AQRP Monthly Technical Report

PROJECT TITLE	Source-sector NOx emissions analysis with sub-kilometer scale airborne observations in Houston during TRACER-AQ	**PROJECT #**	22-023
PROJECT PARTICIPANTS	George Washington University Ramboll	**DATE SUBMITTED**	6/12/2023
REPORTING PERIOD	**From:** May 1, 2023 **To:** May 31, 2023	**REPORT #**	10

A Financial Status Report (FSR) and Invoice will be submitted separately from each of the Project Participants reflecting charges for this Reporting Period. I understand that the FSR and Invoice are due to the AQRP by the 15th of the month following the reporting period shown above.

Detailed Accomplishments by Task for reporting period

Task 1: Simulate NO_2, HCHO, O_3 at 444 × 444 m^2 spatial resolution using WRF-CAMx
The final WRF-CAMx simulation was completed in May 2023. There is model output for the two GCAS measurement periods: August 30 – September 11, 2021 and September 23 – September 27, 2021 with additional days of spin-up prior to each episode that will not be utilized. This latest model run includes updated emissions based on CEM hourly data for two additional power plants. Model output for all days in August and September for which there is GCAS data has been provided to the full team. See Figure 1c. QA/QC of the model output is on-going.

Task 2. Process the GCAS measurements
The reprocessing of the GCAS aircraft measurements with very minor adjustments was completed in February 2023, and all new files were made available to the full team, and posted on the TRACER-AQ data archive (https://www-air.larc.nasa.gov/cgi-bin/ArcView/traceraq.2021).

In May, GCAS measurements were re-processed with the initial CAMx model output. The team is exploring the differences now, but the average increase in the AMF is 5% and the average difference in the vertical column density is 2.2×10^{14} molecules cm^{-2}. These files will be updated with the most up-to-date model run in June 2023 and used for the final version of the products delivered in Tasks 4, 5 and 6.

Task 3. Process the satellite NO_2 data
The satellite air mass factor has been processed for all days in September using the CAMx model output, and the resulting data has been provided to the team. This task is now fully completed.

Task 4. Calculating NO_X from NO_2 airshed measurements
NO_X emissions from several point sources (W.A. Parish Power Plant, Texas City, Bayview ExxonMobil, Lyondell Basell Channelview, and Mont Belvieu) were calculated from the new GCAS data. The team was able to generate reasonable NO_X emissions estimates from these point sources.

We are now completing an in-depth comparison between the GCAS data, TROPOMI satellite data, and CAMx model output at the location of the W.A. Parish plant to better understand uncertainties in the three datasets before making any firm conclusions. See Task 5.

Additionally, NO_2 divergence has been calculated for the Houston area. On-going work is determining which assumptions should be made in order to calculate NO_X emission rates. The flux divergence was calculated using the new GCAS retrievals that use the CAMx Air Mass Factors. This led to an improved characterization of ship emissions and reduced noise in the background. We also performed the method on the CAMx fields themselves in order to better constrain the emission estimates and identify calibration factors.

This task will complete in June 2023.

Task 5. Comparison of NO_2, HCHO, O_3 between model, aircraft, and satellite
An in-depth comparison between the aircraft, satellite, model, and Pandora instruments for NO_2 is on-going. Please see the Preliminary Analyses section for more updates.

Task 6. Use of machine learning to estimate emission factors for individual sectors
Task 6 was initiated in May 2023. Preliminary tests have been conducted with the new CAMx simulations. A multi-linear regression model was set up to estimate scaling factors for each of 16 source sectors in order to obtain an optimal match between CAMx simulations and GCAS retrievals. We are currently testing the code and performing sensitivity tests.

