JANUARY 2021

TRACER-AQ Science Plan

AN INTERAGENCY COOPERATIVE AIR QUALITY FIELD STUDY IN THE HOUSTON, TX METROPOLITAN REGION

Version 1

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Note: Extensive Collaborator and Participant List in Appendices A1 and A2

Purpose of this Document

The TRACER-AQ Science Plan is meant to encompass all current planning and logistics for the TRACER-AQ field study in summer 2021 in Houston, Texas. It includes motivation/background for the study, science objectives, planned measurements, a preliminary intensive operations plan, and the science team and collaborators during summer 2021 and beyond. As this study is still growing and our decisions related to operations are preliminary, the science team will update as information becomes available and iterated through the versioning number of the document. Always remember to check for the latest updates going forward.

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Introduction

Tracking Aerosol Convection interactions ExpeRiment (TRACER) is a Department of Energy (DOE) Atmospheric Radiation Measurement (ARM) user facility led campaign that will take place from June 2021-2022 (with intensive operations occurring from June through September 2021) to study the impact of aerosols on microphysical processes within convective clouds in the region near Houston, Texas (see DOE/TRACER Science Plan). The Houston region commonly has isolated convection in the presence of variable aerosol environments with measurements strategically placed to capture urban, rural, and marine driven aerosol conditions.

Houston lies within a humid subtropical climate regime, where sea-breeze dynamics often interacts with local urban and industrial emissions to degrade air quality. Therefore, the state of air quality in this region is also an important research topic and better understanding of pollution challenges are crucial for public health in addition to NASA's goal of expanding capacity toward space-based air quality monitoring and related health applications. Therefore, NASA has committed contributions to TRACER by planning a parallel and complementary air quality (AQ) component (TRACER-AQ) during late summer 2021. This is a cross-collaborative effort between NASA's Tropospheric Composition Research Program and the Health and Air Quality Applied Sciences Program, with the goal of researching emissions, chemistry, and meteorology relevant to ozone and PM air quality and supporting the use of these Earth observations by air quality managers and the public health sector. NASA intends to coordinate both ground-based and aircraft observations within the larger existing air monitoring network. Many of the Houston air quality monitoring sites are operated by the Texas Commission on Environmental Quality (TCEQ) and TRACER/TRACER-AQ objectives largely overlap with TCEQ priorities, including the assessment of the regional air quality (aerosols and trace gases) and their nexus with emissions, chemistry, and meteorological patterns. The TCEQ also plans to further contribute to the TRACER-AQ campaign by supporting targeted detailed experiments that will be conducted during the campaign timeframe. With these combined inter-agency

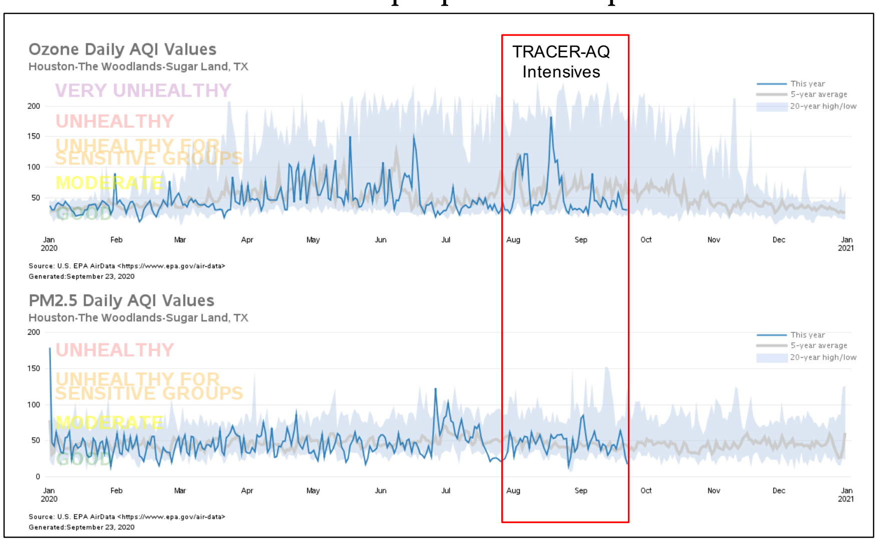


Figure 1: Ozone Daily Air Quality Index (AQI) (top) and PM2.5 Daily AQI (bottom) (through mid-September 2020), the five-year average, and the max/min during the last 20 years. Timeline for the proposed TRACER-AQ intensives are highlighted in red. Sources: US EPA

efforts, measurement platforms will include aircraft, ground-based sites, mobile laboratories, and boat-based observations.

Currently, Houston is designated as in attainment for the National Ambient Air Quality Standards (NAAQS) for $PM_{2.5}$ (particulate matter with diameters that are 2.5 micrometers and smaller) though does periodically experience elevated $PM_{2.5}$ levels as shown in Figure 1 (bottom panel). Although $PM_{2.5}$ concentrations do not often reach regulatory exceedance levels, ozone (O_3) exceedances occur more frequently during the summertime months as shown in Figure 1(top panel).

The Houston area is classified as nonattainment with a marginal classification for the 2015 8-hr ozone standard and nonattainment with a serious classification for the 2008 ozone standard. As shown in Figure 1 above, ozone has typically exceeded the NAAQS ozone standard from spring through early fall, in episodes lasting anywhere from a day to a week under calm, hot, and sunny conditions. An area meets the eight-hour standard when the three-year average of the annual fourth highest daily maximum eight-hour ozone concentration measured at a monitoring site is less than 71 parts per billion (ppb). The current ozone design value, based on 2017-2019 data, for Houston is 79 ppbv and was recorded at Aldine (a monitoring site on the northside of Houston). Ozone design values in Houston exceeded 100 ppbv before 2006 but have decreased in the last 15 years due to declining local emissions of ozone precursors (TCEQ SIP, 2020).

There is typically a bimodal peak of ozone exceedances each year, where the latter peak is late summer/early fall driven by synoptic conditions (Wang et al., 2016; Lei et al., 2018; Bernier et al., 2019). This latter peak has been explored during previous air quality studies in the region and will be targeted for TRACER-AQ intensive measurements in September 2021 (see Figure 1, red box). Historically, Houston has been a popular location for large air quality studies. Each study allows for a detailed reassessment of local air quality challenges that evolve due to changes in regulations, industry, and meteorological variability. Previous major investigations corresponding with the late summer peak in ozone exceedances of the last two decades include TexAQS 2000,(e.g., Daum et al., 2004;), TexAQS2006/GoMACCS (e.g., Williams et al., 2009; Langford et al., 2009; Senff et al., 2010; Kim et al., 2011; Langford et al., 2011), and DISCOVER-AQ 2013 (e.g., Mazzuca et al., 2016; Li et al., 2016; Leong et al., 2017; Kotsakis et al., 2017).

Relevance and Intrinsic Merit

In the last four years NASA has led several mesoscale campaigns with an emphasis on collaboration with state and federal air quality agencies, regional consortiums, research and academic institutions, in coastal urban environments subject to air quality issues intensified by land/water breezes. These focused regional studies include the Lake Michigan Ozone Study (LMOS) in 2017, the Long Island Sound Tropospheric Ozone Study (LISTOS) in 2018, and the Ozone Water-Land Environmental Transition Study (OWLETS) 2017 and 2018 (EM Magazine, 2020). These collaborative field efforts exemplify inter-agency and inter-state cooperative efforts to advance scientific understanding of air pollution near urban-coastal environments using a community grassroots approach.

With Houston being an urban-coastal site, the advantages of conducting this air quality field study includes a better characterization of the emissions heterogeneously distributed along the Houston Ship Channel, Galveston Bay, and nearby industrial regions and their interaction with mesoscale coastal dynamic processes which together impact air quality and public health. Furthering partnerships with federal/state and local agencies are also excellent opportunities for collaborative research with strengths in air quality monitoring, ground-based measurements, geostationary satellite observations (e.g., TEMPO), and modeling.

Scientific Questions and Motivating Focus Areas

Leveraging off of the deployment framework and intensive strategies of previous field campaigns in coastal urban areas and the research priorities of local partners, a set of scientific focus areas and motivating questions are proposed that can be answered within the resources provided for the TRACER-AQ/TRACER effort. These questions will lead to progress in three centralized focus areas: scientific understanding of atmospheric composition, advancing the use of models and satellite retrievals of the current atmospheric state, and further understanding of the intersection of air quality and socioeconomic factors within this local community.

