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Extended Observation Data for the 2022 Modeling Platform Performance Evaluation

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RAMBOLL

Extended Observation Data for the 2022 Modeling Platform Performance Evaluation

Final Report

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LIST OF ACRONYMS AND ABBREVIATIONS

AGL	Above Ground Level
AMSL	Altitude above mean sea level
CAMx	Comprehensive Air Quality Model with Extensions
CST	Central Standard Time
CSV	Comma-separated Values
EPA	Environmental Protection Agency
FCAA	Federal Clean Air Act
GPS	Global Positioning System
LCC	Lambert Conformal Conic
MAQL	Mobile Air Quality Laboratory
MPE	Model Per
NOx	Nitrogen Oxides
PGM	Photochemical grid model(s)
ppbC	parts per billion Carbon
ppbv	parts per billion
PM2.5	Particulate Matter with diameter smaller than 2.5 μm
PTR-SRI-MS	Proton Transfer Reaction Mass Spectrometer with a Selective Reagent Ionization
SOF	Solar Occultation Flux
sUAS	small Unmanned Aircraft System
TRACER-AQ2	Tracking Aerosol Convection Interactions ExpeRiment-Air Quality
TCEQ	Texas Commission on Environmental Quality
UHPB	University of Houston Pontoon boat
VOC	Volatile Organic Compounds
WD	Wind direction
WS	Wind speed

PROJECT SUMMARY

TCEQ is developing an air quality modeling platform for 2022 for attainment demonstration purposes under the Federal Clean Air Act (FCAA). Evaluating model performance is a crucial step in the air quality modeling process. TCEQ provided Ramboll with air quality measurement data collected in Houston during 2022, which Ramboll processed into files to be used in TCEQ's Model Performance Evaluation (MPE).

EXECUTIVE SUMMARY

TCEQ is developing an air quality modeling platform for 2022 for attainment demonstration purposes under the Federal Clean Air Act (FCAA). The air quality modeling platform provides estimates of ozone, particulate matter, and their precursor concentrations using photochemical grid models (PGMs) such as the Comprehensive Air Quality Model with extensions (CAMx). Evaluating model performance is a crucial step in the development of the modeling platform. A model performance evaluation involves comparing simulated values of a parameter to estimated or measured values of the same parameter and quantifying the difference using various statistical measures.

The Tracking Aerosol Convection Interactions ExpeRiment-Air Quality (TRACER-AQ2) field campaign conducted air quality measurements from stationary and mobile platforms (including drones, ozonesondes, Pandora profilers, mobile labs, and shipping boats) in Houston from April through October 2022 to assess a wider spatial footprint than stationary monitors offer alone. An important objective of the project summarized in this report is to consolidate and reformat the TRACER-AQ2 dataset to allow TCEQ to perform a more comprehensive and detailed Model Performance Evaluation (MPE) for their modeling platform. This project will also help the TCEQ to evaluate multiple CAMx simulations against TRACER-AQ2 field data from which to guide the technical configuration of the modeling platform.

TCEQ provided Ramboll TRACER-AQ2 measurements collected in seven main datasets. Table 2 provides a brief description of contents and the number of files in each dataset. We provide more detail for each individual dataset in subsequent sections. For each data category, Ramboll provided one or more plain text files processed as comma-separated values (CSV) format. We grouped available measurements within each dataset that have identical date and time stamps in single CSV files. We made several general changes that introduced consistent formats in all column headers, number of significant digits and units across all datasets. An important modification that will facilitate comparison with model results is the inclusion of grid cell column and row information that correspond to TCEQ's 4 km computational domain. We also added rotated wind speed and direction that are consistent with the modeling domain's Lambert Conformal Conic (LCC) projection. As Ramboll processed these datasets, we identified certain aspects that deviated from this general approach or required alternatives to format the data. We documented those differences in the individual platform sections. We provided a final inventory of the processed files in a data manifest Excel spreadsheet accompanying this report, which includes their final format, the file names that belong to each category, and any other relevant metadata.

Ramboll has two recommendations for TCEQ to consider for future projects: 1) Apply the processing methods developed under this project to other air quality measurement campaign datasets; and 2) Assist TCEQ in assessing model performance evaluation using the new dataset.

1.0 INTRODUCTION

TCEQ is currently developing an air quality modeling platform for the year 2022 for attainment demonstration purposes under the Federal Clean Air Act (FCAA). The air quality modeling platform provides estimates of ozone, particulate matter, and their precursor concentrations using photochemical grid models (PGMs) such as the Comprehensive Air Quality Model with extensions (CAMx). Evaluating model performance is a crucial step in the development of the modeling platform. A model performance evaluation involves comparing simulated values of a parameter to estimated or measured values of the same parameter and quantifying the difference using various statistical measures.

The Tracking Aerosol Convection Interactions ExpeRiment-Air Quality (TRACER-AQ2) field campaign conducted air quality measurements from stationary and mobile platforms (including drones, ozonesondes, Pandora profilers, mobile labs, and shipping boats) in Houston from April through October 2022 to assess a wider spatial footprint than stationary monitors offer alone. These additional air quality measurements can be used by TCEQ to improve scientific understanding of ozone and particulate matter formation as well as to evaluate and inform photochemical modeling. Quality-assured data from the field campaign are available in an electronic format at the TCEQ.

The TRACER-AQ2 datasets collected are listed in Table 1 for the following monitoring platforms: Mobile Air Quality Lab 1 (MAQL1), Mobile Air Quality Lab 2 (MAQL2), water vessels from University of Houston (UH Pontoon Boat, RMS Victory, Red Eagle), small Unmanned Aircraft System (sUAS), and FluxSense Mobile Lab. These platforms were outfitted with analytical instruments including Pandora profilers, ceilometers, volatile organic compounds (VOC) resin tubes samplers, and weather stations.