Preliminary Analyses

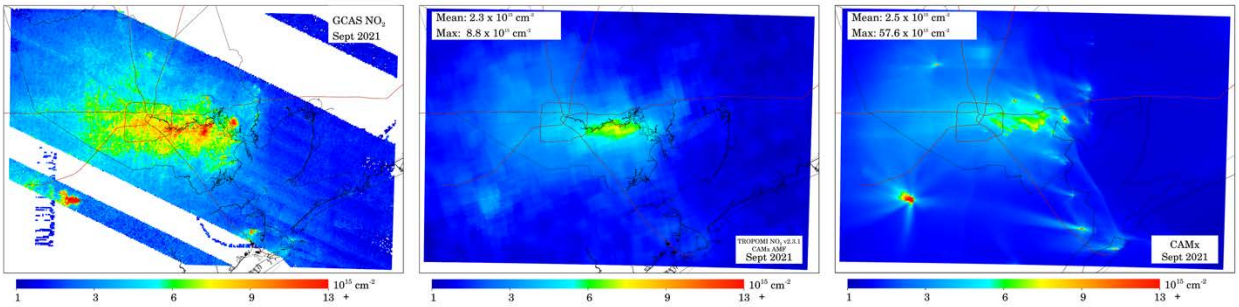

Figure 1. Vertical column NO_2 averaged during the early afternoon for September 2021. Left panel shows the monthly average from the aircraft (GCAS). Center panel shows the monthly average from the satellite (TROPOMI) with an air mass factor re-processed using the CAMx model simulation. Right panel shows the monthly average from the CAMx model simulation. All datasets are on the same grid.

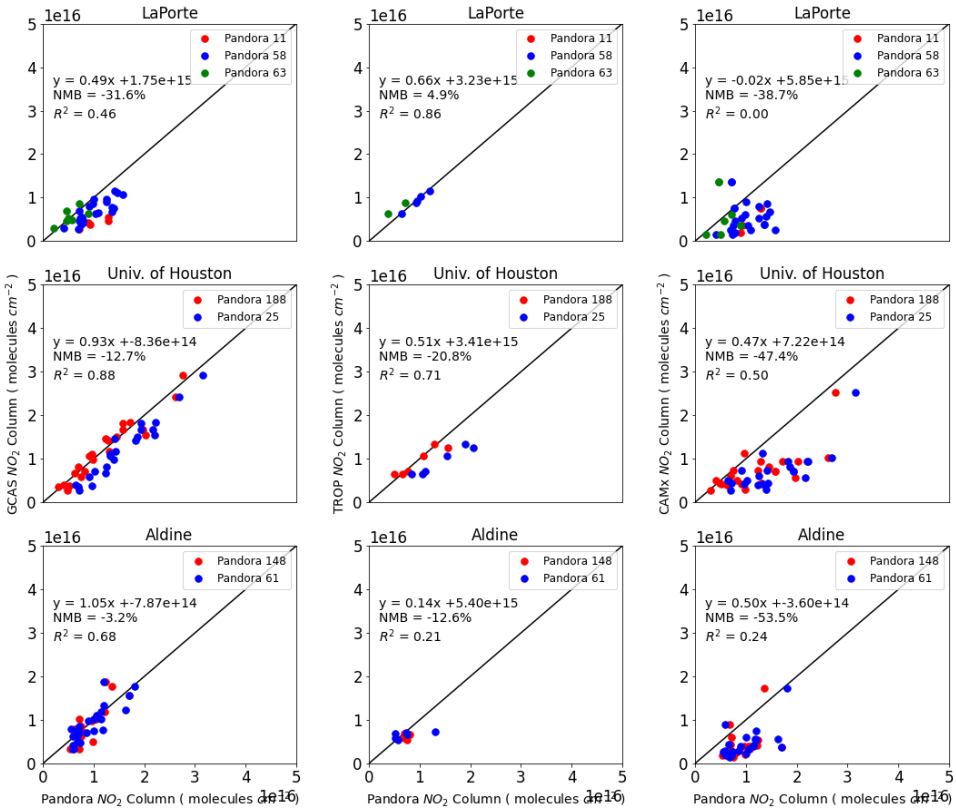

Figure 2. Comparison of the vertical column NO_2 between the Pandora instruments and the (left column) GCAS measurements, (center column) TROPOMI measurements, (right column) model output for all collocations in time and space during September 2021. Each row represents a different Pandora location: (top) LaPorte, (center) University of Houston, (bottom) Aldine.