Focus Area 1: Ozone Photochemistry and Meteorology

Question 1a. *How and why have the mechanisms (chemistry and/or dynamics) that produce high ozone in the region changed over time and what is the current role of over-water ozone formation?*

Question 1b. *How do mesoscale and synoptic conditions impact the vertical distribution of trace gases and aerosols over the Galveston Bay and continental Houston sites?*

Focus Area 2: Modeling and Satellite Evaluation

Question 2a. *Are chemical transport modeling platforms used by the research and air quality management communities accurately representing the spatial and temporal evolution of ozone and PM and the associated meteorology in the SE Texas region?*

Question 2b. *Are satellite measurements over Houston of the trace gases, (e.g., NO_2, HCHO, and SO_2) accurately retrieved from current UV-VIS sensors like OMI and TROPOMI? How can these results help local air quality and public health entities use these existing platforms to address their current air quality challenges?*

Question 2c. *How can measurements from TEMPO in the coming years help the Houston community better understand their challenges with respect to air quality and health, specifically related to, diurnal pollution patterns, and local emissions, and the near-range transport of secondary pollutants?*

Focus Area 3: Intersection of Air Quality and Socioeconomics Factors

Question 3a. *How has the relationship between NO_2 pollution levels and socioeconomic factors within Houston described in Demetillo et al. (2020) evolved since 2013? Do these findings extend to the spatiotemporal distribution of HCHO and/or ozone over Houston?*

Question 3b. *How does sampling at different times of the day impact the narrative of air quality disparities compared to a once-daily satellite overpass?*

Focus Area 1: Ozone Photochemistry and Meteorology

Question 1a. *How and why have the mechanisms (chemistry and/or dynamics) that produce high ozone in the region changed over time and what is the current role of over-water ozone formation?*

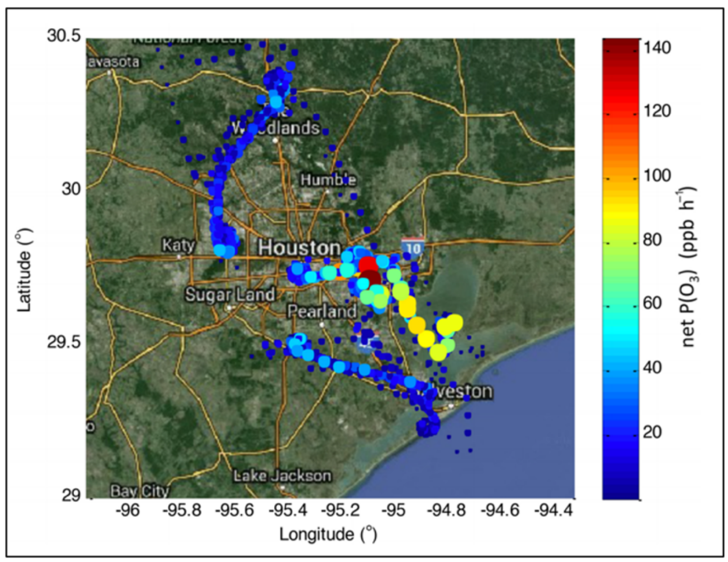


Figure 2: Spatial distribution of net ozone production calculated using the P-3B flight track during DISCOVER-AQ 2013 (Mazzuca et al., 2016).

In coastal urban areas like Houston, ozone pollution depends on chemistry and meteorology. The greater Houston region population recently exceeded 7 million inhabitants and is home for a number of petrochemical and other industries, many located at or near the Houston Ship Channel and Galveston Bay. Traffic and industrial emissions emit ozone precursors, such as nitrogen oxides (NOx: NO+ NO_2) and volatile organic compounds (VOC), that have been the target of study during previous air quality field campaigns. In recent years, due to implemented regulations, NOx levels have decreased approximately 30% since 2007 and VOC measurements decreased 30% from 2007-2012 but have since rebounded 10% despite continued reported emission decreases in the emissions inventory (TCEQ, 2020b).

The ratio of NOx and VOCs is critical for understanding local ozone formation and uncertainties associated in known emissions. As Houston, TX comprises a complex and spatially heterogeneous portfolio of industrial and urban emissions leading to variable pollution production rates ($P(O_3)$). For example, during the DISCOVER-AQ campaign, box model calculations of net ozone production rates were estimated using the chemical in situ observations from the NASA P-3B aircraft as constraints. Figure 2 illustrates these calculated rates along the flight track for all flight days during the Houston deployment. There are several P(O_3) hot spots over the Houston Ship Channel located to the east/southeast of downtown Houston and near Galveston Bay. This is expected because of large emissions of NOx and VOCs from the Houston Ship Channel, where the highest P(O_3) was observed – up to ~ 140 ppbv h^{-1}. Similar instantaneous ozone production rates have been observed in two previous studies in Houston in 2000, 2006, and 2009 (Kleinman et al., 2002; Mao et al., 2010; Ren et al., 2013). Similar analysis can be compared with previous studies to update the conceptual model for ozone exceedances in the Houston area though at this stage will be limited to ground-based in situ measurements.

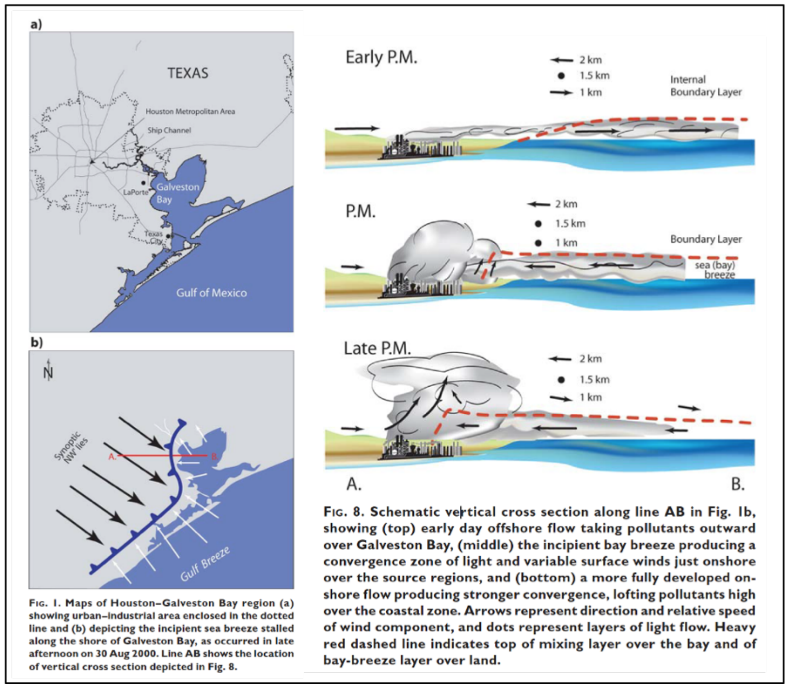


Figure 3: Banta et al. (2005) illustrated the classic case study specifically for the Houston/Galveston Bay region from the TexAQS 2000 air quality study.

Meteorologically, local ozone production is linked to days with weak synoptic flow/stagnation – often with a continental flow component that competes with the development of mesoscale boundaries related to sea- and bay-breezes. Banta et al. (2005) illustrated a classic case study specifically for the Houston/Galveston Bay region from the TexAQS 2000 air quality study (Figure 3). At a synoptic level, this can occur when frontal boundaries are able to penetrate into southeast Texas, which is often aided by the western extent of the Bermuda High retracting far enough east in the late summer weakening the influence of southerly flow from the Gulf of Mexico (Wang et al., 2016; Lei et al., 2018). In summer when frontal passages are less frequent, sea breeze recirculation will still occur under weak synoptic flow related to the buildup of high pressure over central Texas (Li et al., 2020). During recirculation, emissions are advected over the water through weak continental flow or through the occurrence mesoscale land-breezes confining ozone precursors in the marine boundary layer. As the thermal contrast between the land and water increases into the day, a sea/bay-breeze can advect pollution back ashore. On-going weak continental flow over land can also oppose the penetration of the sea-bay breeze leading to stagnation over this coastal environment leading to further buildup of pollution.

Measurements in this study will map emissions of NO_2 and additional complex trace chemicals, such as formaldehyde (HCHO), from a top-down perspective and include extensive ozone measurements over the water and near the coast to capture the relationship between emissions and meteorology in more detail than standard regulatory measurements. A more detailed review of the chemical and meteorological impacts of on ozone pollution in the Houston area can be found in Chapter 5 of TCEQ's latest State Implementation Plan revision as well as documented conceptual model for achieving NAAQS attainment (TCEQ, 2020a).

Question 1b. *How do mesoscale and synoptic conditions impact the vertical distribution of trace gases and aerosols over the Galveston Bay and over continental Houston sites?*

During TRACER-AQ/TRACER, meteorological, aerosol, and ozone vertical profiles will be observed from ground-, balloon-, and aircraft-based measurements to characterize their vertical distribution and the role of vertical dynamics in relation to surface-based air quality.

The role of the sea/bay-breeze and convection in planetary boundary layer evolution and its relation to air quality has been previously examined in Houston during several studies (e.g. Langford et al., 2010; Mazzuca et al., 2016; Caicedo et al., 2019). For example, during DISCOVER-AQ 2013, the NOAA/CSL TOLNet lidar was sited La Porte, TX. After 10:00 LT on September 25th (Figure 4), ozone values increased near the surface due to daytime photochemical ozone formation that accumulated as a result of calm winds. In addition to horizontal advection and ozone production rates, any potential downward mixing of ozone in the residual layer can lead to additional buildup and mixing between recirculation flows can contribute to the high surface ozone measurements.