Table 1. Measuring platform, instruments, and measurements from the TRACER-AQ2 field campaign.

Platform	Instruments	Measurements
MAQL1	Hantzsch reaction and fluorescence light technique	Formaldehyde (HCHO)
MAQL1	Rapid Alkene Detector (RAD)	Highly reactive Volatile Organic Compounds (VOC; lumped ethene, propene, butadiene, and isoprene)
MAQL1	Peak Performer 1 Reducing Compound Photometer	Isoprene
MAQL1	AROMA uses CRDS Cavity Ring-Down Spectroscopy (Speciation and Rapid Scan modes)	Speciation Mode: Isoprene, Benzene, Toluene, Ethylbenzene, Xylene and Styrene RapidScan Mode: Alkanes, Aromatics, Dienes, Ethylene Oxide and Methane
MAQL1	Pandora	Nitrogen dioxide (NO_2), HCHO
MAQL1	Thermovironment Trace gas analyzers	Nitric oxide (NO), Oxides of nitrogen (NO_X), Total Reactive Nitrogen (NO_Y), NO_X/NO_2, Ozone, Sulfur Dioxide (SO_2), and Carbon Monoxide (CO)

Platform	Instruments	Measurements
MAQL1	Other parameters	Photolysis rate of nitrogen dioxide (jNO_2), temperature, relative humidity (RH), pressure (P), wind speed (WS), wind direction (WD), Global Positioning System (GPS), and Boundary Layer Height
MAQL2	Proton Transfer Reaction Mass Spectrometer with a Selective Reagent Ionization (PTR-SRI-MS)	Formaldehyde, acetonitrile, acetaldehyde, acetone, isoprene, methyl vinyl ketone plus methacrolein, benzene, toluene, styrene, C2-alkylbenzenes, C3- alkylbenzenes, C4-alkylbenzenes, monoterpenes, propene, ethylene, and 1,3- butadiene
MAQL2	Tricolor Absorption Photometer	Aerosol absorption
MAQL2	Tricolor nephelometer	Aerosol scattering
MAQL2	Trace gas analyzers	NO, NO_X/NO_2, NO_Y, Ozone, SO_2, and CO
MAQL2	Other parameters	jNO_2, temperature, RH, pressure, wind speed, wind direction, and GPS, and Boundary Layer Height
Red Eagle	2B Technology Model 205 dual-beam ozone analyzer with a blue light converter (BLC)	Ozone, Odd Oxygen Family (O_X), NO_2 (calculated)
Red Eagle	Weather station	Temperature, relative humidity, pressure, and wind speed and direction, GPS
Red Eagle	Vaisala CL-51 ceilometer	Boundary layer/cloud height (BLH)
Red Eagle	Ozonesonde launch	Vertical profiles of Ozone, temperature, and RH; GPS location, and GPS-derived wind speed and direction
RMS Victory	2B Technology Model 205 dual-beam ozone analyzer with BLC	Ozone, O_X, NO_2 (calculated)
RMS Victory	Weather station	Temperature, relative humidity, pressure, and wind speed and direction, GPS
UH Pontoon Boat	Trace gas analyzers	Ozone, NO, NO_X/NO_2, CO
UH Pontoon Boat	Pandora spectrometer	Columnar values of NO_2, Ozone, and formaldehyde
UH Pontoon Boat	Radiometer	jNO_2
UH Pontoon Boat	Vaisala CL-51 ceilometer	Boundary layer/cloud height
UH Pontoon Boat	Weather Station	Temperature, relative humidity, pressure, and wind speed and direction, GPS
UH Pontoon Boat	Ozonesonde launch	Vertical profiles of Ozone, temperature, and RH; GPS location, and GPS-derived wind speed and direction
sUAS	Ozonesonde with radiosonde	Ozone, temperature, pressure, and RH, GPS location, and altitude
sUAS	Resin tubes	VOCs
FluxSense Mobile Lab	Solar Occultation Flux (SOF)	Gas columns through the atmosphere by means of infrared light absorption
FluxSense Mobile Lab	SkyDOAS (Differential Optical Absorption Spectroscopy)	Gas columns through the atmosphere by means of ultraviolet light absorption
FluxSense Mobile Lab	MeFTIR (Mobile extractive Fourier Transformed Infrared spectrometer)	VOCs
FluxSense Mobile Lab	Mobile extractive White cell DOAS (MeDOAS)	Alkanes, ethylene, propylene, isobutene, formaldehyde, methane, benzene, toluene, ethylbenzene, pxylene, and m-xylene)

An important objective of this project was to prepare datasets from the TRACER-AQ2 field study that would allow TCEQ to perform a more comprehensive and detailed Model Performance Evaluation (MPE) of the modeling platform. Together with the national set of standard surface-based monitor measurements, these TRACER-AQ2 measurements may inform technical choices in the development and improvement of the 2022 modeling platform.

This report describes how each TRACER-AQ2 dataset was processed and consolidated to facilitate TCEQ's evaluation of their 2022 modeling platform.

2.0 APPROACH

In this section we briefly summarize the datasets received from TCEQ and then describe the processing we performed on each to prepare them for an eventual evaluation of the 2022 TCEQ's modeling platform. Ramboll received from TCEQ TRACER-AQ2 measurements collected in seven main datasets. Table 2 provides a brief description of what is included and the number of files in each dataset.