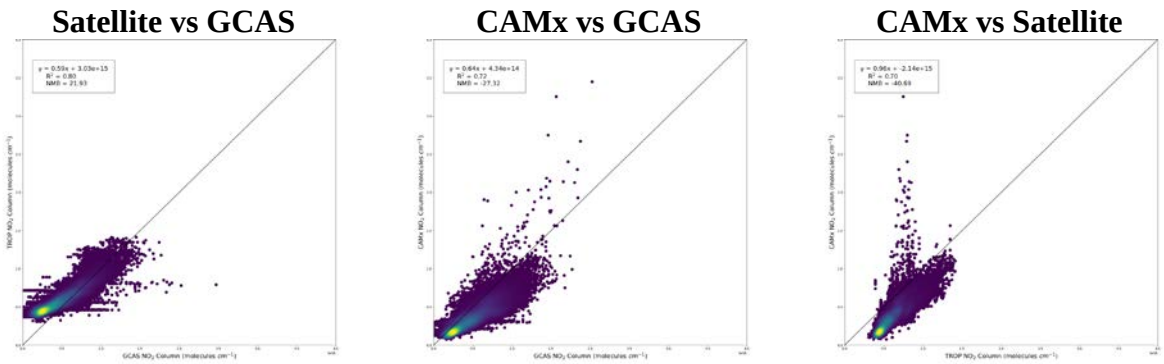

Figure 3. Comparison of the vertical column NO_2 between the (left) satellite and GCAS, (center) CAMx and GCAS, and (right) CAMx and satellite. CAMx appears to have smaller column NO_2 values than both GCAS and the satellite, except in the presence of point source plumes. The satellite has larger column NO_2 values than GCAS in rural areas, and may be

related to missing column NO_2 measurements above the aircraft which was not accounted for in this analysis.

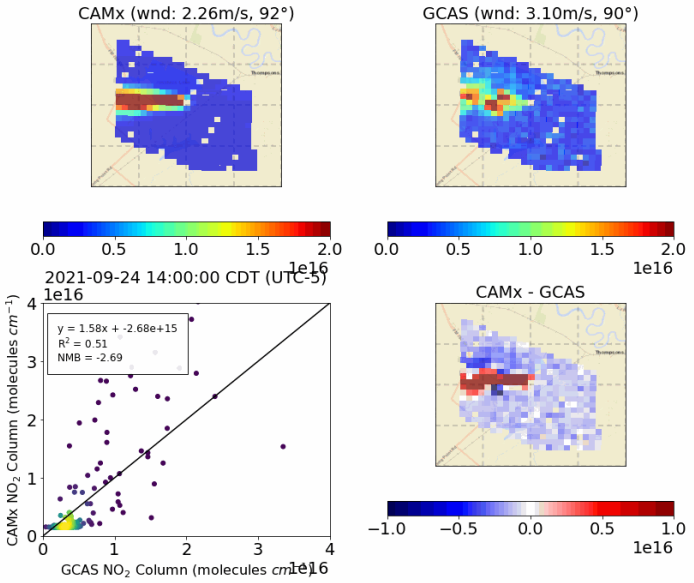

Figure 4. Comparison of the vertical column NO_2 at the location of the W.A. Parish Power Plant on September 24, 2023 between the (top left) model and (top right) GCAS. There is excellent agreement in the location of the wind plume direction. (Bottom left) Scatterplot comparison between the two plots in the top row. (Bottom right) Difference plot between the two plots in the top row.

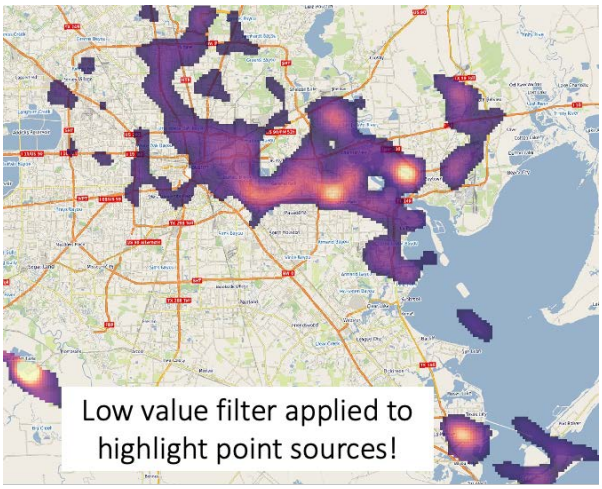

Figure 5. Smoothed NO_2 flux divergence – incremental addition of NO_2 in each grid cell – using all the measurements from the GCAS aircraft. Lighter color are larger values, darker colors are smaller values; ***a low value filer is applied to highlight point sources***. Additional assumptions will need to be made to derive NO_X emission rates.

