies, were integrated into MEGAN v3.1. In general, MEGAN v3.1 estimated lower isoprene emissions and higher terpene emissions than MEGAN v3. The lower MEGAN v3.1 values are primarily due to an improved assignment of non-emitters. A lack of observations in the MEGAN v3 database resulted in non-emitters, such as maple trees, being assigned a moderate (average of all trees) isoprene emission factor due to no data being available. MEGAN 3.1 domain total isoprene emissions were about 10% lower than BEIS for the contiguous U.S. In Texas, MEGAN v3.1 isoprene was slightly lower than MEGAN v3 and much lower than MEGAN v2.1 or BEIS. MEGAN v3.1 total monoterpene emissions were about 36% higher than MEGAN v3 for the contiguous U.S. primarily due to the addition and revision of emission factors input to the MEGAN-EFP emissions database. In Texas, the MEGAN v3.1 monoterpene emissions were higher than MEGAN v3 and lower than MEGAN v2.1 and BEIS.

In the 2020-2021 biennium, BVOC emission estimation tool updates again returned to addressing land cover. AQRP Project 20-007 developed methods for updating urban land covers, using digital imagery. Urban areas are the most challenging for BVOC emissions estimation, due to heterogeneity and a lack of vegetation information, and yet they have historically been the least studied. Recent ground surveys of urban tree inventories and increasingly higher resolution remote sensing data products have substantially improved the potential for characterizing the land cover inputs required for biogenic emission models. In AQRP Project 20-007, urban tree inventories and aerial and satellite imagery were used to develop a high spatial resolution (~1 km) gridded inventory of time-varying Leaf Area Index (LAI), total vegetation cover, and the relative abundance of high BVOC emitting trees (e.g., live oaks, deciduous oaks, sweetgum, palms, pines, juniper) and other vegetation cover types for three Texas urban areas: Austin, Houston, San Antonio. The project found that uncertainties in land cover data, including LAI and tree cover distributions, continue to make a significant contribution to overall uncertainties in Texas BVOC emission estimates and that land cover datasets based on 30-meter (and coarser) resolution imagery tend to underestimate tree cover in urban areas by 35% or more. Sub-meter resolution can capture tree cover associated with individual trees and is suitable for quantifying urban tree cover and virtual urban tree surveys are a cost-effective approach.

2.1.3 Evaluation of MOVES NO_x Emissions (AQRP Project 16-010)

Recent chemical transport modeling studies that apply the U.S. Environmental Protection Agency's (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 of 2 or more (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, 2014) 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 photochemical modeling episode for September 2013, AQRP Project 14-014 (Choi, 2014) 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 the 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 under-predicted 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. regions (e.g., Fujita et al., 2012; Kota et al., 2014) and Texas (e.g., Rappenglueck 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; Rappenglueck 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 work suggests that the overestimate of NO_x emissions from on-road mobile sources reported to the NEI are caused by the use of national default input data to MOVES; county-level NO_x emissions are improved by using local activity data (Koupal et al., 2014). In support of Texas air quality modeling applications, the TCEQ (Kite, 2017) and the 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, the employment of best available local data for MOVES in the recent AQRP Project 16-010 analysis by Bai et al. (2017) resulted in 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 sensitivity analysis demonstrated that the predicted emissions were more sensitive to vehicle fleet mix and age distribution compared 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), the 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 photochemical modeling episode for September 2013 to assess the accuracy of the TCEQ's NO_x emissions inventory with respect to NO_x concentrations in the Houston area. A sensitivity simulation that reduced NO_x emissions from Texas on-road mobile sources worsened the statistical agreement between predictions and observations collected at both the surface and via aircraft platforms indicating degradation of the fine resolution TCEQ emissions inventory. 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 Project 16-007)

There has been an increased focus by the EPA on VOC emissions from storage tanks associated with crude oil and natural gas production and petroleum refinery operations (U.S. EPA, 2011a; U.S. EPA, 2011b; U.S. EPA, 2015b; U.S. 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; U.S. 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 (U.S. EPA, 2015d). The 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 16-007 (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: American Society for Testing and Materials (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 of 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) were in agreement with estimates for the "known" material; the method had a relatively flat slope as a function of temperature and 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 Windblown Dust (AQRP Project 20-011)

Visibility impairment is predominantly caused by particulate matter (PM) in fine and coarse size ranges. Project 20-011 developed improvements to emission estimation methods for PM that originates from windblown dust. Whereas fine PM commonly includes a multitude of primary and secondary inorganic and organic compounds from a variety of sources, including crustal (soil-derived) components, the majority of coarse PM derives from direct emissions of crustal material. Current emission modeling exhibits especially large underestimates of coarse crustal PM concentrations, indicating a need to improve emission estimates from dust sources. Soil emissions are especially difficult to estimate given the variety of source mechanisms and environmental conditions that lead to high spatial and temporal variations. Improving dust emissions and modeled concentrations requires refined vegetative and soil datasets and emission parameterizations. Visibility simulations benefit from enhanced wind-blown dust (WBD) modeling and explicit treatment of elemental species (e.g., Ca, Fe, Mn), which influence secondary PM chemistry (e.g., sulfate, nitrate) and enable more refined model evaluation because they are explicitly monitored. The CAMx WBD emission model provides an existing framework to efficiently test updated parameterizations and to incorporate enhanced and/or more locally specific land cover, soil, and activity data. CAMx test runs using the updated WBD model created in Project 20-011 revealed that key parameters controlling dust emissions are wind drag partitioning and, to a lesser extent, the amount of vegetative dust suppression. Specifying vegetation cover for each individual emissive land use/land cover (LULC) type within each grid cell, rather than relying on grid-composite values was particularly important. This additional refinement greatly improved simulated crustal PM concentrations throughout the western U.S.

Model-observation agreement for fine and coarse WBD concentrations has improved substantially with the updated WBD model over the original version. The new model is capable of generating sufficient dust on par with measured concentrations in all seasons. Generally, the model systematically over predicted fine dust components and total coarse mass in the spring and autumn, but under predicted during the summer when measured levels increase. Model performance for coarse mass tended to be better than for individual fine dust elemental

components or their sums. There were no clear performance tendencies for fine elemental concentrations, but overall, the relative elemental compositions were appropriately characterized.