Table 2. Description of measurements included in TRACER-AQ2 data provided by TCEQ

Data Category	Number of Files	Description
1. FluxSense Data	2243	Various VOC pollutant concentrations (units: $\mu g/m^3$) and column amounts (units: mg/m^2) (e.g., benzene, BTEX, NO_2, HCHO)
2. Ozonesonde Data	46	Meteorological and ozone sonde data
3. Pandora NO_2 and HCHO Data	4	NO_2 and Formaldehyde concentrations (mol/m^3) and column amounts (mol/m^2), meteorological data, ozone data
4. Mobile Lab Data (Resin Tubes)	1	Various VOC pollutant concentrations (ppbv) (e.g., isoprene, benzene, toluene, PCBTF)
4. Mobile Lab Data (PM)	4	Absorption and Total Scattering coefficient data at various wavelengths (Mm^{-1})
4. Mobile Lab Data (VOC)	6	VOC concentrations (ppbv, ppmv, some units not provided) (e.g., isoprene, formaldehyde, benzene, toluene, alkanes, aromatics)
4. Mobile Lab Data (Meteorology)	3	Meteorological data, various pollutant concentrations (ppbv) (e.g., NO_X, O_3, SO_2)
5. Offshore Air Quality Measurements	1	Meteorological data, various pollutant concentrations (ppbv) (CO, NO_X, O_3)
6. Commercial Vessels Offshore AQ Data	2	Meteorological data, various pollutant concentrations (ppbv) (CO, NO_X, O_3)
7. Drones Data	24	Meteorological and ozone data

For each data category, Ramboll processed the provided files and in several cases, consolidated them for convenience. We formatted the data in a consistent manner in one or more comma-separated values (CSV) plain text files. We grouped available measurements within each data category that have identical date and time stamps (hereafter "datetime stamps") into a single CSV file. Datetime stamps are expressed in Central Standard Time (CST) following this format:

YYYYMMDD HH:MM:SS

Where YYYYMMDD is the date, and HH:MM:SS is the time in 24-hour format. Additionally, the following general changes were performed as needed for all datasets:

1. Any day and time columns were processed with a consistent format as described above and provided in two columns: one with the date and one with the hours, minutes and seconds.
2. Data were provided in their individual native time resolution. Ramboll did not average or aggregate any dataset in time.

3. We prioritized the use and implementation of metric system units (meters, seconds, degrees Celsius, etc.).
4. We converted any ppmv/ppbv concentration data for carbon-containing species to ppmC/ppbC by multiplying the volume concentration by the number of carbons per molecule. Otherwise, we kept pollutant concentrations in their native units.
5. We retained most volatile organic compounds (VOC) species in the deliverables, but several species should be compared lumped instead of individually. We have provided TCEQ a file with the recommended mapping between measured and modeled species.
6. All fields (column names) were updated and revised for consistency. For instance, datasets that include latitude were renamed from the several identifiers currently used (GPSLat, RE_LAT_DDeg_1min_avg, etc.) to a single term (latitude).
7. Additional data columns were added with the horizontal (X) and vertical (Y) distance in meters from the origin of the Lambert Conformal Conic (LCC) projection used in TCEQ's 4 km computational domain. Also, data columns were added to include the integer indices for the grid cell columns and rows that correspond to the latitude and longitude coordinates in relevant datasets.
8. Pollutant names were revised for consistency, giving preference to their chemical formulas (i.e. O3 instead of ozone) except when several pollutants are aggregated and do not represent a single chemical compound (i.e. Total alkanes).
9. For datasets where temperature and relative humidity were provided, we added a column with the dew point temperature calculated using the Magnus-Tetens empirical approximation.
10. We rotated any observed wind speed and direction to be consistent with the Lambert Conformal Conic projection used by WRF and CAMx. This rotation allows wind measurements to be compared directly to model estimates in a consistent manner.
11. For datasets with wind speed and direction, we added data columns with the explicit U and V components of the corresponding wind vectors.

Measurements from several platforms raise concerns about spatial representativeness when comparing fine scale measurements to coarser CAMx grid cells. We recommend that vertical column measurements, like Solar Occultation Flux (SOF), be compared to columns computed from three-dimensional CAMx outputs. This approach helps reduce errors that may occur in CAMx's vertical distribution of pollutant concentrations. Mobile lab measurements may be less comparable to CAMx than SOF when the measurements are collected along roads with significant traffic, which CAMx may not accurately represent. For instance, NO_X concentrations measured from mobile platforms near roads may be significantly underpredicted by the model and one should not conclude the model performance is not adequate for the modeling project's objectives.

As Ramboll processed these datasets, we found certain aspects that deviated from this general approach or required alternatives to format the data. We documented those differences in the processing approach sections for individual platforms below. We provided TCEQ a final inventory of the processed files in a data manifest Excel spreadsheet, which includes their final format, the

number of files that belong to each category, and relevant metadata. The following subsections provide more detail on how each dataset category was processed.

2.1 Flux Sense

FluxSense Mobile data provided by TCEQ contains measurements from SOF, SkyDOAS, MeFTIR and MeDOAS instruments. Ramboll identified 1,888 files out of the 2,243 total files to be processed in this dataset, sharing a similar format. The unused files were either duplicates or contained measurements of propene (C_3H_6) which is not explicitly represented in the CAMx Carbon Bond chemical mechanisms (CB6/CB7) and thus not considered for MPE purposes. Table 3 describes the fields from the original data files that were processed as part of this dataset and the corresponding fields in the processed files. The Flux Sense data was organized such that each processed file and its name represents measurements for a single pollutant or pollutant group at a single measurement site.