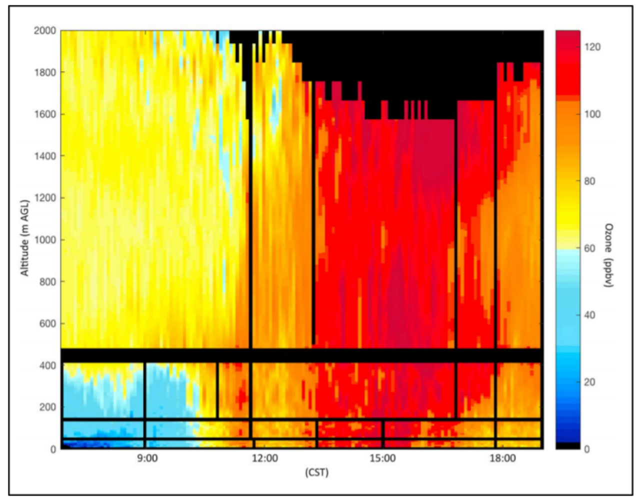


Figure 4: Ozone Lidar Time series from the NOAA/CSL TOPAZ Instrument at La Porte, Texas in 2013 (Caicedo et al. 2019)

Focus Area 2: Modeling and Satellite Evaluation

Question 2a. *Are chemical transport modeling platforms used by the research and air quality management communities accurately representing the spatial and temporal evolution of ozone and PM and the associated meteorology in the SE Texas region?*

As a requirement for State Implementation Plans (SIPs), TCEQ must demonstrate a plan for attainment of NAAQS, which may use photochemical modeling to predict future air quality (EPA, 2018). The TRACER-AQ campaign can provide information that can be used to validate, evaluate, and improve these model analyses. Additionally, operational chemical modeling platforms, such as the National Air Quality Forecast Capability at NOAA (NAQFC) and newer platforms like the GMAO GEOS-Composition Forecast (GEOS-CF), NOAA RAP-Chem analysis, and other research modeling platforms can utilize measurements from TRACER-AQ to assess both their meteorological and chemical analyses to identify strengths and weaknesses in the modeling performance.

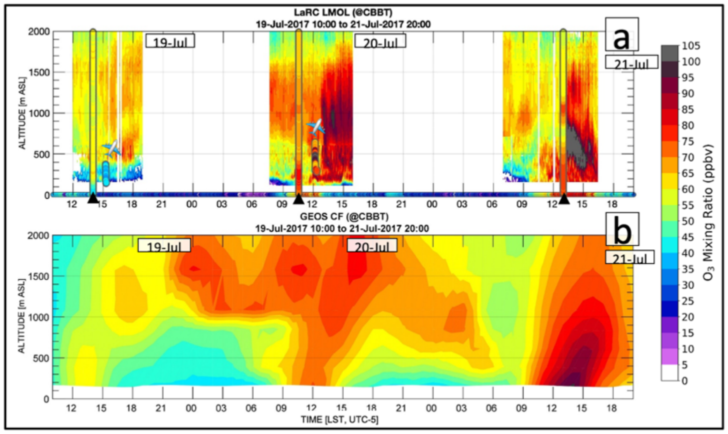


Figure 5: Synchronous profiles of O_3 from the (a)TOLNet/LaRC Langley Mobile Ozone Lidar (LMOL), ozonesondes, and airborne profiles over at the Chesapeake Bay Bridge Tunnel and (b) the GEOS-CF vertical profile from 10:00 LST July 19th to 20:00 LST July 21st 2017 for the first 2000 m ASL. Edited from Dacic et al. (2020)

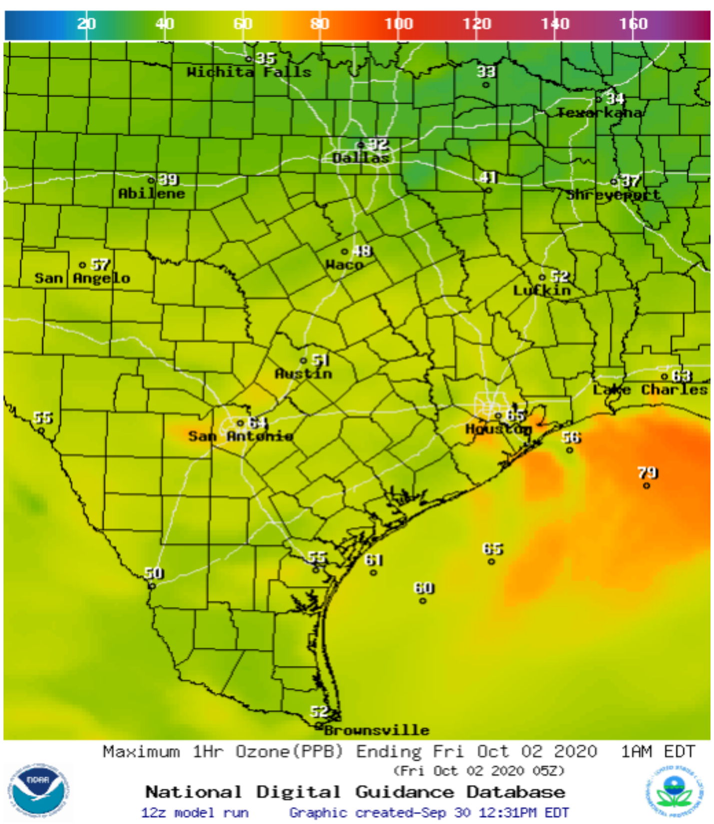


Figure 6: Elevated Ozone Offshore of Southeast Texas during October 2, 2020 from the NOAA NAQFC (airquality.weather.gov)

Dacic *et al.* (2020) was the first to use data from a similar small collaborative campaign, OWLETS-1, to evaluate the NASA GEOS-CF in an coastal area with complex ozone chemistry in relation to the land-water boundaries and dynamics with ozone profiles collected from TOLNet associated O_3 lidars and other complementary ozone profile measurements (Figure 5).

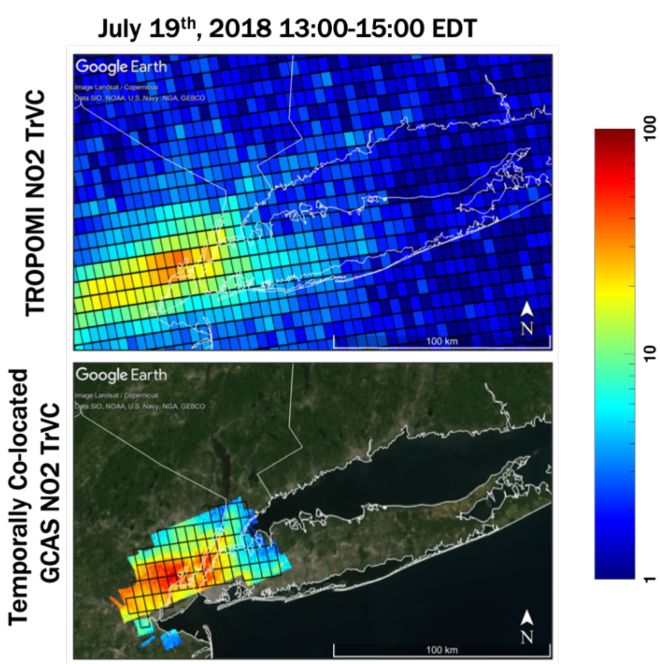
Based on previous work, it is expected that comparisons between observations and simulations will yield the largest discrepancies near coastal areas where the highly localized ozone concentrations are observed and linked to the strength and timing of the bay/sea breeze progression. Additionally, anticipated observations will characterize vertical downmixing from the remnants of the nighttime residual layer during morning hours into the convective boundary layer and from the lofted offshore return flow into the subjacent bay breeze flow.

Regional photochemical models regularly produce elevated ozone concentrations over the Gulf of Mexico and Galveston Bay (e.g., Figure 6), where surface monitoring does not exist for verification and can act as an uncharacterized ozone source. Ship- and aircraft-based ozone and precursor measurements will help evaluate the offshore air quality and compare to model predictions.

Question 2b. *Are satellite measurements over Houston of the trace gases (e.g., NO_2, HCHO, and SO_2) accurately retrieved from current UV-VIS sensors like OMI and TROPOMI? How can these results help local air quality and public health entities use these existing platforms to address their current air quality challenges?*

The spatial resolution of select satellite products have started to approach the sub-urban spatial scales that can be fully sampled within a small temporal window from the nearly instantaneous satellite overpass (e.g., Sentinel-5P TROPOMI satellite for trace gases and GOES-16 for aerosol optical depth). Dense and detailed observations taken during field campaigns are isolated in time and space but these intensive measurements can assist in developing strategies and applications for using space-based air quality observations from UV-VIS sensors, like OMI or TROPOMI (e.g., Janz et al., 2019; Judd et al., 2020; Tack et al., 2020; Verhoelst et al., 2020) and prepare for future observations from the NASA TEMPO Mission, which will be the first geostationary air quality monitoring instrument measuring over greater North America.

