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**	7/11/2023
REPORTING PERIOD	**From:** June 1, 2023 **To:** June 30, 2023	**REPORT #**	11

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 CAMx simulation "run3" was completed last month. QA/QC of the model output is complete.

Task 2. Process the GCAS measurements
The GCAS aircraft measurements were re-processed with the a priori information from the CAMx "run3" simulation. Using the CAMx information yielded minor changes (~5% increase), but meaningfully important. This task is now complete.

Task 3. Process the satellite NO_2 data
The TROPOMI satellite measurements were re-processed with the a priori information from the CAMx "run3" simulation. The adjustments were minor (~15% increase) compared to the operational measurements, but meaningfully important. This task is now complete.

Task 4. Calculating NO_X from NO_2 airshed measurements
Comparisons between GCAS NO_2 and CAMx NO_2 at the location of the W.A. Parish Power Plant show a small normalized mean bias (-2.7% and +11.2% during the two September 24 overpasses). This agreement is encouraging because the W.A Parish Power Plant's emissions are input into the CAMx simulation using the CEM hourly measurements. This suggests that the GCAS measurements are doing well in capturing the magnitude of point source emissions.

Using GCAS measurements as the "truth", we observe a NO_2 underestimate in the CAMx simulation near the Bayview ExxonMobil facility. Comparisons at other facilities show better agreement.

NO_2 divergence has been calculated for the Houston area. See Preliminary Figures. In order to convert NO_2 divergence to NO_X emission rates, there needs to be an assumed NO_2 lifetime. On-going work is determining the best-estimate for the NO_2 lifetime in order to calculate NO_X emissions.

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. We find that the aircraft NO_2 measurements have the best agreement ($r^2 = 0.81$) with the Pandora NO_2 column measurements with a very small normalized mean bias of +2.4%. Satellite NO_2 measurements have slightly worse agreement ($r^2 = 0.62$) with the Pandora NO_2 column measurements with a small normalized mean bias of –11.4%; the low normalized mean bias may be due to satellite pixel size which is unable to capture the neighborhoods with the worst pollution and/or a small low bias in the version 2.3.1 algorithm related to the coarse surface reflectivities, which have been updated in the algorithm in July 2022.

CAMx NO_2 has the worst agreement ($r^2 = 0.23$) with the Pandora NO_2 column measurements and a normalized mean bias of –21.7%. The relatively low r^2-value could be related to the difficulty of identically simulating plume dispersion, especially dispersion related to the Gulf breeze. Some of the low bias may be related to background NO_2, but since the background NO_2 in the Houston urban environment is a small fraction of the total column (<10% in most cases), we think that this may be related to a NO_X emissions underestimate from certain sectors. Further, the bias between CAMx and Pandora is better on weekends (–7.3%) than weekdays (–27.5%), suggesting that activities more active on weekdays may a cause of this bias.

When doing a direct comparison between NO_2 columns from GCAS and CAMx, CAMx has a normalized mean bias of –27%.

The remaining work will investigate the uncertainties of the GCAS, TROPOMI, and Pandora measurements to characterize their biases.

Please see the Preliminary Analyses section for more updates.

Task 6. Use of machine learning to estimate emission factors for individual sectors
Initial work has been done to correlate the individual NO_X sectors using the CAMx source apportionment. This task will constitute the majority of the work during July 2023.