Table 3. Fields included in the FluxSense dataset

Original Field Name	Processed File Field Name	Processed Field Description	Processed Field Units
Day	DATE	Date in Central Standard Time	MM/DD/YYYY
Time	TIME	Time in Central Standard Time	HH:MM:SS
GPSlat	LATITUDE	Latitude	Degrees
GPSLon	LONGITUDE	Longitude	Degrees
TotalAlkanes (ug/m3)	TotalAlkanes (ug/m3)	Total Alkanes concentration	$\mu g/m^3$
Benzene (ug/m3)	Benzene (ug/m3)	Benzene concentration	$\mu g/m^3$
BTEX (ug/m3)	BTEX (ug/m3)	Benzene, Toluene, Ethylbenzene, and Xylenes concentration	$\mu g/m^3$
HCHO (mg/m2)	HCHO (mg/m2)	HCHO column amount	mg/m^2
NO2 (mg/m2)	NO2 (mg/m2)	NO_2 column amount	mg/m^2
C2H4 (mg/m2)	C2H4 (mg/m2)	C_2H_4 column amount	mg/m^2
TotalAlkanes (mg/m2)	TotalAlkanes (mg/m2)	Total Alkanes column amount	mg/m^2
WS (m/s)	WS	Wind speed	m/s
DIR	WD	Wind direction	Degrees
N/A	U	Wind Speed X-component	m/s
N/A	V	Wind Speed Y-component	m/s
N/A	LCC-X	X-component to LCC projection origin	m
N/A	LCC-Y	Y-component to LCC projection origin	m
N/A	i	Grid cell column index	N/A
N/A	j	Grid cell row index	N/A

2.2 Ozonesonde Data

Ozone profiles and meteorological parameters were measured using ozonesondes and provided by TCEQ. Ramboll identified 46 files in this dataset, with each file sharing a similar format. The above mean sea level (AMSL) altitude was changed from kilometers to meters. The original files have two values for the altitude: one from GPS and one pressure-derived. Although both are similar, we chose the pressure-derived values for the deliverable because they are more consistent and do not show negative altitude values at the surface like the GPS data, except for four files that are corrected by removing any the rows with data when the altitude is negative. The ozonesonde data processed files were named such that they correspond with the unprocessed filenames. Table 4 describes the fields from the original data files and the corresponding fields in the processed files.

Table 4. Fields included in the Ozonesonde dataset.

Original Field Name	Processed Field Name	Processed Field Description	Units
N/A	Date	Date in Central Standard Time	MM/DD/YYYY
Time	Time	Local time in Central Standard Time	HH:MM:SS
Altitude	Altitude (AMSL)	Altitude above mean sea level	km
N/A	Elevation	Site/Launch point elevation	km
N/A	Altitude (AGL)	Altitude above ground level	km
Temperature	Temperature	Ambient temperature	Degrees Celsius
N/A	Dewpoint	Dewpoint temperature	Degrees Celsius
RH	RH	Ambient relative humidity	%
Ozone_MR	O_3	Ozone concentration	ppmv
GPSLon	Longitude	Longitude	Degrees
GPSLat	Latitude	Latitude	Degrees
Pressure	Pressure	Ambient pressure	mbar
WindDirection	WD	Wind direction in LCC projection	Degrees
WindSpeed	WS	Wind speed in LCC projection	m/s
N/A	U	Wind speed x-component	m/s
N/A	V	Wind speed y-component	m/s
N/A	LCC-X	X-Component to LCC projection origin	m
N/A	LCC-Y	Y-Component to LCC projection origin	m
N/A	i	Grid cell column index	N/A
N/A	j	Grid cell row index	N/A

2.3 Pandora NO_2 and HCHO

Two Pandora instruments collected nitrogen dioxide (NO_2) and formaldehyde (HCHO) concentrations and data were provided by TCEQ in two files per pollutant (4 total files). Each file pair shares a similar format. Table 5 and Table 6 describe the original data file fields included as part of this dataset and the processed field names and descriptions. The dataset includes a surface concentration index value that indicates the validity or type of measurement made. A value of -6 in this index indicates no surface concentration was retrieved and we noticed this is the most common value reported.

Table 5. Fields included in the Pandora NO_2 dataset.

Original Field Description	Processed Field Name	Processed Field Description	Processed Field Units
UTC date and time for measurement center	Date	Date in Central Standard Time	MM/DD/YYYY
UTC date and time for measurement center	Time	Time in Central Standard Time	HH:MM:SS
Effective duration of measurement	Effective Measurement Duration	Measurement Duration	seconds
Nitrogen dioxide surface concentration	NO_2 Surface Concentration (mol/m3)	NO_2 Surface Concentration	mol/m^3
Nitrogen dioxide surface concentration index	NO_2 Surface Concentration Index	Surface Concentration Index	N/A
Nitrogen dioxide tropospheric vertical column amount	NO_2 Vertical Column (mol/m2)	NO_2 Vertical Column	mol/m^2
Location latitude	Latitude	Latitude	degrees
Location longitude	Longitude	Longitude	degrees
N/A	LCC-X	X-component to LCC projection origin	m
N/A	LCC-Y	Y-component to LCC projection origin	m
N/A	i	Grid cell column index	N/A
N/A	j	Grid cell row index	N/A

Table 6. Fields included in the Pandora HCHO dataset.