GCAS is a unique tool for evaluating UV-VIS trace gas measurements from satellite sensors. Additionally, Pandora with its ground-based direct-sun view was developed as a ground-based validation reference measurement. Both of these assets were recently used for TROPOMI product validation in 2018 near New York City. For TRACER-AQ, Houston-specific evaluations will be conducted to demonstrate the ability of TROPOMI to resolve gradients in retrieved species like NO_2 and HCHO. Figure 7 below shows how the GCAS and TROPOMI data were spatially and temporally matched to TROPOMI (from Judd et al., 2020). These results showed a low bias in the TROPOMI Standard Product of approximately 20-30%, where 12-14% was due to the vertical profile assumption in the retrieval. These types of analyses can add confidence for use of satellite data by end-users.



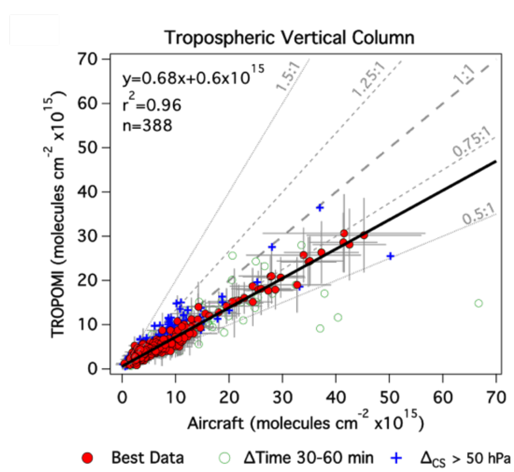
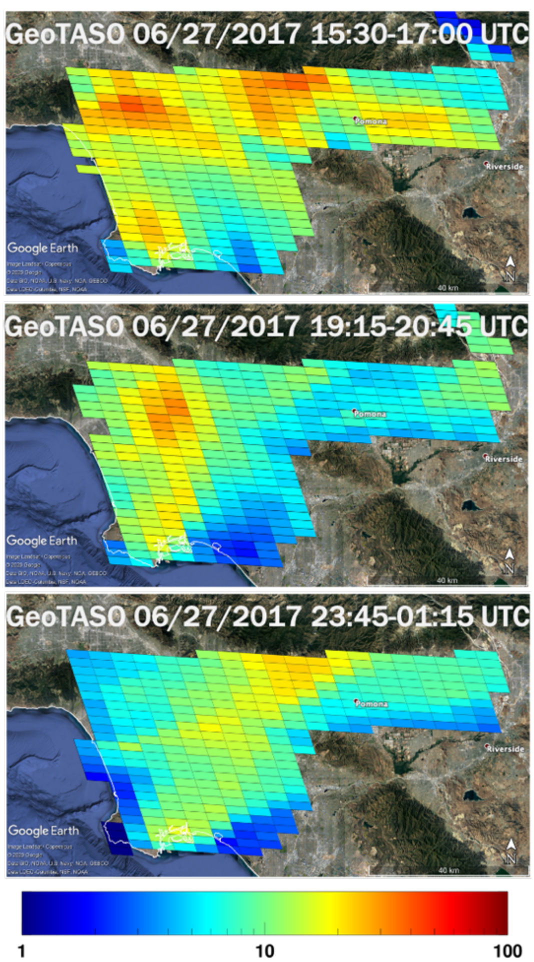


Figure 7: (left) Spatially and temporally matched GCAS observations to TROPOMI data and (right) scatter plot of aircraft to satellite comparison results. Source: Adapted from Judd et al. (2020)

Question 2c. *How can geostationary measurements from TEMPO (and beyond) in the coming years help the Houston community better understand their challenges with respect to air quality and diurnal pollution patterns?*

Airborne observations linked with the repetitive sampling strategy throughout the day (e.g. those presented in Figure 8) are an airborne proxy for geostationary air quality observations and are used to characterize TEMPO observations prior to launch and strengthen the ties of this capability into the local air quality community. The sampling strategy developed for these missions are repeated raster sampling spanning morning to late afternoon. These gapless rasters allow for the data to be binned to the footprints expected for TEMPO (or any satellite-based instrument). During TRACER-AQ, the instrumentation on board the NASA G-V aircraft will collect up to 77 hours of flight data measuring the spatial distribution of NO_2, HCHO, O_3, and aerosols multiple times throughout flight days. The maps below show the diurnal evolution of NO_2 in the Los Angeles Basin in June 2017 (adapted from Judd et al., 2018) binned to the TEMPO field of regard and the expected TEMPO footprints over the Houston region. These data can be useful for future data users of NASA TEMPO data products for their health and air quality needs.



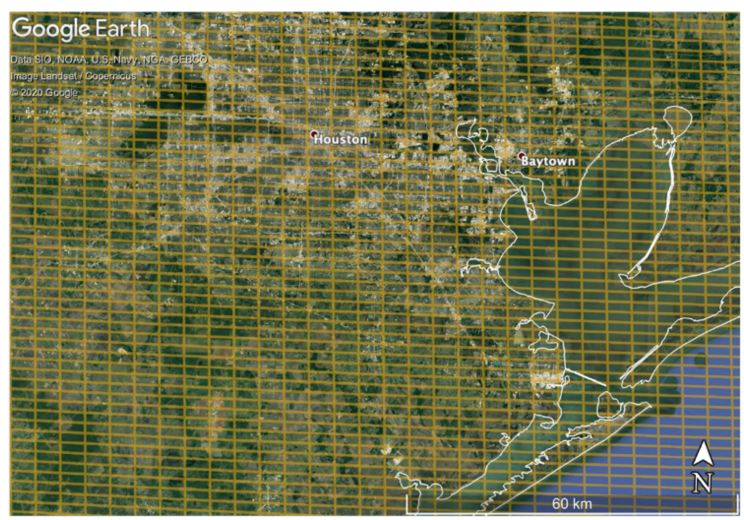


Figure 8: (left) Airborne spectrometer retrieved NO_2 tropospheric vertical columns over the Los Angeles Basin on June 27th, 2017 mapped to the estimated TEMPO field of regard (left) repeated three times during this day (morning, midday, and late afternoon). (above) The expected TEMPO field of regard in Houston, which will have the ability to differentiate between pollution over the water, over the ship channel, greater Houston, and the surrounding suburban and rural areas.

Focus Area 3: Intersection of Air Quality and Socioeconomics Factors

Question 3a. *How has the relationship between NO_2 pollution levels and socioeconomic factors within Houston (for example, those described in Demetillo et al., 2020) evolved since 2013? Do these findings extend to the spatiotemporal distribution of HCHO and ozone over Houston?*

Question 3b. *How does sampling at different times of the day impact the narrative of air quality disparities compared to a once-daily satellite overpass?*

In a number of cities around the world, there have been documented disparities in air pollution exposure with community demographics. Local to Houston, Demetillo et al. (2020) identified that the distribution of NO_2 unequally burdened low income/non-white/Hispanic communities using high resolution measurements from GCAS and TROPOMI (Figure 9). Data from GCAS is dated from 2013 and NOx emissions have likely evolved since that time period. Although the Demetillo analysis did account for this, the original measurement strategies were not collected evenly across the Houston region. Here, sampling strategies will facilitate greater spatiotemporal coverage, finer spatial resolution, and a more robust analysis with NO_2 disparities. These data will also be applied to investigate inequalities in the HCHO distribution. An additional observation in Demetillo et al. (2020) was that the atmospheric conditions leading to the greatest NO_2 inequalities corresponded to the highest levels of ozone throughout Houston. Therefore, analysis could also be expanded consider the distribution of ozone concentrations using the dense ground in situ network and airborne HSRL-2 measurements The NO_2 and HCHO airborne data will be combined to investigate the relationship between precursor inequality, ozone production chemical regime, and regional ozone pollution, potentially revealing air quality and health co-benefits to reducing NO_2 disparities. Systematic samplings