Crustal elements (e.g., calcium and iron) in WBD impact the chemistry of secondary inorganic (sulfate, nitrate, ammonium) and potentially organic compounds. Improved WBD emissions result in both increases and decreases in all of the secondary inorganic particulate species. For sulfate, impacts are generally small with perhaps some tendency toward concentration increases more than decreases. Nitrate concentrations tend to be higher in all months, especially in the western U.S., due to increased abundance of neutralizing cations that convert gaseous nitric acid to particulate nitrate. Effects on ammonium are opposite and smaller, with generally more concentration decreases than increases in the western U.S. for all months. WBD cations tend to displace ammonia as neutralizing agents for sulfate and nitrate.

2.1.6 Energy Sector Emissions in Mexico (AQRP Project 18-023)

Energy reform in Mexico has transformed the country's energy sector. Development of Mexico's energy sector has the potential to substantially transform the magnitude and spatial distribution of emissions from the oil and gas and power generation sectors. Emission inventories for Mexico have become essential for air quality modeling in Texas and elsewhere in the U.S. AQRP Project 18-023 developed a bottom-up assessment of emissions for the upstream and midstream oil and gas sectors and electric power sector in Mexico for supporting air quality modeling applications. Emission sources included onshore and offshore oil and gas exploration and production well sites, well flaring, natural gas compressor stations, natural gas processing plants, and electricity generating units (EGUs). Emissions estimates were developed for 2016, the base year of the EPA's national air quality modeling platform.

Figure 2.2 shows an example of the mappings that were developed for the electricity generation sector. Natural gas was the dominant fuel for electricity generation in Mexico in 2016, accounting for over 70% of fuel use. Coal fired electricity generators, however, are large NO_x sources in the region near the Texas-Mexico border, especially the Carbon II and Rio Escondido facilities. This makes tracking transitions in Mexico from coal to natural gas fuels important for air quality in Texas. Figure 2.3 shows an example of the mappings that were developed for oil and gas production. Compared to the EGU emissions, VOC and other emissions from oil and gas production operations are relatively remote from Texas, although long range transport could result in some impacts.

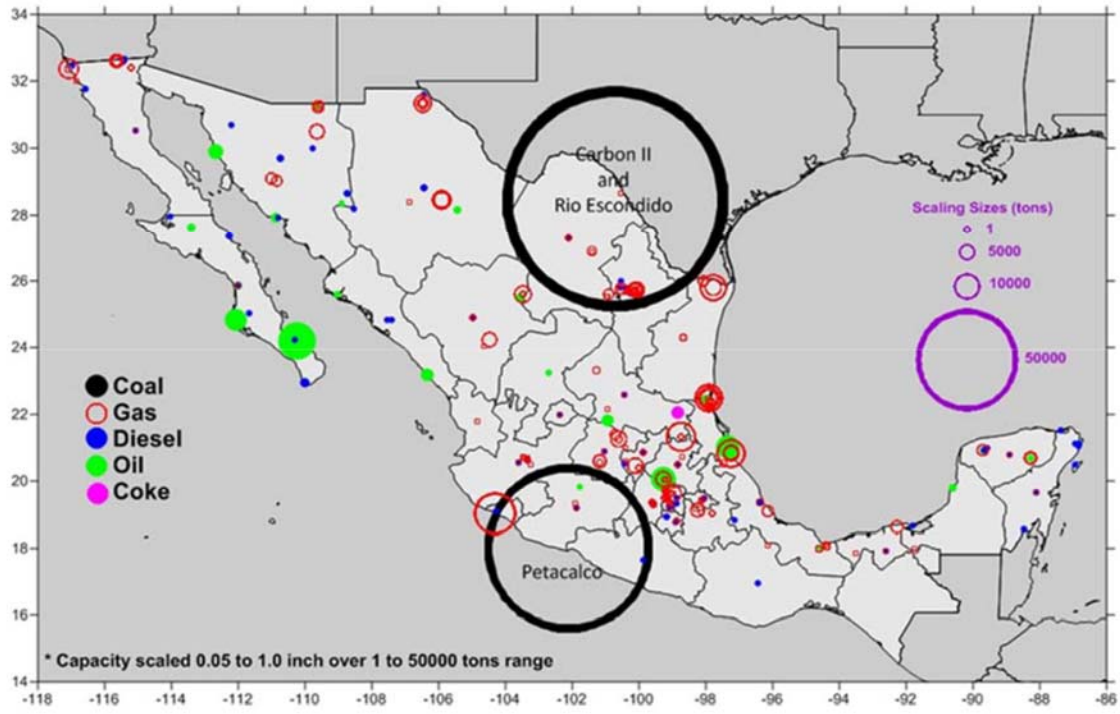

Figure 2.2 NO_x emissions (tons) from thermal electricity generation in Mexico during 2016; location symbols are sized by emissions.

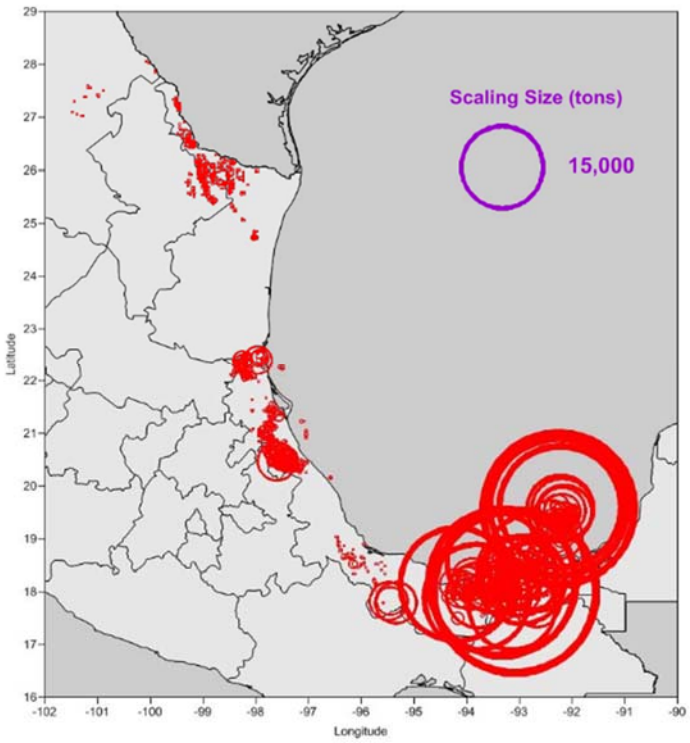

Figure 2.3 Annual 2016 VOC emissions (individual wells aggregated to 4 km by 4 km grid cells). Location symbols are proportionally sized by emissions