Original Field Description	Processed Field Name	Processed Field Description	Processed Field Units
UTC date and time for measurement center	Date	Date in Central Standard Time	MM/DD/YYYY
UTC date and time for measurement center	Time	Time in Central Standard Time	HH:MM:SS
Effective duration of measurement	Effective Measurement Duration	Measurement Duration	seconds

Original Field Description	Processed Field Name	Processed Field Description	Processed Field Units
Formaldehyde surface concentration	Formaldehyde Surface Concentration (mol/m3)	Formaldehyde Surface Concentration	mol/m^3
Formaldehyde surface concentration index	Formaldehyde Surface Concentration Index	Surface Concentration Index	N/A
Formaldehyde tropospheric vertical column amount	Formaldehyde Vertical Column (mol/m2)	NO_2 Vertical Column	mol/m^2
Location latitude	Latitude	Latitude	degrees
Location longitude	Longitude	Longitude	degrees
N/A	LCC-X	X-component to LCC projection origin	m
N/A	LCC-Y	Y-component to LCC projection origin	m
N/A	i	Grid cell column index	N/A
N/A	j	Grid cell row index	N/A

2.4 Mobile Laboratory Measurements Data

TCEQ provided mobile laboratory resin tube measurements for VOC, other pollutants, and meteorological data. Ramboll identified a total of 10 files to be processed for this dataset. The final processed file structures are described in individual categories below. As feasible, data were combined based on timestamp. The position of the mobile lab is specified in 10 seconds intervals, and some of the measurements are integrated over longer intervals. In those cases, the data aggregated over longer intervals were repeated for each time stamp within the interval.

2.4.1 MAQL1 Meteorological and VOC Data

The MAQL1 Meteorological and VOC data were provided in 4 files. The meteorological data file included latitude and longitude coordinates and various meteorological data in 10-second time increments, and the other three files included pollutant concentration data at 10-second and 5-minute time increments. All pollutant concentrations were merged along with the meteorological data based on time stamps. Table 7 describes the fields from the original data files that were processed as part of this dataset and the corresponding fields in the processed file. Ramboll estimate the dewpoint temperature and added to this dataset.

Table 7. Fields included in the MAQL1 Meteorological and VOC Dataset.

Original Field Name	Processed Field Name	Processed Field Description	Units
maql1_time_CST_1min	Date	Date in Central Standard Time	MM/DD/YYYY
maql1_time_CST_1min	Time	Local time in Central Standard Time	HH:MM:SS
maql1_altitude_masl_10s	Altitude	Altitude above mean sea level	km
maql1_temp_degC_10s	Temperature	Ambient temperature	Degrees Celsius
N/A	Dewpoint	Dewpoint temperature	Degrees Celsius
maql1_rh_percent_10s	RH	Ambient relative humidity	%
maql1_no_ppbv_10s	NO	Concentration of NO	ppbv
maql1_no2_ppbv_10s	NO_2	Concentration of NO_2	ppbv
maql1_noy_ppbv_10s	NO_Y	Concentration of NO_Y	ppbv
maql1_o3_ppbv_10s	O_3	Concentration of O_3	ppbv
maql1_so2_ppbv_10s	SO_2	Concentration of SO_2	ppbv
maql1_hcho_ppbv_10s	HCHO	Concentration of HCHO	ppbC
MAQL1_propene_equivalent_ppbv_10s	Propene Equivalent	Concentration of Propene equivalent	ppbC
maql1_isoprene_ppbv_5min	Isoprene	Concentration of Isoprene	ppbC
maql1_longitude_dd_10s	Longitude	Longitude	Degrees
maql1_latitude_dd_10s	Latitude	Latitude	Degrees
maql1_press_mbar_10s	Pressure	Ambient pressure	mbar
maql1_wd_deg_10s	WD	Wind direction in LCC projection	Degrees
maql1_ws_mps_10s	WS	Wind speed in LCC projection	m/s
N/A	U	Wind speed x-component	m/s
N/A	V	Wind speed y-component	m/s
N/A	LCC-X	X-Component to LCC projection origin	m
N/A	LCC-y	Y-Component to LCC projection origin	m
N/A	i	Grid cell column index	N/A
N/A	j	Grid cell row index	N/A

2.4.2 MAQL1 AROMA Data

TCEQ provided the MAQL1 AROMA data in 2 files. The Rapid Scan file includes latitude and longitude coordinates and VOC data in 2-minute time increments. The speciated VOCs file includes VOC data averaged over 2 minutes, approximately every 10 minutes. The data were merged based on time stamps. All the data with a Sample ID of "Isoprene Cal" were excluded from processing. Table 8 describes the fields from the original data files that were processed as part of this dataset and the corresponding fields in the processed file.

Table 8. Fields included in the MAQL1 Meteorological and VOC Dataset.

Original Field Name	Processed Field Name	Processed Field Description	Units
DateTime	Date	Date in Central Standard Time	MM/DD/YYYY
DateTime	Time	Local time in Central Standard Time	HH:MM:SS
Alkanes (ppbv)	Alkanes	Dewpoint temperature	Degrees Celsius
Aromatics (ppbv)	Aromatics	Ambient relative humidity	%
Ethylene Oxides (ppbv)	Ethylene Oxides	Concentration of NO	ppbv
Methane (ppmv)	Methane	Concentration of NO_2	ppbv
Isoprene (ppbv)	Isoprene	Concentration of NO_Y	ppbv
Benzene (ppbv)	Benzene	Concentration of O_3	ppbv
Toluene (ppbv)	Toluene	Concentration of SO_2	ppbv
Ethylbenzene (ppbv)	Ethylbenzene	Concentration of HCHO	ppbC
Xylene (ppbv)	Xylene	Concentration of Propene equivalent	ppbC
Styrene (ppbv)	Styrene	Concentration of Isoprene	ppbC
Longitude (deg)	Longitude	Longitude	Degrees
Latitude (deg)	Latitude	Latitude	Degrees
N/A	LCC-X	X-Component to LCC projection origin	m
N/A	LCC-y	Y-Component to LCC projection origin	m
N/A	i	Grid cell column index	N/A
N/A	j	Grid cell row index	N/A