Preliminary Analyses

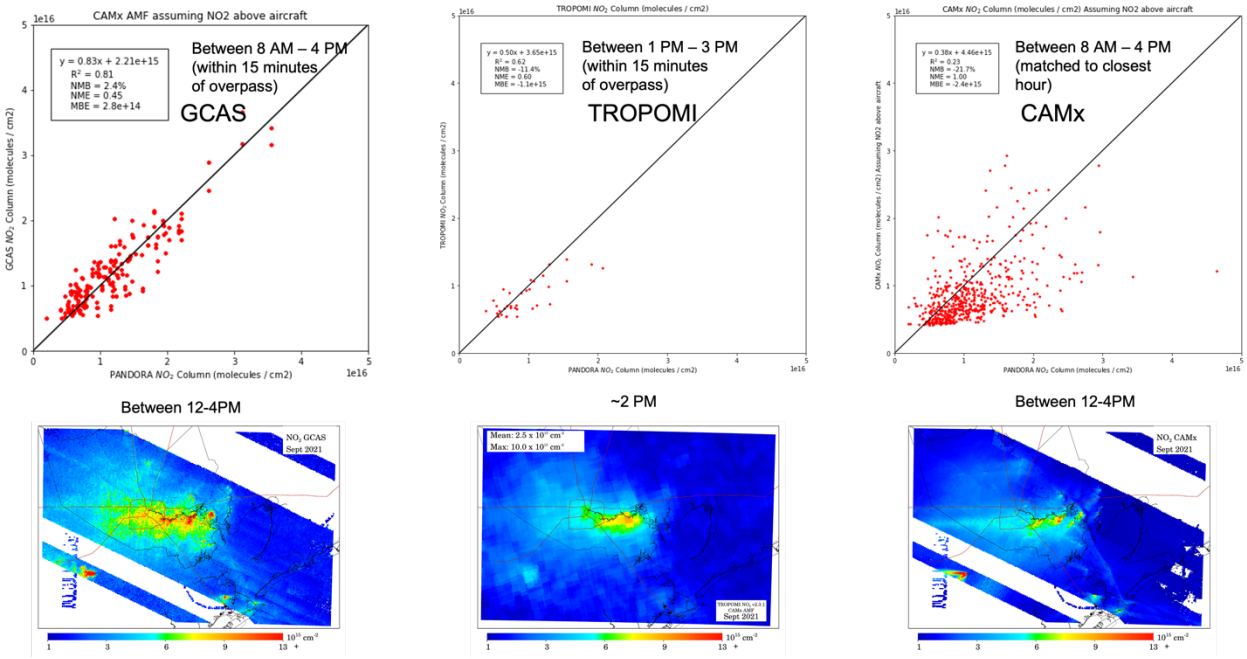

Figure 1. (Top row) Comparisons of total vertical column NO_2 from (left) GCAS, (center) TROPOMI, and (right) CAMx compared to coincident Pandora measurements during September 2021. (Bottom row) Spatial plots of the tropospheric vertical column NO_2 averaged during September 2021.

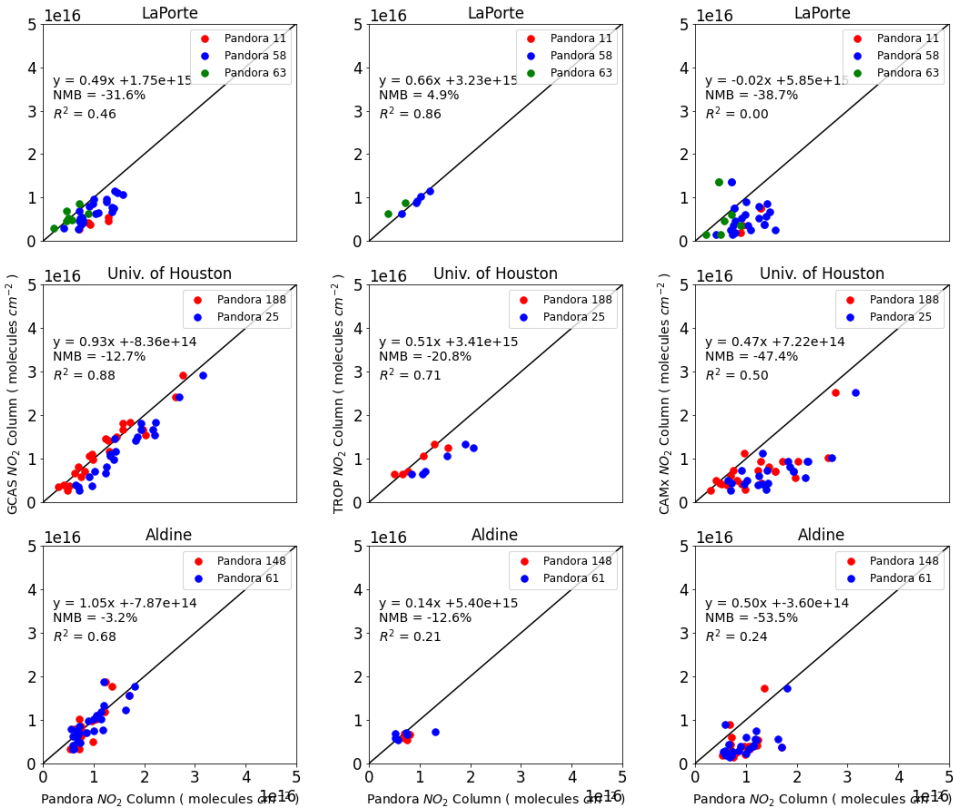

Figure 2. Comparison of the vertical column NO_2 between the Pandora instruments and the (left column) GCAS measurements, (center column) TROPOMI measurements, (right column) model output for all collocations in time and space during September 2021. Each row represents a different Pandora location: (top)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

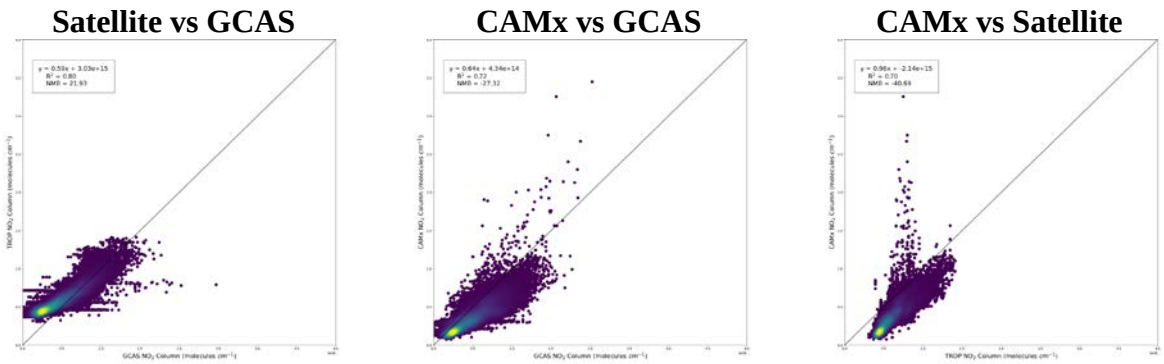

Figure 3. Comparison of the vertical column NO_2 between the (left) satellite and GCAS, (center) CAMx and GCAS, and (right) CAMx and satellite. CAMx appears to have smaller column NO_2 values than both GCAS and the satellite, except in the presence of point source plumes. The satellite has larger column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