2.1.7 Use of Satellite Data in Emission Inventory Performance Evaluations (AQRP Project 20-020)

Because of their radiative properties, NO_2 and SO_2 are among a small group of gas-phase air pollutants that may be reliably detected from space. These gases have short atmospheric lifetimes, such that satellite-based observations are useful an indicator of concentrations in the immediate vicinity of sources. Although the characterization of gas-phase emissions has emerged as one of the leading areas for air quality utilization of satellite data, multiple atmospheric processes affect the relationship between satellite-derived column abundance and near surface. AQRP Project 20-020 examined methods for using satellite data to evaluate emission inventories and developed best-practice recommendations. The project evaluated methods to compare satellite NO_2 with emission inventories developed by the TCEQ. The project found that a 3-D model is the only tool for evaluating emission inventories on regional and daily scales. Gaussian plume methods succeed for well-detected sources over longer timescales. This approach offers a lower-cost strategy to account for meteorology and chemistry. The project also sought to provide guidance on the use of specific satellite products and found that The TROPOspheric Monitoring Instrument (TROPOMI) is useful for assessing overall spatial patterns in NO_x emissions and in modeled NO_2, including differences among cities.

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3. Tropospheric Chemistry

Since its inception, the AQRP 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 2016-2021 AQRP related to tropospheric chemistry as well as relevant results from previous AQRP project cycles.

3.1 AQRP Projects during 2016-2021 and Related Previous Projects

3.1.1 Alkyl Nitrates from Anthropogenic and Biogenic Precursors (AQRP Project 16-019)

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 hydroxyl radical (OH)-initiated oxidation of anthropogenic or biogenic VOC precursors in the presence of NO_x during the daytime and ozone or nitrate radical (NO_3)-initiated oxidation of VOC precursors primarily at nighttime (Perring et al., 2013). VOC precursors to ANs, including alkanes, alkenes, and aromatics, vary by location with anthropogenic or biogenic emission source regions (Day et al., 2010; Perring et al., 2013). ANs 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 ANs (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 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). ANs 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 (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 six-hours to one-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 NO_3-monoterpene chemistry, and (3) splitting of paraffinic carbon into fractions with low and high AN yield. More rapid AN 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. Splitting terpenes was also important for $PM_{2.5}$ concentrations in these areas but had little impact on ozone. Updating AN yields from alkanes 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 Project 16-031)

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).

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 U.S. (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, α-pinene ozonolysis SOA which is a major biogenic SOA (Hallquist et al; 2009) and toluene and naphthalene SOA produced from photochemical oxidation which are important markers for anthropogenic SOA. 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 Southern Oxidant and Aerosol Study (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 References

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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 2016-2021 AQRP as well as those from previous AQRP project cycles that put these findings into context.

4.1 AQRP Projects during 2016-2021 and Related Previous Projects

4.1.1 Effects of Regional Background Ozone and Meteorological Events on Houston Area Air Quality (AQRP Project 16-008, 18-010)

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 the maximum daily averaged eight-hour (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 during this time period 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) further found that 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.

In addition to long range transport and stagnation events, recirculation events (e.g., flow reversals, rotating winds) can have a significant impact on ozone formation in the Houston-Galveston-Brazoria (HGB) area. AQRP Project 18-010 confirmed that clockwise wind rotation is a strong feature in the lower atmosphere over coastal Texas. Recirculation takes place when the local-scale winds are strong enough to equal or exceed the large-scale wind speeds and happens during the warm season (April-September), mostly with wind speeds less than 2.5 m/s. In order to investigate the impacts of wind rotation and resultant pollutant evolution, four specific cases in 2000, 2013 and 2016 were analyzed in AQRP Project 18-010. Multiple planetary boundary layer (PBL) parameterization schemes were examined along with the ability of the Weather Research and Forecasting (WRF) meteorological model to resolve the recirculation. The WRF models were found to struggle to show any recirculation in the boundary layer near Houston. Analysis of the case studies showed that aged ozone, transported into the HGB region by recirculating flows can be as high as 50% (or ~20 ppb) of the peak time non-background ozone at Galveston. This level of aged non-background ozone is almost as high as the fresh ozone predicted in the vicinity of the urban Houston area on high ozone days. Continued improvement of recirculating wind patterns will be important for understanding ozone formation in the HGB region.

4.1.2 Impacts of Regional Biomass Burning Events on Particulate Matter Concentrations in Texas
(AQRP Projects 16-024, 18-031, 20-005)

As described in Section 2 of this report, which addressed emissions, fires within Texas continue to have large and variable impacts on air quality in Texas. Emissions from fires outside the state, transported into Texas can also be large and variable. To develop tools to improve tracking of fire plumes into the State, AQRP Project 16-024 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 Goddard Earth Observing System, with atmospheric chemistry (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.

In addition to the tools developed in AQRP project 16-024, there are multiple tools developed by other organizations to track wildfire plumes based on satellite and other remote sensing observations. However, because the products use different techniques to identify smoke plumes, they may disagree on the extent of the area covered by biomass burning smoke. In addition, currently available products do not provide information on the height of the smoke plumes or estimates of the surface impacts of the observed smoke. AQRP Project 20-005 evaluated the ability of remote sensing smoke products to accurately and consistently identify regions impacted by smoke. A sampling of three smoke products in the Texas/Gulf of Mexico region indicates little

spatial agreement in presence of smoke and/or horizontal extent. However, including additional remotely-sensed smoke-relevant variables such as NH_3, CO, and brown carbon into a smoke presence analysis adds further value to assessing presence and horizontal extent of smoke.