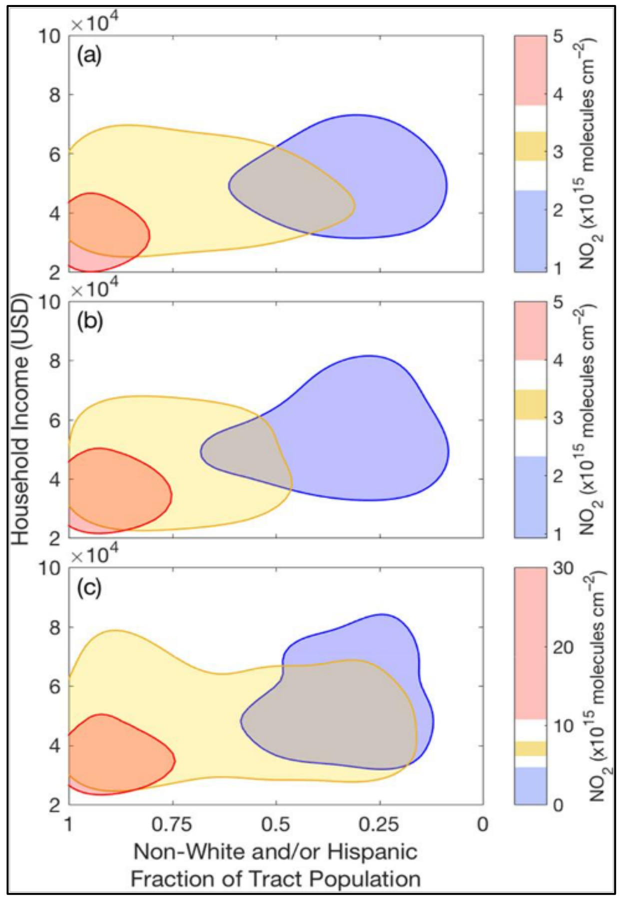


Figure 9: (From Demetillo et al., 2020): HMA population as a function of census tract annual household income (USD) and non-white/Hispanic or non-Hispanic white fractions separated by a census-tract-averaged NO_2 column quintile: high NO_2 (80–100% highest column densities) (red), mid-quintile NO_2 (40–60%) (yellow), and low NO2 (0–20%) (blue). (a, b) Annual (June 2018 to May 2019) weekday (Tuesday–Friday) TROPOMI observations across the HMA (a) and along the GCAS flight track (b). (c) Composite distribution of all 35 GCAS circuits. Color bars represent vertical column densities (molecules cm^{-2}) corresponding to the NO_2 quintiles

from the aircraft will produce as proxy measurement for geostationary observations, which can lay groundwork for space-based research on diurnal variations in disparities.

Platforms and Measurements

A combined and integrated 4D observing system is developing to successfully meet the scientific questions posed in the previous section. Data from surface air quality monitoring network stations, airborne lidar/raster mapping capabilities, and additional ground-based remote sensing instrumentation deployed during TRACER-AQ will allow for a unique spatial and temporal study of the progression of both meteorological and air quality conditions in the Houston region.

This section covers brief details on measurements that will be conducted in Houston during summer 2021 relevant to air quality research. A more detailed list of instrumentation can be found in the Appendix of this document. Aside from NASA efforts for TRACER-AQ, additional externally led efforts will be simultaneously conducted during the TRACER-AQ IOP.

Airborne Measurements

The NASA Airborne Science Program provides aircraft systems for both satellite calibration/validation studies as well as process level studies at the spatial and temporal resolutions needed to improve the understanding of underlying scientific mechanisms (i.e., air quality for this study). For TRACER-AQ, the Johnson Space Center (JSC) Gulfstream-V (G-V) will be carrying two remote sensing instruments: the GEOstationary Coastal and Air Pollution Events (GEO-CAPE) Airborne Spectrometer (GCAS) and the High Spectral Resolution Lidar-2 (HSRL-2). Below are brief details about the capabilities of each instrument.

GCAS

GCAS is an ultraviolet-visible-near infrared (UV-VIS-NIR) airborne spectrometer used as a test-bed for similar air quality satellite observations in geostationary orbit (e.g., TEMPO). This instrument has two channels: the UV-VIS (Air Quality) channel spans the 300-490 nm with a 0.6 nm spectral resolution and the VIS-NIR (Ocean Color) channel spans 480-900 nm with 2.8 nm spectral resolution. Background information on the mechanical design of GCAS can be found in Kowalewski and Janz (2014). Nadir of the aircraft, GCAS has a field of view of 45°. This field of view in conjunction with aircraft altitude determines the swath width, which during prior campaigns was slightly over 7 km from a flight altitude of 28,000 ft. The G-V has the capability of flying well above this altitude (ceiling of 51,000 ft).

Heritage trace gases retrieved from GCAS are below aircraft columns of nitrogen dioxide (NO_2) and formaldehyde (HCHO), with spatial resolutions as fine as 250 x 250 m. Previous work and background on retrievals are described in Nowlan et al. (2018), Judd et al. (2019), Janz et al. (2019). The measurement strategy for this campaign will be to collect raster datasets repeated throughout the day to get the spatial and diurnal evolution of these trace gases over the

Houston region. Figure 10 shows examples of NO_2 and HCHO rasters during the previous deployment of GCAS in New York City for the Long Island Sound Tropospheric Ozone Study. Note that NO_2 is displayed on a log scale color bar and the HCHO data are gridded to 1 km resolution to improve the signal to noise ratio.

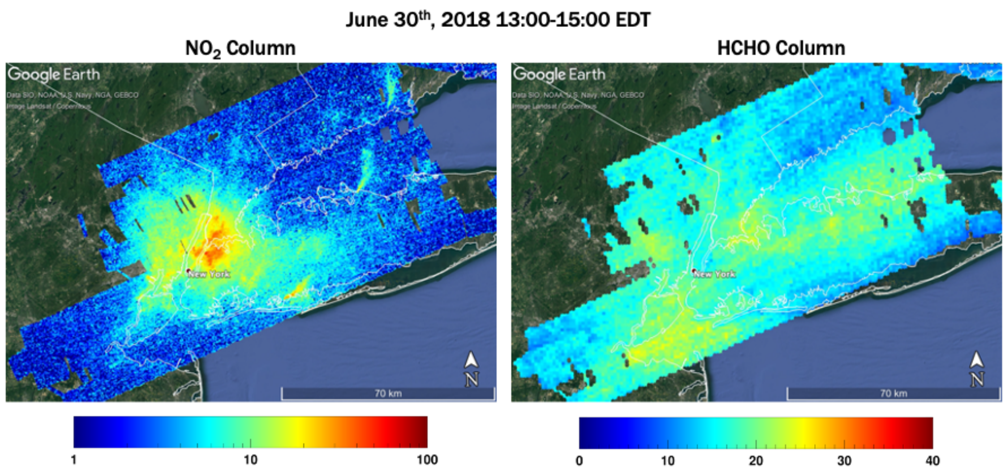


Figure 10: NO_2 Tropospheric Vertical Column (left) and HCHO Tropospheric Vertical Column (right) over the New York City/Long Island region from the afternoon of June 30th, 2018. NO_2 data are shown at approximately 250 x 250 m resolution, whereas HCHO are binned at 1 x 1 km resolution.

HSRL-2/Ozone DIAL

The airborne High Spectral Resolution Lidar (HSRL)-2 measurements provide vertical profiles of aerosol characteristics below the aircraft (including type classification) as well as have the ability to derive mixed layer heights. NASA also aims to incorporate UV-DIAL capabilities to profile ozone from the aircraft, which can help in mapping out the spatial and vertical distribution of ozone below aircraft altitude. Example data products from this instrument are shown in Figure 11. The HSRL capabilities enable measurements of aerosol backscatter, (532 nm, 1064 nm), extinction (532 nm), and depolarization (355 nm, 532 nm, 1064nm) to characterize the aerosol and cloud distributions.

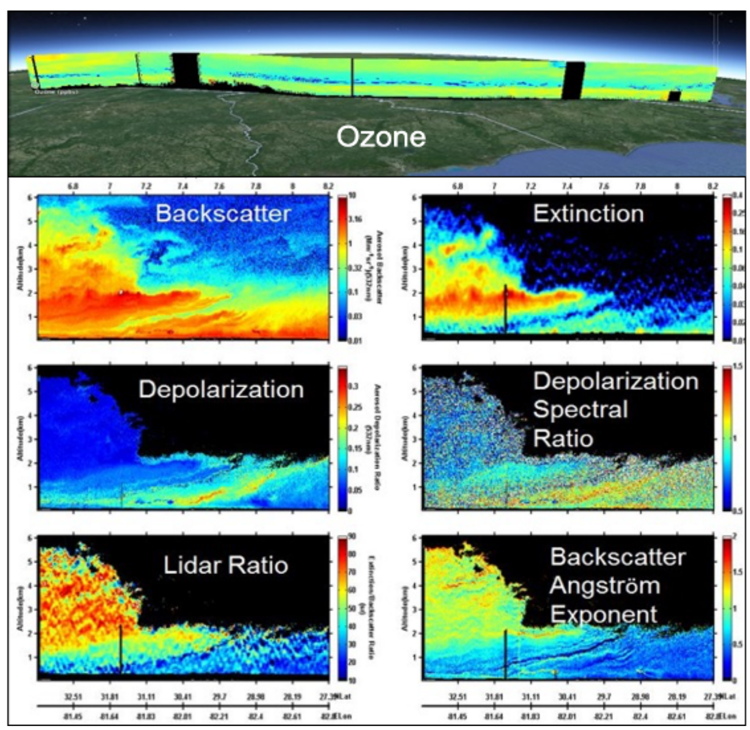


Figure 11: Ozone profiles and extended aerosol products derived from the HSRL-2/Ozone DIAL platform.