2.4.3 Resin Tubes

Resin tube data include VOC concentrations that were provided in a single file. Table 9 describes the fields in the original data file and the corresponding fields in the processed file. The resin tube data were merged with the MAQL2 meteorological data described below (Sample ID: "Ground Data") and the Red Eagle Commercial Vessel data (Sample ID: "Red Eagle") based on date, time and Sample ID. Some of the records for "Ground Data" data did not have a corresponding Sample ID in the Sample Info tab. Since we could not assign a datetime stamp, some of these data were excluded from our deliverable.

Table 9. Fields included in the Resin Tube Dataset.

Original Field Name	Processed Field Name	Processed Field Description	Units
Isoprene	Isoprene	Concentration of Isoprene	ppbC
Benzene	Benzene	Concentration of Benzene	ppbC
Toluene	Toluene	Concentration of Toluene	ppbC
Ethylbenzene	Ethylbenzene	Concentration of Ethylbenzene	ppbC
m&p-Xylene	m&p-Xylene	Concentration of m&p-Xylene	ppbC
o-Xylene	o-Xylene	Concentration of O-Xylene	ppbC
Styrene	Styrene	Concentration of Styrene	ppbC
a-Pinene	a-Pinene	Concentration of a-Pinene	ppbC

2.4.4 MAQL2 Meteorological and VOC (Resin Tube) Data

The MAQL2 Meteorological and VOC (Resin Tube) data were provided in 2 files. The meteorological data file included various meteorological data in 5-minute time increments, and the resin tube data in 10-minute time increments. The resin tube data were merged with the meteorological data based on time stamps. Latitude and longitude records were added based on information available in the TRACER-AQ2 Analysis in the Houston Final Report[1]. Table 10 describes the fields from the original data files and the corresponding fields in the processed file. Ramboll added the dewpoint temperature to this dataset.

Table 10. Fields included in the MAQL2 Meteorological and VOC Dataset.

Original Field Name	Processed Field Name	Processed Field Description	Units
maql2_time_mid_cst_5min	Date	Date in Central Standard Time	MM/DD/YYYY
maql2_time_mid_cst_5min	Time	Local time in Central Standard Time	HH:MM:SS
maql2_temp_degC_5min	Temperature	Ambient temperature	Degrees Celsius
N/A	Dewpoint	Dewpoint temperature	Degrees Celsius
maql2_rh_percent_5min	RH	Ambient relative humidity	%
maql2_no_ppbv_5min	NO	Concentration of NO	ppbv
maql2_no2_ppbv_5min	NO_2	Concentration of NO_2	ppbv
maql2_noy_ppbv_5min	NO_Y	Concentration of NO_Y	ppbv
maql2_o3_ppbv_5min	O_3	Concentration of O_3	ppbv
maql2_so2_ppbv_5min	SO_2	Concentration of SO_2	ppbv
Isoprene	Isoprene	Concentration of Isoprene	ppbC
Benzene	Benzene	Concentration of Benzene	ppbC
Toluene	Toluene	Concentration of Toluene	ppbC
Ethylbenzene	Ethylbenzene	Concentration of Ethylbenzene	ppbC
m&p-Xylene	m&p-Xylene	Concentration of m&p-Xylene	ppbC
o-Xylene	o-Xylene	Concentration of O-Xylene	ppbC
Styrene	Styrene	Concentration of Styrene	ppbC
a-Pinene	a-Pinene	Concentration of a-Pinene	ppbC
N/A	Longitude	Longitude	Degrees
N/A	Latitude	Latitude	Degrees
maql1_press_mbar_10s	Pressure	Ambient pressure	Mbar

[1] TRACER-AQ2 Analysis in Houston. Final Report. Prepared for TCEQ. May 31, 2024

Original Field Name	Processed Field Name	Processed Field Description	Units
maql2_wd_deg_5min	WD	Wind direction in LCC projection	Degrees
maql2_ws_mps_5min	WS	Wind speed in LCC projection	m/s
N/A	U	Wind speed x-component	m/s
N/A	V	Wind speed y-component	m/s
N/A	LCC-X	X-Component to LCC projection origin	m
N/A	LCC-y	Y-Component to LCC projection origin	m
N/A	i	Grid cell column index	N/A
N/A	j	Grid cell row index	N/A

2.4.5 MAQL2 PTR-MS Data

The MAQL2 PTR-MS data were provided in one file. The PTR-MS data include VOC concentrations in 30-second time increments. Latitude and longitude records were added based on information available in the TRACER-AQ2 Analysis in the Houston Final Report[1]. Table 11 describes the fields from the original data files that were processed as part of this dataset and the corresponding fields in the processed file.

Table 11. Fields included in the MAQL2 PTR-MS Dataset.