Project 18-031 also found that observational tracking of smoke plumes could be enhanced by using chemical markers of smoke. AQRP Project 18-031 examined the use of measurements of black carbon (BC) and brown carbon (BrC) in particulate matter to track smoke plumes. BrC is the carbon fraction of an aerosol that selectively absorbs short wavelengths of light (i.e., ultraviolet or UV). Light absorption by atmospheric aerosols, dominated by BrC rather than BC, is an indicator of influence from biomass burning. The influence of biomass burning plumes was identified using absorption Ångström exponents (AAE) and scattering Ångström exponents (SAE) (Sandradewi et al. 2008, Laing et al. 2016). When light absorption by atmospheric aerosols is dominated by BrC rather than BC, such as when there is increased influence from biomass burning on aerosols, the AAE is much greater than one. When the aerosol absorption is dominated by BC, like in motor vehicle exhaust, the AAE is close to one. The newest technology for real-time monitoring of aerosol absorption is the tricolor absorption photometer (TAP). The TAP measures absorption at UV, green and red wavelengths to more specifically target this biomass burning influence. Project 18-031 deployed two TAPs, a seven-channel aethelometer (Magee Scientific AE42), and a three-wavelength nephelometer (TSI 3563) to characterize aerosol optical properties, including multi-wavelength light absorption and scattering, in El Paso during a March-June 2019 field campaign. The aerosol optical properties were supplemented by measurements of trace gas concentrations, analysis of satellite fire data products and back trajectories. This information was used to assess the extent of biomass burning influence during the field program. The field trial demonstrated that AAE allowed for biomass burning events to be identified, even in a complex urban atmosphere when changes in concentration alone are not indicative. The TAP and nephelometer instrument suite provided a relatively low maintenance solution to conducting a long-term biomass burning observational assessment.

4.1.3 Improved Representation of Atmospheric and Land Surface Processes for Meteorological Modeling (AQRP Project 16-039)

As described in Section 4.1.1, AQRP 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 Rappenglueck, 2014; Haman et al., 2014), planetary boundary layer schemes (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 Rappenglueck, 2014; TCEQ, 2011). 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, 2011). AQRP Project 16-039 (McNider et al., 2017) 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 U.S. was applied as an alternative to U.S. Geological Survey (USGS) data to capture seasonal and inter-annual 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. The satellite data assimilation (i.e., insolation, vegetation fraction, skin temperature nudging of soil moisture and heat capacity) have in general improved WRF model performance with respect to 2-m temperature and humidity, wind speed, and skin temperatures and 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.

4.1.4 Simulation of Clouds and Precipitation (AQRP Project 20-026)

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., 2014)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.

In AQRP Project 20-026 (Lu et al., 2021), cloud fields generated by the WRF model were feed into the Cloud Feedback Intercomparison Project (CFMIP) Observation Simulator Package (COSP), so that modeled clouds could be directly compared to satellite observations. With modeled and observed cloud fields, a GAN (Generative Adversarial Network) deep learning technique was used to assess model parameterizations that led to the best predictions of observations. GAN changed the texture of modeled cloud fields by adding fine scale features and improved modeled cloud fields associated with frontal systems. However, GAN sometimes fails

to simulate localized deep convection systems during the summer and also fails to reproduce cloud fields associated with hurricanes because of very limited examples in long-term simulations.

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5. Chemical Transport Modeling

5.1 AQRP Projects during 2016-2021 and related Previous Projects

5.1.1 Direct Decoupled Method (DDM) Enhancements in CAMx: Local Chemistry Sensitivity and Deposition Sensitivity (AQRP Project 18-007)

Three-dimensional (3-D) chemical transport models, used in the development and evaluation of air quality management plans, require numerous inputs and parameters. Estimating the uncertainty in a model's predictions due to the effect of the uncertainties in all the inputs and parameters is important to understand the accuracy of a model and whether or not its predictions agree with observations. Nevertheless, such an uncertainty analysis is a challenge due to the hundreds or even thousands of inputs and parameters, the possibility of interactions among them, and the relatively long computer runtimes for 3-D models. There have been previous studies of the effects of uncertainties in some or many of the inputs to 3-D models, though apparently none using the Comprehensive Air Quality Model with Extensions (CAMx) or its current chemical mechanism, Carbon Bond 6 revision 4 (CB6r4). The objective of Project 18-007 was to estimate the uncertainties in CAMx predictions for eastern Texas due to uncertainties in the CB6r4 mechanism, emissions, boundary concentrations, and deposition velocities. A new tool for probing uncertainty in chemical mechanisms within CAMx, the CAMx Chemistry Sensitivity Analysis (CSA), was developed as part of this work. The tool provides computational efficiency comparable to box/trajectory models while maintaining the simplicity of full integration into CAMx. CSA calculates, using the Decoupled Direct Method (DDM), the sensitivity of chemical change (e.g., ozone formation) in individual grid cells to any or all rate constant(s) and reaction stoichiometric coefficient(s) in the gas-phase chemical mechanism. CSA is complementary to an existing probing tool in CAMx, Chemical Process Analysis (CPA). CPA analyzes rates of individual reactions or groups of reactions to provide quantities that help understand the oxidant chemistry, e.g., ozone destruction and production rates.

The sensitivity of ozone formation to hundreds of parameters were examined and the 50 parameters that generated the largest variations in ozone formation were examined in more detail. A thousand different combinations of variations in the top 50 individual parameters were identified and analyzed. Three "high ozone" and three "low ozone" sets of parameters (from the thousand permutations) were selected for detailed simulation. The three "high ozone" and three "low ozone" sets of parameters correspond to plus and minus one standard deviation of the ozone productivity from the mean value of the thousand parameter sets. The high and low mechanisms were used in separate CAMx simulations for June 2012 and the results analyzed to determine one standard deviation of uncertainty in ozone predictions due to uncertainty in the chemistry. The uncertainty (one standard deviation) on high ozone days is 10-11 ppb in the Gulf near Galveston and 7 ppb-8 ppb in much of the rest of the domain. As a percent of the ozone concentration, the uncertainty is more uniform, 11%-14% over the whole domain. Based on this assessment, uncertainties in chemistry are comparable to uncertainties in emissions and processes such as deposition in chemical transport models, suggesting that focused chemical mechanism development and evaluation may improve the degree of confidence in chemical transport models.