The profiling capabilities of the HSRL-2/Ozone DIAL platform aim to successfully describe several chemical and dynamical properties of the state of the atmosphere that can be used to better understand several of the scientific questions in this document. For instance, air quality models predict ozone build-up over water where local deposition is low and regions are often cloud free. However, validation of these predictions with measurements are scarce.

Ground-Based Measurements

Synchronous remote sensing, balloon-borne, and surface observations of trace gases, wind, aerosol, and temperature at specific ground sites will directly reveal the temporal evolution of air quality features across the Houston area

NASA Tropospheric Ozone Lidar Network (TOLNet)

Continuous tropospheric O_3 profiles add a critical component needed to understand processes relevant to air quality and pollution transport. To address these fundamental science and policy questions relating to O_3, ground-based remote sensing efforts from O_3 lidars will be utilized in conjunction with balloon-borne and surface sampling techniques

TOLNet systems from NASA GSFC/TROPOZ, NASA LaRC/LMOL, and NOAA Chemical Science Laboratory/TOPAZ (https://www-air.larc.nasa.gov/missions/TOLNet/) have been identified for these efforts through support from NASA (TROPOZ and LMOL) and TCEQ (TOPAZ). TOLNet O_3 lidars provide accurate (within 5%–10%; Sullivan et al. 2015b) observations vertically through the atmosphere from the surface to 5-8 km depending on daytime or nighttime conditions and can generate consistent long-term datasets. These instruments are portable and have been deployed previously in air quality campaigns in coordination with state and local agency's interests, such as the Fires, Asian, and Stratospheric Transport–Las Vegas Ozone Study (FAST-LVOS) in coordination with Clark County, Nevada; Department of Air Quality and the California Baseline Ozone Transport Study (CABOTS) in coordination with the California Air Resources Board (CARB), OWLETS I & II, LISTOS, and supplementary investigations with the Maryland Department of the Environment. For TRACER-AQ, the three TOLNet systems will be located at La Porte, University of Houston (UH), and Aldine.

Pandora Spectrometers

Pandora spectrometers consist of a ground-based UV-VIS spectrometer capable of operating in direct-sun DOAS or multi-axis(MAX)-DOAS mode (Herman et al., 2009; Herman et al., 2015; Hönninger et al., 2004). Operational products include total column O_3 and NO_2 from direct sun columns that will soon evolve to include HCHO total column. These instruments in MAX-DOAS mode can also retrieve information about the vertical distribution of these pollutants. In Houston, there are two existing Pandora instruments operated by the University of Houston Air Quality Research Group at the University of Houston-Main Campus and a ground site near Liberty, TX. The NASA Pandora Project aims to deploy at least 3 more instruments including one instrument capable of sampling on a boat over the under-sampled Galveston Bay. Another three are planned to be deployed courtesy of Dr. Elena Lind from Virginia Tech. The current goal is to have at least two instruments at each TOLNet lidar location with one dedicated to profiling observations.

Ozonesondes

Support for up to 70 ozonesondes is available courtesy of TCEQ over the course of the 2021 ozone season. Ozonesondes are weather balloons with an instrumented payload to measure ozone, temperature, pressure, wind speed and direction, relative humidity, and location. Measurements are taken every second as the balloon rises through the atmosphere before it bursts 20+ kilometers in altitude (in some cases over 30 km). Launches will be coordinated via communication with TCEQ and the science team based on the air quality forecast. Possible launch sites include the TOLNet lidar locations (at least 7 designated per site in September though FAA dependent at Aldine), boat measurements in Galveston Bay or the Gulf of Mexico, or perhaps from mobile laboratories operating in places of interest on that respective day. The final siting and frequency of launches is an on-going area of discussion.

Parallel Partner-led Efforts

TRACER (PI: Michael Jensen, BNL)

The broad research goal of the TRACER campaign is to fully observe the evolution of convective clouds and the environment, including thermodynamic, kinematic and aerosol properties, in which they initiate, grow, and decay to better understand how aerosols impact convective strength and precipitation. ARM facility field operations include a year-long deployment of the first ARM mobile facility (AMF1) to La Porte, Texas, which will include more than 60 instruments, providing comprehensive in situ and remote sensing observations of clouds, aerosols, precipitation, radiation and meteorology. In addition, a C-band scanning precipitation radar will be deployed near Pearland, TX as well as another precipitation radar system. During intensive operations (summer 2021), additional ARM instrument assets and DOE Atmospheric System Research (ASR) funded efforts will deploy with partners bringing manned and unmanned aircraft, mobile-laboratory facilities, a tethered balloon system, mobile-laboratory facilities, radar systems, detailed aerosol number and composition measurements, and additional radiosonde measurements. The ARM mobile facility instrument suite will include a radar wind profiler, Doppler lidar, ceilometer, and atmospheric emitted radiation interferometer from which high-resolution measurements of boundary layer characteristics including boundary layer depth, thermodynamic structure, winds and turbulence will be collected that can be used to characterize mixing from the surface through the free troposphere. In addition, a detailed focus on observations of aerosol size distribution, composition and optical properties over the full annual cycle (with more intensive operations in summer 2021) can also help TCEQ in evaluating their borderline PM2.5 levels. Two DOE ASR funded TRACER-related projects sub-experiments so far have actively participated in TRACER-AQ planning efforts with associated cross benefits to both studies. These are briefly summarized below:

TRACER-MAP (PI: Rebecca Sheesley, Baylor University)

This effort will deploy a mobile air quality laboratory in the TRACER domain to characterize the impact of convection on gas-aerosol chemistry pre- and post-storm. The trailer will measure O_3, NO, NO_X, NO_Y, CO, SO_2, VOCs & HCHO (PTR-MS), aerosol composition (HR-ToF-AMS), CCN, aerosol optical and physical properties, PBL height (ceilometer), jNO_2, WS/WD, and PTU. Deployment will be coordinated with the forecast team to place the trailer for 3-5 day periods in areas likely to see convective conditions under a variety of aerosol loadings and composition. This program is scheduled for July-August 2021 and coincides with 65 DOE supported O_3 sonde launches on convective days during the same period from the AMF1. Avenues for extending these measurements to September 2021 are currently being pursued.

Ultrafine Aerosol Particle Formation & Impacts in Houston (PI: Jim Smith, UC Riverside)

This effort includes measurements of ambient gas and size-resolved ultrafine particle composition during TRACER at La Porte. This team will also measure size-resolved growth of particles resulting from exposure to photochemically treated, filtered ambient area using the CAGE chamber (Sirmollo et al., 2020). This information gained will lead to a process-level modeling study to describe particle formation and growth in the Houston atmosphere.

TCEQ Supported Studies

BC^2 (University of Houston and Baylor University)

This effort is to measure PM2.5 optical properties to calculate scattering and absorption Angstrom exponents. Together, these measurements can identify periods of dust or biomass burning influence whether in a rural or urban setting. Coupled with satellite and ground based AOD measurements to address whether the plume is lofted or at ground level. During 2021 the new network will operate April-October and consist of four sites, one in El Paso and three in Houston (Aldine, Galveston, Liberty). Each site will have complimentary measurements as well as capacity to host guest researchers and equipment.

Galveston Offshore Ozone Observations (GO^3) (University of Houston)

This effort will deploy automated O_3/Ox measurement systems on two commercial boats. A crew boat will operate between Galveston Island and the offshore areas where the large ships anchor while waiting to enter the Houston Ship Channel or at the lightering area where tankers can load/unload product. A shrimp boat that operates in Galveston Bay will be equipped with a similar O_3/Ox package plus a CL-51 ceilometer to collect routine mixed layer heights in the bay. A combination weather/compass/GPS will provide location and local conditions with true winds calculated. It may be possible to add a Pandora to this payload as well. A third boat owned by UH will be used to conduct targeted sampling within Galveston Bay and will be equipped to launch O_3 sondes from the Bay to evaluate gradients within the marine boundary layer and free troposphere. Additional O_3 sonde launches may occur from the offshore crew boat and UH boat in the Bay in coordination with G-V flights during TRACER-AQ.

TRACER-Mobile (PI: Yuxuan Wang, University of Houston)

This effort would extend the TRACER-MAP campaign as well as additional air quality observations through the September 2021 TRACER-AQ program including added support for a second mobile laboratory that would measure O_3, NO, NO_X, NO_Y, CO, SO_2, HCHO, VOCs (sorbent tubes), PBL height (TBD, pending Goddard ceilometer availability), jNO_2, WS/WD, and PTU. Additional instrumentation may augment this payload. This second mobile laboratory would operate August-September 2021 and focus on mesoscale circulation influence on atmospheric chemistry by probing the evolution of the bay and sea breezes as they propagate inland, in addition to investigating the impact of convection on atmospheric chemistry.