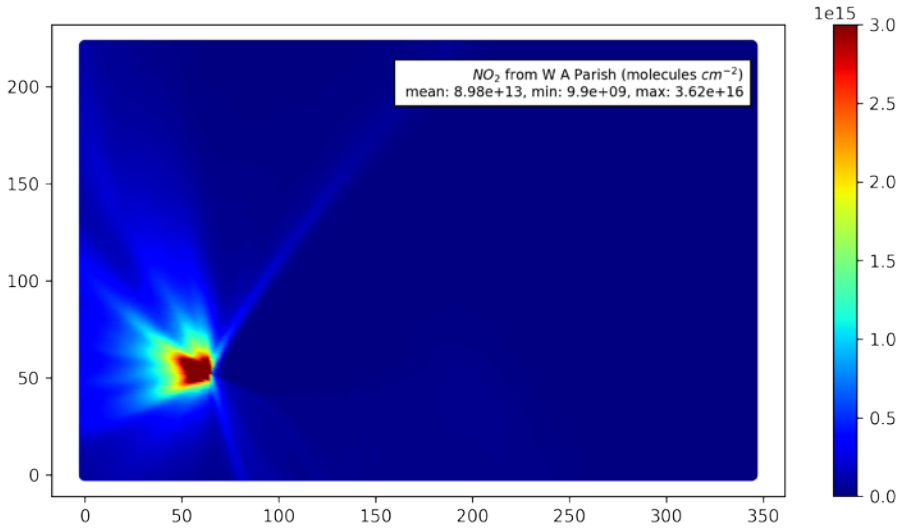

Figure 6. CAMx simulated source apportioned NO_2 columns from W A Parish power plant from between 8am and 5pm on GCAS flight days. Redder colors indicate higher NO_2 columns contributed by emissions from W A Parish in CAMx simulation while bluer colors indicate lower NO_2 columns. The x and y axes correspond to grid cells in the CAMx domain. Mean, minimum and maximum values are indicated in the top right.

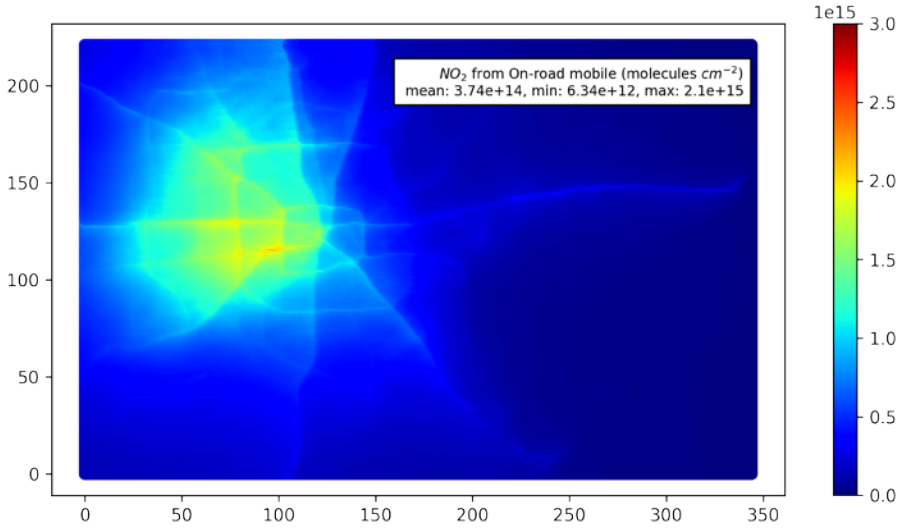

Figure 7. CAMx simulated source apportioned NO_2 columns from on-road vehicle emissions from between 8am and 5pm on GCAS flight days. Redder colors indicate higher NO_2 columns contributed by emissions from on-road vehicles in CAMx simulation while bluer colors indicate lower NO_2 columns. The x and y axes correspond to grid cells in the CAMx domain. Mean, minimum and maximum values are indicated in the top right.