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6. Field Studies

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. In the period covered by this report (2016-2021), the AQRP supported multiple projects and two field measurement campaigns in the region from Corpus Christi to San Antonio. Prior to these AQRP field campaigns, this region that had seen limited scientific field studies. The AQRP also supported measurements made in Galveston Bay and in the coastal waters of the Gulf of Mexico.

6.1 AQRP Projects during 2016-2021 and Related Previous Projects

6.1.1 The 2017 San Antonio Field Study (SAFS) Measurement Campaign (AQRP Projects 17-SAFS, 16-032, 16-053)

The San Antonio area is one of the most rapidly growing metropolitan regions in the U.S. During recent years, ground-level monitoring stations in and around San Antonio have continued to measure maximum daily averaged eight-hour (MDA8) ozone concentrations greater than 70 parts per billion by volume (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 16-053: Yacovitch and Herndon, 2017; AQRP Project 16-032: Wood, 2017) supported the collection of measurements by the Aerodyne Research, Inc. (ARI) mobile laboratory. The suite of instruments aboard the mobile laboratory (Table 6.1) were selected by Yacovitch and Herndon (2017) to improve the understanding of ozone and particulate matter formation in central Texas, and to quantify the local ozone production that impacts the design value monitors that exceed the ozone NAAQS in central Texas.

Table 6.1 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
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/ 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 6.1) with the timing at each location determined in daily coordination with the TCEQ and AQRP. To complement the suite of ARI measurements, the TCEQ sponsored a second mobile laboratory operated by The University of Houston, Rice University, and Baylor University that primarily sampled at the University of Texas at San Antonio (UTSA) and also included monitoring at a location just to the south of the San Antonio urban core. The measurement dataset included meteorological data, organic and inorganic gas phase compounds, particle composition and size, and ambient VOC canister measurements. In order to provide information on meteorological conditions above the surface, the 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.

Preliminary analyses highlighted by Wood (2017) quantified the ozone production rate in the Greater San Antonio area using measurements of hydroperoxyl radical (HO_2) and organic peroxy radicals (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 destruction rates of radicals containing hydrogen and oxygen (HO_x) suggested that conditions were almost always NO_x-limited. Yacovitch and Herndon (2017) noted that isoprene and its photoproducts 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, did not add significantly to atmospheric hydroxyl radical reactivity contributed by biogenic VOCs during May 2017. Additional analyses of the 2017 SAFS data were conducted during the 2018-2019 biennium as described in Section 6.1.2.

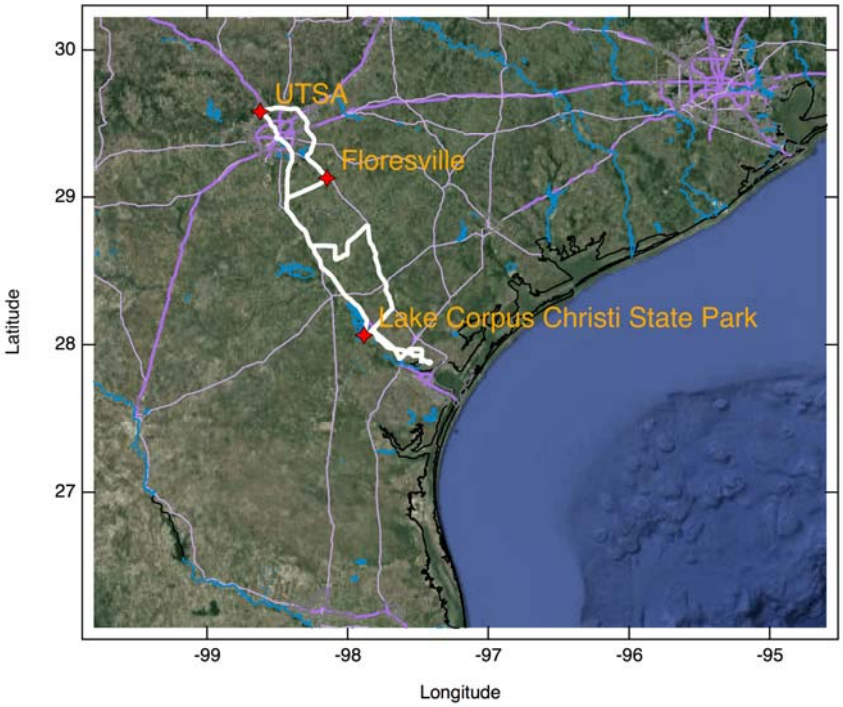

Figure 6.1 Measurement locations for AQRP Project 16-053 during May 2017. Red diamonds indicate the locations where the mobile laboratory was stationed. The white line indicates the route of the mobile laboratory.

6.1.2 Analyses of Data Collected in the 2017 San Antonio Field Study (SAFS) Measurement Campaign (AQRP Projects 19-025, 19-040)

During, May 2017, research groups from Drexel University, Aerodyne Research, University of Houston, Rice University, Baylor University, and others participated in the San Antonio Field Study (SAFS) with the overall goal of characterizing ozone formation in the greater San Antonio area. AQRP Projects 19-025 and 19-040 focused on analysis of data from the Aerodyne and Drexel teams.

The three major findings, based on observations were:

(i) Ozone production rates were calculated at the UTSA, Floresville, and Lake Corpus Christi sites, and were generally under 15 ppb/hr. Multiple lines of evidence show that UTSA was usually NO_x-limited except for time periods when HO_x radical production was low, typically in the morning or because of overcast conditions.

(ii) Ozone production during these periods was typically less than 5 ppbv/hr. Biomass burning plumes were clearly sampled during the campaign, but there was

little evidence that ozone production in these plumes was enhanced when compared to air not influenced by burning emissions.

(iii) Hydroxyl radical reactivity was dominated by biogenic VOCs at both UTSA and Floresville, with isoprene sometimes accounting for over 50% of total OH reactivity. Contributions from alkanes, alkenes, and aromatics were 1% or less at the UTSA site.