Original Field Name	Processed Field Name	Processed Field Description	Units
Time	Date	Date in Central Standard Time	MM/DD/YYYY
Time	Time	Local time in Central Standard Time	HH:MM:SS
Ethene	Ethene	Concentration of Ethene	ppbC
Formaldehyde	Formaldehyde	Concentration of Formaldehyde	ppbC
Acetaldehyde	Acetaldehyde	Concentration of Acetaldehyde	ppbC
Acetone	Acetone	Concentration of Acetone	ppbC
DMS	DMS	Concentration of DMS	ppbC
Isoprene	Isoprene	Concentration of Isoprene	ppbC
Benzene	Benzene	Concentration of Benzene	ppbC
Toluene	Toluene	Concentration of Toluene	ppbC
Styrene	Styrene	Concentration of Styrene	ppbC
m-Xylene	m-Xylene	Concentration of m-Xylene	ppbC
C3-Benzene	C3-Benzene	Concentration of C3-Benzene	ppbC
C4-Benzene	C4-Benzene	Concentration of C4-Benzene	ppbC

Original Field Name	Processed Field Name	Processed Field Description	Units
Monoterpene	Monoterpene	Concentration of Monoterpene	ppbC
N/A	Longitude	Longitude	Degrees
N/A	Latitude	Latitude	Degrees
N/A	LCC-X	X-Component to LCC projection origin	m
N/A	LCC-y	Y-Component to LCC projection origin	m
N/A	i	Grid cell column index	N/A
N/A	j	Grid cell row index	N/A

2.5 Offshore Air Quality Measurements

The Galveston Bay offshore air quality measurements provided by TCEQ were collected between April and October 2022 on board of the University of Houston Pontoon boat (UHPB). All measurements were consolidated into a single file. Table 12 describes the fields from the original data files and the corresponding fields in the processed file.

Table 12. Fields included in UHPB offshore measurements.

Original Field Name	Processed Field Name	Processed Field Description	Units
UHPB_Date_Time_CST_1min	Date	Date in Central Standard Time	MM/DD/YYYY
UHPB_Date_Time_CST_1min	Time	Local time in Central Standard Time	HH:MM:SS
UHPB_AirTemp_degC_1min_avg	Temperature	Air temperature	Degrees Celsius
UHPB_Dewpoint_degC_1min_avg	Dewpoint	Dewpoint	Degrees Celsius
UHPB_RH_percent_1min_avg	RH	Relative Humidity	%
UHPB_NOx_ppbv_1min_avg	NO_X	NO_X concentration	ppbv
UHPB_NO_ppbv_1min_avg	NO	NO concentration	ppbv
UHPB_NO2_ppbv_1min_avg	NO_2	NO_2 concentration	ppbv
UHPB_O3_ppbv_1min_avg	O_3	Ozone concentration	ppbv
UHPB_CL51_BL_HEIGHT_1_1min_avg	Boundary Layer Height 1	Boundary layer height	m
UHPB_CL51_BL_HEIGHT_2_1min_avg	Boundary Layer Height 2	Boundary layer height	m
UHPB_CL51_BL_HEIGHT_3_1min_avg	Boundary Layer Height 3	Boundary layer height	m
UHPB_CL51_CLOUD_1_1min_avg	Cloud Base Height 1	Cloud base height	m
UHPB_CL51_CLOUD_2_1min_avg	Cloud Base Height 2	Cloud base height	m

Original Field Name	Processed Field Name	Processed Field Description	Units
UHPB_CL51_CLOUD_3_1min_avg	Cloud Base Height 3	Cloud base height	m
UHPB_CL51_MEAN_LAYER_HEIGHT_1min_avg	Mean Boundary Layer Height	Mean boundary layer height	m
UHPB_LON_DDeg_1min_avg	Longitude	Longitude	Degrees
UHPB_LAT_DDeg_1min_avg	Latitude	Latitude	Degrees
UHPB_Pressure_Millibar_1min_avg	Pressure	Ambient pressure	mbar
UHPB_WD_deg_1min_avg	WD	Wind direction	Degrees
UHPB_WS_knots_1min_avg	WS	Wind speed	m/s
N/A	U	Wind speed x-component	m/s
N/A	V	Wind speed y-component	m/s
N/A	LCC-X	X-Component to LCC projection origin	m
N/A	LCC-y	Y-Component to LCC projection origin	m
N/A	i	Grid cell column index	N/A
N/A	j	Grid cell row index	N/A

2.6 Commercial Vessel Offshore Air Quality Measurements

The Red Eagle and the RMS Victory commercial marine vessels were equipped to measure ozone, oxidants and meteorological parameters between April and October 2022. Two data files were provided, one for each vessel, that are similar in content, but the data for the Red Eagle vessel included additional ceilometer measurements. Table 13 and Table 14 describe the fields from the original data files and the corresponding fields in the processed file. The resin tube data were merged with the Red Eagle data based on time stamps.

Table 13. Fields included in the Red Eagle CMV and VOC (Resin Tubes) offshore measurements.

Original Field Name	Processed Field Name	Processed Field Description	Units
RE_Date_Time_CST_1min	Date	Date in Central Standard Time	MM/DD/YYYY
RE_Date_Time_CST_1min	Time	Local time in Central Standard Time	HH:MM:SS
RE_AirT_degC_1min_avg	Temperature	Air temperature	Degrees Celsius
RE_Dewpoint_degC_1min_avg	Dewpoint	Dewpoint	Degrees Celsius
RE_RH_percent_1min_avg	RH	Relative Humidity	%