Identified Measurement Gaps

The science team for TRACER-AQ is based on a grass-roots approach and we welcome collaborations from the air quality and health sector partners who have the motivation and resources to fill gaps in our measurement strategy. Identified gaps in the current committed measurement portfolio that could further assist in the investigation of TRACER-AQ science objectives include, but are not limited to:

- **Vertical profiling of trace gases**: In situ information provided by low-altitude platform outfitted with chemical and meteorological measurements could help link and interpret column and surface-based measurement (e.g., Mazzuca et al., 2016; Abdi-Oskouei et al., 2020; Benish et al., 2020). Additional in situ chemical and wind profiling near the coastal interface would improve the overall interpretation of perturbations caused by the onset of the bay/sea-breeze and its associated penetration depth inland. Suggested platforms that have previously been used to sample the lower atmosphere include UAV, tethered balloons, and small aircraft. Though there are challenges to overcome with respect to airspace-restrictions.
- **Wind profiling**: In general, spatiotemporal patterns of pollution will be understood most effectively with the combination of ozone, aerosol backscatter and wind profiles at each "super site". Currently the La Porte site has plans to consist of all three, while the UH-Launch trailer and Aldine sites are limited in vertical wind measurements.
- **Speciated highly reactive volatile organic compounds (HRVOCs):** HRVOCs can produce ozone pollution much more efficiently due to their fundamental reactivity and are generally underestimated in the modeling inventories. These measurements would be a critical addition to the TRACER-AQ effort and improve interpretation of measurements. TCEQ has had success in adjusting the modeling inventories to account for unreported HRVOC emissions and later test-driving controls on emissions of these specific compounds presented, however this presents a set of unique challenges to emissions modelers, since emission processing software typically is not designed to apply adjustments or controls to individual VOC species. Sub-hourly measurements of Ethylene and propylene (in addition to VOCs such as BTEX (Benzene, Toluene, Ethylbenzene, and Xylenes) are generally the most important contributors to total reactivity-weighted concentration in Houston (TCEQ 2020a). Additionally, ground based HCHO in-situ measurements paired with mixing layer height measurements would benefit analyses of correlative column-based measurements from Pandora and GCAS.

Intensive Operations Plan

Figure 12 shows the proposed locations for intensive measurements within the Houston, TX domain for TRACER-AQ and partner-led campaigns. The collaborative approach to TRACER-AQ requires the development of measurement strategies to optimize the overall scientific and technical value of the study. The GCAS and HSRL-2/DIAL instruments on the NASA G-V are capable of mapping high spatial resolution measurements of trace gas and aerosol composition over the Houston area. The fast ground speeds of > 400 kts on the G-V allow for high temporal resolution through a repeated raster sampling strategy. For TRACER-AQ in September 2021, the JSC G-V can fly up to 77 science flight hours. Requirements for flight are dependent on solar zenith angle and cloud coverage over the area of interest. Solar zenith angles must be less than 70 degrees (encompassing 9:00 AM - 5:00PM LT by the end of September). Therefore, each flight could be up to 8 hours which would allow for at least 9+ flight days during this month-long deployment. Sampling of the Houston outflow as it is transported downwind and recirculated is also conceptually feasible both during the week as well as on weekends.

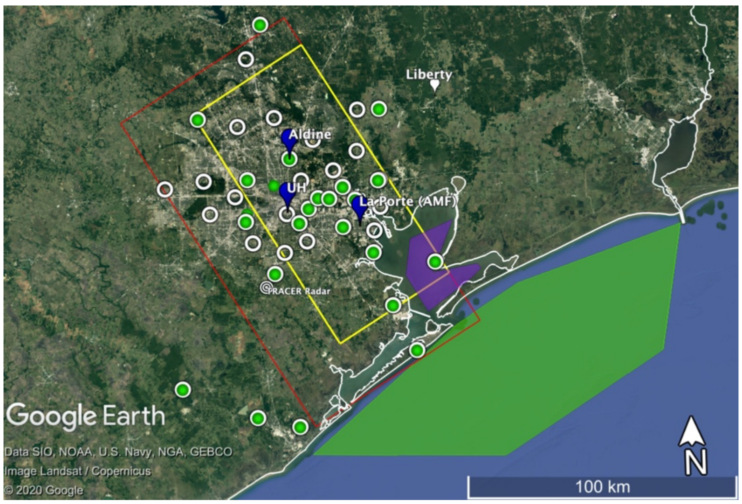


Figure 12: Google Earth Map showing the proposed locations for intensive measurements within the Houston, TX domain for TRACER-AQ and partner-led campaigns. Major enhance ground-based monitoring efforts will be at Aldine, UH, and La Porte (blue balloons). Red and Yellow outlined polygon represent the spatial area that could be covered by the NASA aircraft in 2 and 1 hour, respectively (areas mapped will likely be different than shown), and the green and red filled polygons are proposed domains for boat measurements sponsored by TCEQ/AQRP. White open circles represent ozone regulatory monitoring sites and those filled with green also have NOx measurements co-located.

Ultimately, top-down mapping of ozone and its precursors on the NASA G-V will reveal their spatial extent and the repeated measurements throughout the day will help in characterizing the transport and chemical evolution from source to receptor. Red and yellow outlined polygons in Figure 12 represent the areal extent that can be flown at 2-hour and 1-hour repeats, respectively. These flight areas will require adjustment to from what is shown to cover the most polluted regions of Houston, the background Liberty site for a clean reference, as well as extensions over Galveston Bay and the Gulf of Mexico.

For the duration of TRACER-AQ flights, the aircraft team will likely have one or two common flight plans to execute repeatedly over the region to allow for the accumulation of temporal and spatial statistics. These modes of sampling are sufficient to address the scientific questions posed above, but the science team also has maintained the option for more exploratory flight plans if, for instance, models indicate interesting features or survey flights indicate the influence of anomalous sources worthy of direct sampling. Alternative options for flight areas not associated with the TRACER area may cover offshore drilling platforms of Louisiana and Texas that were the focus during the NASA SCOAPE campaign, as well as emissions sampling over the San Antonio area.

Flight decisions and daily operations will depend on and leverage forecasts from DOE TRACER. This will incorporate use of daily weather and air quality guidance following notated metrics voiced in the TRACER Forecasting Guidance Document to assist in the decision-making pertaining to intensive operations daily. To date, there have been two practice forecasting exercises to prepare for intensive operations in Houston to develop metrics required by various science teams. Following daily briefings during intensive operations, we expect that an additional intensive operation meeting will take place to make measurement decisions for the following day (with brief outlooks into Days 2-5). Forecasting resources have been compiled and are provided here.

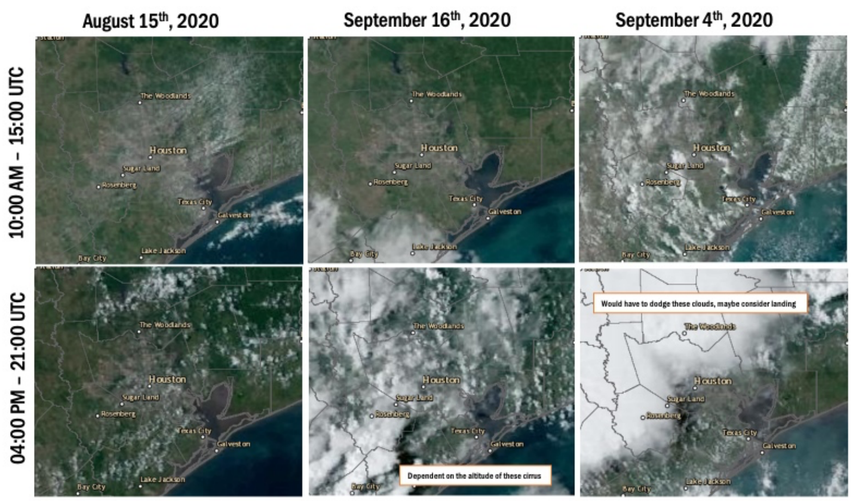


Figure 13: Morning and afternoon GOES ABI snapshots from NOAA Aerosol watch over the Houston region from August 15th, September 16th, and September 4th, 2020.

Most ground- and boat-based operations will occur simultaneously with G-V flights. G-V flight determination will be mostly based on expected cloud coverage of less than 50% over the greater Houston area from 9am-5pm LT, daily. Partial day flights will be considered if cloud conditions are clear in the morning and cloud up in the afternoon and vice versa. Figure 13 shows example images from the GOES-16 ABI instrument (NOAA Aerosol Watch) demonstrating a variety of cloud conditions for various days to illustrate flight feasibility during each condition. The best-case scenario in Houston is a case like August 15th, 2020. There were a few sporadic cumulus clouds throughout the day, but not extensive enough to obscure visualization of the surface. September 16th had ideal conditions in the morning, but through the development of low-level cumulus clouds and high-level cirrus clouds in the afternoon, the flight conditions would be up for debate. If the cirrus were above flight level, then the flight likely would continue. September 4th is an example of an unlikely flight day, but a morning flight could be but likely would have finished early with the arrival of convection from the NE that afternoon. Cloudier conditions than this example would be considered not feasible for flight.