Zero-dimensional (0-D) photochemical modeling constrained by the SAFS datasets was conducted and led to the following conclusions:

(iv) Two versions of the carbon bond mechanism (CB6r3 and CB05) and the GEOS-Chem mechanism produced peroxy radical concentrations that agreed within 5% of observations. Interestingly, the master chemical mechanism (MCM 3.3.1), which is the most up-to-date and explicit mechanism, overestimated observed peroxy radicals by 27%. Each mechanism was able to reproduce the general observed relationship between ozone production and NO.

(v) Ozone production rates at the Travelers' World site, as calculated by the box model, were significantly higher than at UTSA, peaking between 40 and 80 ppbv/hr, depending on the mechanism. CB6r2, CB05, and GEOS-Chem each suggest possible ozone production in the VOC-limited regime on the order of 20 –30 ppbv/hr at this site.

(vi) The dominant peroxy radicals for ozone production at both UTSA and Travelers' World, according to MCM 3.3.1, CB6r3, and GEOS-Chem are HO_2 and radicals derived from isoprene, although isoprene plays a more dominant role at UTSA. Peroxy radicals from alkanes comprised a larger fraction of ozone production at Travelers' World, but still less than half that of isoprene.

Three-dimensional air quality modeling was conducted with the Community Multiscale Air Quality model (CMAQ) and led to the following conclusions:

(vii) Consistent with previous studies, the "base" NO_x emissions used as inputs for CMAQ were found to be too high, overestimating concentrations at surface monitors by approximately 50%. Reducing these emissions by 30% brought modeled NO_x to within about 10% of observations.

(viii) Reducing NO_x emissions by a further 20% lead to median reductions in surface ozone in San Antonio of 2 ppbv over May 2017. Emissions from power plants outside of San Antonio only produced a median of 0.25 ppbv ozone at the surface, although there was significant daily variation, with contributions up to 3 ppbv. NO_x emissions from oil and gas operations upwind of San Antonio seem to have minimal impact on San Antonio ozone.

(ix) The relationship between surface ozone production and NO for high HO_x production was similar between CMAQ and observations, with maximum values of about 15 ppbv. Vertical profiles of ozone production show that the highest ozone production rates are limited to near the surface.

6.1.3 The 2021 San Antonio Field Study (SAFS II) Measurement Campaign (AQRP Projects 20-003, 20-028)

Following up on the 2017 San Antonio Field Study (SAFS), which collected data in May 2017, a measurement campaign was initially planned for August 2020. Because central Texas typically

sees its highest frequencies of ozone exceedances in two periods, late spring and mid- to late-summer, the second San Antonio Field Study (SAFS II) was originally designed to collect data under different meteorological conditions than the 2017 SAFS. The pandemic made it impossible for the measurement teams to deploy during August 2020, so the SAFS II measurement campaign was deferred until May 2021. Although SAFS II collected data during the same general meteorological conditions as the 2017 SAFS, pandemic associated changes in traffic and other emission sources in 2021 compared to 2017, could be investigated in future work.

The platform for the 2021 campaign was the University of Houston/Rice University/Baylor University Mobile Air Quality Laboratory 2 (MAQL2). The instrumentation on the MAQL2 included sensors to measure meteorological parameters, inorganic trace gases that can be used as emissions tracers and that are relevant to both particulate matter and ozone formation (including carbon monoxide, carbon dioxide, nitrogen oxides, total reactive nitrogen, SO_2, and ozone itself), volatile organic compounds, and particulate matter composition, concentration and optical properties. The analyses were supplemented by three-dimensional air quality modeling using the Weather Research and Forecasting-GEOS Chem platform. Model output was compared to parameters measured by both the MAQL2 and the regional monitoring network; model runs were used to evaluate air pollution sensitivity to emissions scenarios.

The main focus of the 20-003 project was data collection. Preliminary observations include the importance of off-shore activities for determining the composition of air being transported into the Corpus Christi atmosphere, the importance of local activities on top of these off-shore activities in determining air quality in both Corpus Christi and San Antonio, and large differences in both composition and concentration of air pollutants across the spatial extent of the field campaign. Three-dimensional air quality modeling was able to simulate accurately the meteorology and air quality observations across the campaign once changes in background ozone and in emissions of anthropogenic combustion tracers were considered.

6.1.4 Ozone Measurements over Galveston Bay and the Coastal Waters of the Gulf of Mexico
(AQRP Project 20-004)

Ozone formation and transport over bays and the coastal waters of the Gulf of Mexico significantly impacts ozone concentrations in Texas coastal communities, yet relatively few measurements have been made over water to test model predictions of over-water ozone formation and transport. AQRP Project 20-004 deployed sampling systems on commercial boats operating in Galveston Bay (Larry Willis, commercial shrimper) and the offshore waters adjacent to Galveston Island (Ryan Marine Services, crew launch boat operator) to collect routine measurements of ozone and meteorology, including boundary layer height, during May-September 2021. A third boat, owned and operated by the University of Houston (UH), was utilized for special studies in Galveston Bay as well as for launches of ozonesondes to examine vertical profiles of ozone and confirm ceilometer measurements of boundary layer height. The instrumentation packages include an ozone monitor, GPS, all-in-one weather station, and a ruggedized PC with a cellular data connection. A ceilometer was installed on one of the vessels to measure boundary layer height over the water. The small sampling systems were found to be a highly effective and economical way to collect routine measurements over the water. The selection of boats and operational areas can be tailored to study different areas of interest. High

ozone was found over the water numerous times, once exceeding 130 ppbv over Galveston Bay and 110 ppbv over the Gulf. Several recirculation events of land-bay breeze and land-sea breeze which resulted in elevated ozone levels reaching one or more monitors were also observed. Measurements of Ox (ozone plus NO_2) allowed for the calculation of NO_2 which was found to be elevated over Galveston Bay at times, even when excluding discrete ship exhaust plumes.