Original Field Name	Processed Field Name	Processed Field Description	Units
RE_O3_ppbv_1min_avg	O_3	O3 concentration	ppbv
RE_Ox_ppbv_1min_avg	O_X	Ox concentration	ppbv
RE_NO2_ppbv_1min_avg	NO_2	NO_2 concentration	ppbv
Isoprene	Isoprene	Concentration of Isoprene	ppbC
Benzene	Benzene	Concentration of Benzene	ppbC
Toluene	Toluene	Concentration of Toluene	ppbC
Ethylbenzene	Ethylbenzene	Concentration of Ethylbenzene	ppbC
m&p-Xylene	m&p-Xylene	Concentration of m&p-Xylene	ppbC
o-Xylene	o-Xylene	Concentration of O-Xylene	ppbC
Styrene	Styrene	Concentration of Styrene	ppbC
a-Pinene	a-Pinene	Concentration of a-Pinene	ppbC
RE_LAT_DDeg_1min_avg	Longitude	Longitude	Degrees
RE_LON_DDeg_1min_avg	Latitude	Latitude	Degrees
RE_Pres_Millibar_1min_avg	Pressure	Ambient pressure	mbar
RE_WD_knots_1min_avg	WD	Wind direction	Degrees
RE_WS_deg_1min_avg	WS	Wind speed	m/s
N/A	U	Wind speed x-component	m/s
N/A	V	Wind speed y-component	m/s
N/A	LCC-X	X-Component to LCC projection origin	m
N/A	LCC-y	Y-Component to LCC projection origin	m
N/A	i	Grid cell column index	N/A
N/A	j	Grid cell row index	N/A

Table 14. Fields included in the Victory CMV offshore measurements.

Original Field Name	Processed Field Name	Processed Field Description	Units
Victory_Date_Time_CST_1min	Date	Date in Central Standard Time	MM/DD/YYYY
Victory_Date_Time_CST_1min	Time	Local time in Central Standard Time	HH:MM:SS
Victory_AirT_degC_1min_avg	Temperature	Air temperature	Degrees Celsius
Victory_Dewpoint_degC_1min_avg	Dewpoint	Dewpoint	Degrees Celsius
Victory_RH_percent_1min_avg	RH	Relative Humidity	%
Victory_O3_ppbv_1min_avg	O_3	O_3 concentration	ppbv
Victory_Ox_ppbv_1min_avg	O_X	O_X concentration	ppbv
Victory_NO2_ppbv_1min_avg	NO_2	NO_2 concentration	ppbv
Victory_LON_DDeg_1min_avg	Longitude	Longitude	Degrees
Victory_LAT_DDeg_1min_avg	Latitude	Latitude	Degrees
Victory_Pres_Millibar_1min_avg	Pressure	Ambient pressure	mbar
Victory_WD_knots_1min_avg	WD	Wind direction	Degrees
Victory_WS_deg_1min_avg	WS	Wind speed	m/s
N/A	U	Wind speed x-component	m/s
N/A	V	Wind speed y-component	m/s
N/A	LCC-X	X-Component to LCC projection origin	m
N/A	LCC-y	Y-Component to LCC projection origin	m
N/A	i	Grid cell column index	N/A
N/A	j	Grid cell row index	N/A

2.7 Drones Data

Data collected by drones includes ozone concentrations and meteorological data. Ramboll identified 24 files to be processed for this dataset, each file sharing a similar format. Table 15 describes the original fields and the processed field names and descriptions. The original files have two values for the altitude: one from GPS and another that is pressure-derived. Although both are similar, we chose the pressure-derived values because they are more consistent and do not show negative altitude values at the surface like the GPS values. We decided to remove any of the rows with data when the altitude was negative. The above ground level (AGL) altitude was obtained by

subtracting the elevation from the Altitude (AMSL). Ramboll added the dewpoint temperature to the final dataset.

Table 15. Fields included in the Drone dataset.

Original Field Name	Processed Field Name	Processed Field Description	Processed Field Units
N/A	Date	Date in Central Standard Time	MM/DD/YYYY
Time	Time	Time in Central Standard Time	HH:MM:SS
Altitude	Altitude (AMSL)	Altitude above mean sea level	meters
N/A	Elevation	Site/launch point elevation	meters
N/A	Altitude (AGL)	Altitude above ground level	meters
Temperature	Temperature	Temperature	degrees C
N/A	Dewpoint Temperature	Dewpoint Temperature	Degrees C
RH	RH	Relative Humidity	%
Ozone_MR	O_3	Ozone concentration	ppmv
GPSLon	Longitude	Longitude	degrees
GPSLat	Latitude	Latitude	degrees
Pressure	Pressure	Atmospheric pressure	millibar
N/A	LCC-X	X-component to LCC projection origin	m
N/A	LCC-Y	Y-component to LCC projection origin	m
N/A	i	Grid cell column index	N/A
N/A	j	Grid cell row index	N/A

3.0 SUMMARY AND NEXT STEPS

TCEQ is developing an air quality modeling platform for 2022 for attainment demonstration purposes. An important aspect in this development is the evaluation of the model outputs with available measurements. This model performance evaluation typically compares the model estimates with the routine surface-based monitor measurements. During April through October 2022, the University of Houston conducted the Tracking Aerosol Convection Interactions ExpeRiment-Air Quality (TRACER-AQ2) field campaign in Houston that collected air quality measurements from stationary and mobile platforms, including drones, ozonesondes, Pandora profilers, mobile labs, and shipping boats. Thus, significant insights could be gained by comparing results from the TCEQ modeling platform with the TRACER-AQ2 datasets. As part of this project, Ramboll reviewed the different measurement datasets and under TCEQ direction successfully consolidated, augmented and processed them to facilitate model performance evaluation using TCEQ's software. All files were provided to TCEQ in CSV format with a consistent structure and documented in a data manifest with descriptions for each column, along with other relevant metadata.

Ramboll has two recommendations for TCEQ to consider for future projects: 1) Apply the processing methods developed under this project to other air quality measurement datasets; and 2) Assist TCEQ is assessing model performance evaluation using the new dataset.