Ground based instrumentation deployed to the Houston, TX region aim to be online for scientific measurements by Sept. 1, 2021. Field observations will vary between assets and teams, depending on funding levels and safety precautions that are recognized at the time of the intensive operations. A fraction of the ground-based instrument will operate autonomously and measure continuously throughout their deployment (ground-based in situ trace gas and aerosol measurements, meteorology, Pandora spectrometers). Other operations will be dependent on air quality and meteorological forecasts as described above (TOLNet operation, boat operations, ozonesonde launches, mobile lab sampling).

For TRACER-Mobile, the UH mobile lab will operate in its mobile mode during all flight days. Sampling strategies will be split between tracking sea/bay-breeze boundaries, sampling convective outflows. When not operating in mobile sampling mode, the lab will spend part of its time sampling in stationary mode at ground sites with other co-located measurements. Similarly, the TRACER-MAP mobile facility will likely operate at predetermined ground site locations that would change based on air quality forecasts throughout the intensive operations period.

Ozonesonde launches will be coordinated in conjunction with boat, mobile-lab, and G-V overflight operations. TOLNet LIDAR operations will be based on air quality forecasts and will operate when forecasts dictate that data relevant to our science objectives would be answered but at the very least will be operating for the duration of flight days.

Data Availability

TRACER-AQ data funded by NASA will be archived in the airborne field campaign data repository (https://www-air.larc.nasa.gov/missions/tracer-aq/index.html). This data will be made publicly available within one-year from the end of the mission. All other partners are encouraged to add their data to this public archive or provide links for access to their select data archive, especially before publishing using NASA datasets. Additional standard ARM datasets for TRACER will be available in the ARM data archive in near-real time, value-added products will be produced shortly after the end of the campaign, PI datasets (e.g. ASR projects) will be available 6 months after the end of the campaign.

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Appendix A1: Detailed Participants/Partners List for TRACER-AQ

The table below includes a growing list of partners and collaborators (alphabetic by organization/institution) for this study with a brief description of their role within the TRACER-AQ effort of partner-led efforts.

Organization or Institution	Person of Contact	TRACER-AQ Involvement
Baylor University	Rebecca Sheesley Sascha Usenko	TRACER-MAP
DOE	Mike Jensen Scott Collis Heath Powers Nathan Wales	TRACER PI TRACER Co-I/Forecasting Coordinator ARM Mobile Facility Operations Manager AMF1 project lead for TRACER
NASA	Barry Lefer	Program Manager for ESD R&A Tropospheric Composition, NASA HQ
	John Haynes	Program Manager for ESD Applied Sciences Health and Air Quality Program, NASA HQ
	Laura Judd	TRACER-AQ Airborne Science PI – Associate Program Manager for ESD Applied Sciences Health and Air Quality Program, NASA LaRC
	John Sullivan	TRACER-AQ Ground Science PI – TOLNet Project Scientist –PI for GSFC TROPOZ, NASA GSFC
	Tom Hanisco	NASA Pandora Project, Project Scientist NASA GSFC
	Alex Kotsakis	NASA Pandora Project, Research Scientist, USRA/NASA GSFC
	Scott Janz	GCAS, PI, NASA GSFC
	Matthew Kowalewski	GCAS, NASA GSFC
	Tim Berkoff	LMOL, PI, NASA LaRC
	Guillaume Gronoff	LMOL, NASA LaRC
	John Hair	HSRL-2, Co-PI, NASA LaRC
	Taylor Shingler	HSRL-2, Co-PI, NASA LaRC
	K. Emma Knowland	GMAO GEOS-CF Liaison, USRA/NASA GSFC
	Aaron Naeger	TEMPO Early Adopters Liaison, UAH/NASA MSFC
	E. Judd Welton	MPLNET Project Head, NASA GSFC
NOAA	Andrew Langford Christoph Senff Raul Alvarez	TOPAZ O3 Lidar, NOAA CSL
TCEQ	Doug Boyer Raj Nadkarni Stephanie Shirley Weslee Copeland	TCEQ, Air Quality Modeling Technical Specialist TCEQ, Senior Air Quality Project Manager TCEQ, Senior Technical Specialist TCEQ, Meteorological and Air Quality Forecasting
University of Houston	James Flynn Yuxuan Wang Claudia Bernier Travis Griggs	Science and Logistics Liaison TRACER-Mobile
University of Virginia	Sally Pusede Angelique Demetillo	AQ Disparity Research
Virginia Polytechnic Institute and State University	Elena Lind	VT Pandora Deployment and Non-Operational Product Retrieval Lead

Appendix A2: Detailed TRACER-AQ Instrument and Site Information

Fixed Site	Point of Contact	Observational Type	Main Parameter(s)
UH/Launch Trailer	James Flynn, jhflynn@central.uh.edu	In Situ sampling	O3, NOx, NOy, CO, Met
	Latitude: 29.7239970° Longitude: -95.3391430° Elevation: 11.0 m	Columnar Retrievals Passive Profiling	**NO2, O3, (Pandora)**, AOD (AERONet) **SO2, HCHO, (Pandora, Moody Tower)**
		Profilers	**Tropospheric O3, (TOLNet Lidar, NASA LaRC),** atmospheric backscatter, (Ceilometer CL-51)
La Porte Airport (AMF1 TRACER Deployment)	John Sullivan/NASA GSFC, john.t.Sullivan@nasa.gov, Heath Powers/LANL/ARM Mobile Facility, hpowers@lanl.gov	In Situ sampling	**O3, NO2,** extensive cloud/aerosol/meteorological observations (CCN, CPC, SMPS, etc.)
	Latitude: 29.6720000° Longitude: -95.0647000° Elevation: 5.0 m	Columnar Retrievals	**NO2, O3, (Pandora),** AOD (AERONet)
		Profilers	**Tropospheric O3, (TOLNet Lidar, NASA GSFC), atmospheric backscatter, (Ceilometer Lufft CHM15k), Ozonesondes**
Aldine	James Flynn, jhflynn@central.uh.edu	In Situ sampling	O3, NOx, NOy, PM 2.5, Met
	Latitude: 29.9010364° Longitude: -95.3261373° Elevation: 24.1 m	Columnar Retrievals Passive Profiling	**NO2, O3, (Pandora)** **SO2, HCHO, (Pandora)**
		Profilers	**Tropospheric O3, (TOLNet Lidar, NOAA CSL)**
Liberty	James Flynn, jhflynn@central.uh.edu Yuxuan Wang, ywang246@central.uh.edu	In Situ sampling	O3, NOx, NOy, PM 2.5, Met
	Latitude: TBD Longitude: TBD Elevation: TBD	Columnar Retrievals	**NO2, O3, (Pandora),** AOD (AERONet)
		Profilers	**Micropulse Lidar (MPLNet/NASA GSFC),** atmospheric backscatter, (Ceilometer CL-51),

Aircraft Platform	Point of Contact	Observational Type	Main Parameter(s)
NASA Gulfstream V	Laura Judd, laura.m.judd@nasa.gov		
GCAS	Scott Janz, scott.j.janz@nasa.gov	UV-VIS Spectral + Below Aircraft Column	NO_2 and HCHO
HSRL-2	Jonathan Hair, johnathan.w.hair@nasa.gov Taylor; Shingler, taylor.j.shingler@nasa.gov	Below Aircraft Profiles	HRSL-2/DIAL - aerosol backscatter, (532, 1064nm), extinction (532nm), and depolarization (355, 532, 1064nm), Ozone mixing ratios

Mobile Platform	Point of Contact	Observational Type	Main Parameter(s)
UH Contract Boat	James Flynn, jhflynn@central.uh.edu	In Situ sampling	O3, NOx,
	Proposed Location on Map, Port in Smith Point	Columnar Retrievals	NO2, O3, (Pandora)
		Profilers	atmospheric backscatter, (Ceilometer CL-51)
MAQL2 Trailer (TRACER-MAP)	Rebecca Sheesley/Baylor rebecca_sheesley@baylor.edu),	In Situ sampling	O3, NO2, NO NOy, PTR-MS, CO, SO2, jNO2, Met extensive cloud/aerosol/meteorological observations (CCN, CPC, SMPS, etc.)
	Note: TRACER-AQ contingent on funding extension into September	Columnar Retrievals	n/a
		Profilers	atmospheric backscatter, (Ceilometer CL-51)
MAQL Trailer (TRACER-Mobile)	James Flynn, jhflynn@central.uh.edu Yuxuan Wang, ywang246@central.uh.edu	In Situ sampling	O3, CO, SO2, NO, NOx, Noy, HCHO, VOC, Met,
	Note: TRACER-AQ contingent on funding extension into September	Columnar Retrievals	n/a