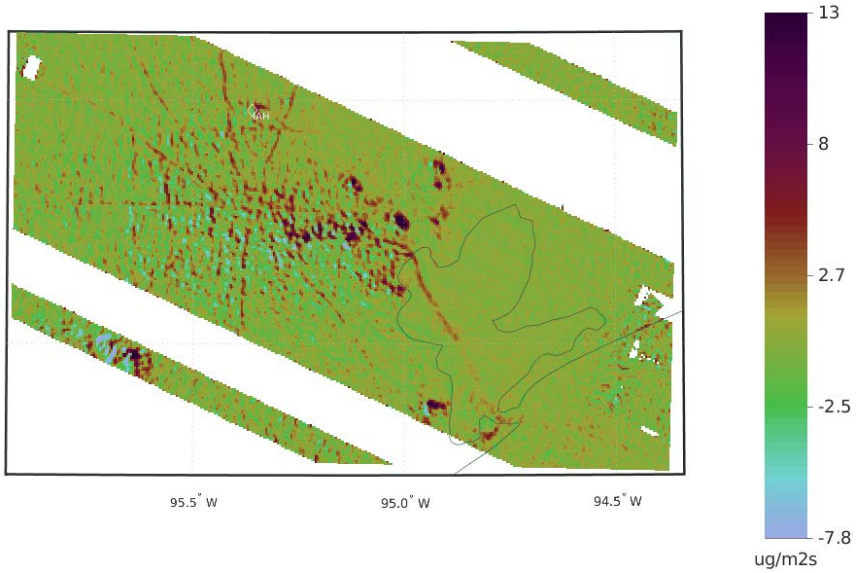

Figure 8. Flux divergence field using GCAS retrievals with CAMx Air Mass Factors. Point sources can be clearly seen, as well as the emissions from ship traffic through the bay and the signature from highways.

Data Collected
None.

Identify Any Problems or Issues Encountered and Proposed Solutions or Adjustments
Project approvals occurred later than anticipated. Development of the WRF-CAMx simulation was delayed by approximately 8-weeks. Model simulation output was delivered to the full team at the end of February 2023 instead of the end of December 2022. Effort for Tasks 3 – 6 will be back-loaded, and we do not anticipate any end-of-project delays.

The TEMPO launch has been delayed to April 2023, and data is not expected to be made available to Early Adopters until September 2023 and therefore will not be available during our project period. The inclusion of TEMPO data was a minor aspect of Task 3 of this project, and therefore exclusion of its data will not affect any end-of-project deliverables.

Goals and Anticipated Issues for the Succeeding Reporting Period
Task 1 – The model output will continue to go through a QA/QC check and a comparison of the model output with the ground monitors will be completed.

Task 2 – Initial analysis completed. We will continue QA/QC and update analysis using the latest CAMx simulation in June.

Task 3 – Completed

Task 4 – NO_X emissions estimates from the point sources and using the flux divergence method will go through additional comparison with the CAMx simulation. This task should be complete in June 2023.

Task 5 – Intercomparison between the aircraft (GCAS), satellite (TROPOMI), and model (WRF-CAMx) will continue. This will constitute the majority of the work during June 2023.

Task 6 – This was initiated in May 2023

Detailed Analysis of the Progress of the Task Order to Date
None.

Do you have any publications related to this project currently under development? If so, please provide a working title, and the journals you plan to submit to.

☐Yes ☒ No

Do you have any publications related to this project currently under review by a journal? If so, what is the working title and the journal name? Have you sent a copy of the article to your AQRP Project Manager and your TCEQ Liaison?

☐ Yes ☒ No

Do you have any bibliographic publications (ie: publications that cite the project) related to this project that have been published? If so, please list the reference information. List all items for the lifetime of the project.

☐ Yes ☒ No

Do you have any presentations related to this project currently under development? If so, please provide working title, and the conference you plan to present it (this does not include presentations for the AQRP Workshop).

☐ **Yes** ☒ **No**

Do you have any presentations related to this project that have been published? If so, please list reference information. List all items for the lifetime of the project.

☐ **Yes** ☒ **No**

Have any personnel changes occurred that were not listed in the original proposal? If so, please include a detailed description of the personnel change(s) below.

☐ **Yes** ☒ **No**

Are any delays expected in the progress of the research? If so, please include a detailed description of the potential delay below.

☐ **Yes** ☒ **No**

Describe any possible concerns/issues (technical or non-technical) that AQRP should be made aware of.

None.

Are you anticipating using all the available funds allocated to this project by the end date? If not, why and approximately what is the amount to be returned?

☒ **Yes** ☐ **No**

Submitted to AQRP by Jeremiah Johnson (co-PI)

Principal Investigator Daniel Goldberg