Boundary layer height measurements from the eastern and western shores of Galveston Bay showed distinctly different average diurnal profiles, with the western shore presenting a more traditional land-based low morning and high afternoon boundary layer while the eastern shore appeared to be more marine influenced with possible impacts from the sea breeze off the Gulf in the late afternoon and evening. Upper layers detected at both locations were quite similar, indicating a larger regional feature decoupled from the surface. Modeling data tended to over-predict ozone, particularly on low ozone days. Possible reasons for this include an under-prediction of boundary layer height over the water.

6.2 References

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AQRP Project 16-053: Yacovitch, I. and S. Herndon, (2017), Identifying and Apportioning Ozone Producing Volatile Organic Compounds in Central Texas, Submitted to the Texas Air Quality Research Program, http://aqrp.ceer.utexas.edu/.

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

AQRP Project 19-025: Yacovitch, T., R. Roscioli, S. Herndon, M. Claflin, B. Lerner, M. Canagaratna, J. Krechmer, and W. B. Knighton, (2019), Submitted to the Texas Air Quality Research Program, http://aqrp.ceer.utexas.edu/.

AQRP Project 19-040: Wood, E., and S. Capps, (2019), Analysis of Ozone Production Data from the San Antonio Field Study, Submitted to the Texas Air Quality Research Program, http://aqrp.ceer.utexas.edu/.

AQRP Project 20-003: Griffin, R., Flynn, J., Sheesley, R., Usenko, S., Wang, Y. (2021), Characterization of Corpus Christi and San Antonio Air Quality During the 2020 Ozone Season, Submitted to the Texas Air Quality Research Program, http://aqrp.ceer.utexas.edu/.

AQRP Project 20-028: E. Wood., Quantification and Characterization of Ozone Formation in Central San Antonio, http://aqrp.ceer.utexas.edu/ (project cancelled).

7. Summary of Projects and Publications from the Texas Air Quality Research Program: 2016-2021

7.1 AQRP Research Projects: 2016-2021

Year	Project Number	Project Title
2016-2017	16-008	High Background Ozone Events in the Houston-Galveston-Brazoria Area: Causes, Effects, and Case Studies of Central American Fires
	16-010	MOVES-Based NO_x Analyses for Urban Case Studies in Texas
	16-011	A Next Generation Modelling System for Estimating Texas Biogenic VOC Emissions
	16-019	The Influence of Alkyl Nitrates from Anthropogenic and Biogenic Precursors on Regional Air Quality in Eastern Texas
	16-031	Condensed Chemical Mechanisms for Ozone and Particulate Matter incorporating the latest in Isoprene chemistry
	17-007	Evaluating Methods for Determining the Vapor Pressure of Heavy Refinery Liquids
	17-024	Improving the Modeling of Wildfire Impacts on Ozone and Particulate Matter for Texas Air Quality Planning
	17-032	Spatial Mapping of Ozone Formation near San Antonio
	17-039	Use of Satellite Data to Improve Specifications of Land Surface Parameters
	17-053	Identifying and Apportioning Ozone Producing VOCs in Central Texas
	17-SAFS	San Antonio Field Study Logistics
2018-2019	18-005	Next Steps for Improving Texas Biogenic VOC and NO Emission Estimates
	18-007	DDM Enhancements in CAMx: Local Chemistry Sensitivity and Deposition Sensitivity
	18-010	A Synthesis Study of the Role of Mesoscale and Synoptic-Scale Wind on the Concentrations of Ozone and its Precursors in Houston
	18-022	Development and Evaluation of the FINN v2 Global Model Application and Fire Emissions Estimates for the Expanded Texas Air Quality Modeling Domain
	19-023	Emission Inventory Development and Projections for the Transforming Mexican Energy Sector
	19-025	Apportioning the Sources of Ozone Production during the San Antonio Field Study
	19-031	Detecting Events and Seasonal Trends in Biomass Burning Plumes using Black and Brown Carbon: (BC)2 El Paso
	19-040	Analysis of Ozone Production Data from the San Antonio Field Study
2020-2021	20-003	Characterization of Corpus Christi and San Antonio Air Quality During the 2020 Ozone Season
	20-004	Galveston Offshore Ozone Observation (GO3)
	20-005	Using Satellite Observations to Quantify Surface PM2.5 Impacts from Biomass Burning Smoke
	20-007	Texas Urban Vegetation BVOC Emission Source Inventory
	20-009	Ozone Measurements and Platform Emission Factors in the Gulf of Mexico
	20-011	Improving Estimates of Wind-Blown Dust from Natural and Agricultural Sources
	20-020	New Satellite Tools to Evaluate Emission Inventories: Is a 3-D Model Necessary?
	20-026	Improve Cloud Modeled by WRF using COSP and Generative Adversarial Network
	20-028	Quantification and Characterization of Ozone Formation in Central San Antonio
	20-SOS	2016-2021 State of the Science

7.2 Publications

16-010
Presentations:
Bai, S., MOVES-Based NO_X Analyses for Urban Case Studies in Texas. *US EPA Emissions Inventory Conference*, Baltimore, MD, August 14-18, 2017.

Bai, S., Reconciling NO_X Emission Inventories with Ambient Observations. *US EPA Emissions Inventory Conference*, Baltimore, MD, August 14-18, 2017.

17-024
Public Presentations:
Alvarado, M, C. Lonsdale, and C. Brodowski, Using Lagrangian Chemical Transport Modeling to Assess the Impact of Biomass Burning on Ozone and $PM_{2.5}$, *American Geophysical Union (AGU) Fall Meeting*, New Orleans, LA, Dec. 11-15, 2017.

Lonsdale, C., C. Brodowski, M. Alvarado, J. Henderson, J. Pierce, E. Ramnarine, J. Lin, and A. Kochanski, New Developments in the Eulerian and Lagrangian Modeling of the Chemistry of Biomass-Burning Plumes, *15th Community Modeling and Analysis Systems (CMAS) Conference*, Chapel Hill, NC, October 15-17, 2017.

Published Presentations:
Brodowski, C.M., M.J. Alvarado, C.R. Lonsdale, J.C. Lin, A.K. Kochanski, An Eulerian vs. Lagrangian Comparison of Modeled Carbon Monoxide in Texas during Biomass Burning Events, *8th International GEOS-Chem Meeting, Cambridge*, MA, May 1-4, 2017.

Lonsdale, C. R., C. Brodowski, M. Alvarado, J. Henderson, J. R. Pierce, and J. Lin, Regional Modeling of Biomass-Burning Aerosol Impacts, Abstract GC51E-1225, *2016 American Geophysical Union (AGU) Fall Meeting*, San Francisco, CA, Dec. 12-16, 2016.

Lonsdale, C., C. Brodowski, M. Alvarado, J. Henderson, J. Pierce, E. Ramnarine, J. Lin, and A. Kochanski, Recent Advances in Modeling the Near-Source Chemistry of Biomass Burning Plumes in Photochemical Transport Models, *European Geosciences Union (EGU) General Assembly 2017*, Vienna, Austria, April 23-28, 2017.

17-032
Presentations:
Anderson, D. and E. Wood, Using Total Peroxy Radicals to Evaluate Ozone Production in Northern Michigan and San Antonio, *Fall 2017 American Geophysical Union (AGU) Conference*, New Orleans, LA, Dec. 11-15, 2017.

17-039
Publications:
McNider, R. T., Pour-Biazar, A., Doty, K., White, A., Wu, Y., Qin, M., Hu, Y., Odman, T., Cleary, P., Knipping, E., Dornblaser, B., Lee, P., Hain, C., and McKeen, S. (2018). Examination of the Physical Atmosphere in the Great Lakes Region and Its Potential Impact on Air Quality—Overwater Stability and Satellite Assimilation, *Journal of Applied Meteorology and Climatology*, *57*(12), 2789-2816.

17-053
Publications:
Anderson, D. C., J. Pavelec, C. Daube, S. C. Herndon, W. B. Knighton, B. M. Lerner, E. C. Wood, 2019. Characterization of ozone production in San Antonio, Texas, using measurements of total peroxy radicals. *Atmos Chem Phys* 19(5): 2845-2860. DOI:10.5194/acp-19-2845-2019.

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Presentations:
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Lindsay, A. et al., 2019. Investigating the impacts of power plants, oil and gas operations, and biogenic emissions on ozone production in San Antonio. *American Geophysical Union. Fall Meeting*, December 12, 2019.

17-SAFS
Publications:
Guo, F., A. Bui, B. Schulze, S. Yoon, S. Shrestha, H. Wallace, Y. Sakai, B. Actkinson, M. Erickson, S. Alvarez, R. Sheesley, S. Usenko, J. Flynn, and R. Griffin, (2021). Urban core-downwind differences and relationships related to ozone production in a major urban area in Texas, *Atmos. Environment.*, 262, 118624, 2021.

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Yoon, S., et al. Apportioned primary and secondary organic aerosol during pollution events of DISCOVER-AQ Houston, *Atmos. Environ.,* 244, 117954, 2021.

Presentations:
Anderson, D., et al., Investigating the impacts of power plants, oil and gas operations, and biogenic emissions on ozone production in San Antonio, *American Geophysical Union Annual Meeting,* San Francisco, CA, December 2019.

Guo, F., et al., Identifying the transport and evolution of oxidized organic aerosol across the urban core of San Antonio, *American Geophysical Union,* online, December 2020. (poster)

Guo, F., et al., Identifying the transport and evolution of oxidized organic aerosol across the

urban core of San Antonio, *American Association for Aerosol Research,* online, October 2020.

Guo, F., et al., Characterization of particulate matter in summer using high-resolution aerosol mass spectrometry in San Antonio, *American Association for Aerosol Research Annual Meeting*, Portland, OR, October 2019.

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18-022
Presentations:
Kimura, Y., C. Wiedinmyer, E. McDonald-Buller. Evaluating the Effects of Fires on Texas Air Quality Using the Fire INventory from NCAR (FINN), *Texas Advanced Computing Center (TACC) Symposium for Texas Researchers*, September 20-21, 2018.

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19-025
Presentations:
Yacovitch, T. et al. Mining High-Resolution Datasets to Understand OH Reactivity in San Antonio, *American Geophysical Union (AGU) Fall Meeting*, December 9, 2019.

19-031
Presentations:
Guo, F., A. Bui, E. Fortner, B. Schulze, S. Shrestha, S. Yoon, R. J. Sheesley, S. Usenko, T. Yacovitch, J. Flynn, R. Griffin. Characterization of Particulate Matter in Summer Using High-Resolution Aerosol Mass Spectrometry in San Antonio. *American Association for Aerosol Research (AAAR),* Portland, OR, Oct. 14-18, 2019.

Shrestha, S., M. C. Guagenti, F. Flynn, S. Alvarez, S. Usenko, R. J. Sheesley. Detecting Biomass Burning Using Intensive Aerosol Optical Properties in El Paso, Texas - (BC)2 El Paso Field Campaign. *American Association for Aerosol Research (AAAR)*, Portland, OR, Oct. 14-18, 2019.

19-040
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Anderson, D.C., J. Pavelec, C. Daube, S. C. Herndon, W. B. Knighton, B. M. Lerner, J. R. Roscioli, T. I. Yacovitch, and E. C. Wood. Characterization of Ozone Production in San Antonio, Texas Using Observations of Total Peroxy Radicals, 2019. *Atmospheric Chemistry and Physics*, 19, 2845-2860, 2019 (https://acp.copernicus.org/articles/19/2845/2019/acp-19-2845-2019.pdf).

20-003
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20-005
Presentations:
Dayalu, A. and M. J. Alvarado. Identifying Smoke-Impacted Regions using the Optical Properties of Brown Carbon Aerosol, *2020 CMAS Fall Meeting*, Virtual, October 29, 2020.

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20-020
Manuscripts:

Holloway, T., (2021), Working title, "Evaluating the NO_x emissions and ozone production sensitivities in Texas using TROPOMI NO_2 and HCHO," planned submission to *Atmospheric Chemistry and Physics*.

Holloway, T., (2021), Working title, "Three Ways of Using Satellite Data to Quantify Emissions," planned submission to *Environmental Manager*.

20-026
Presentations:
Zheng, L and L. Kai, Improve Cloud Modeled by WRF using COSP and Generative Adversarial Network. Presented at *American Geophysical Union (AGU) Fall 2021 Meeting*, December 13-17, 2021.