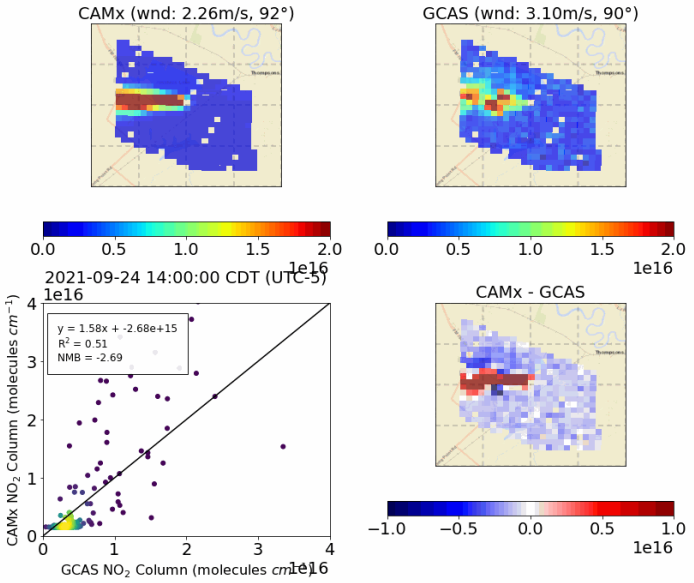

Figure 4. Comparison of the vertical column NO_2 at the location of the W.A. Parish Power Plant on September 24, 2023 between the (top left) model and (top right) GCAS. There is excellent agreement in the location of the wind plume direction. (Bottom left) Scatterplot comparison between the two plots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

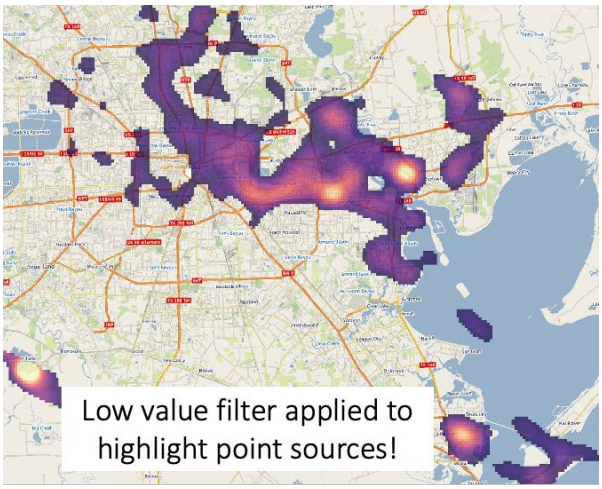

Figure 5. Smoothed NO_2 flux divergence – incremental addition of NO_2 in each grid cell – using all the measurements from the GCAS aircraft. Lighter color are larger values, darker colors are smaller values; ***a low value filer is applied to highlight point sources***. Additional assumptions will need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

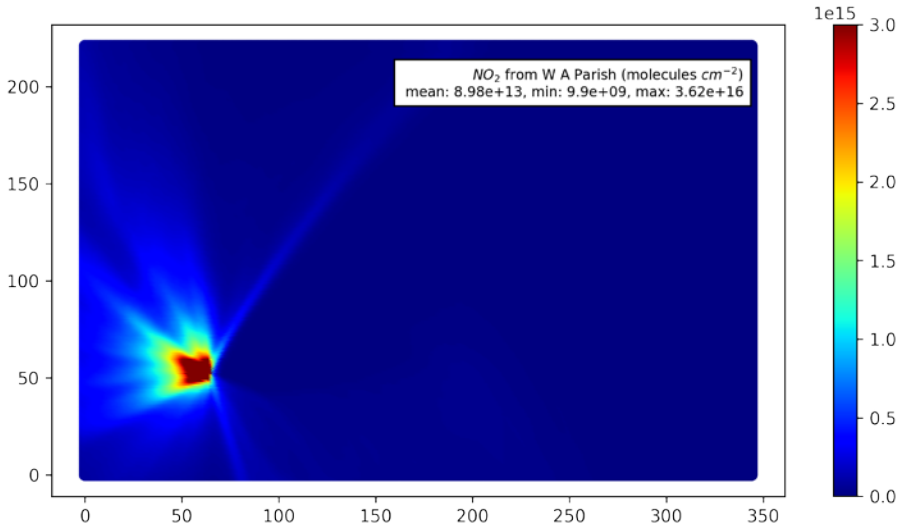

Figure 6. CAMx simulated source apportioned NO_2 columns from W A Parish power plant from between 8am and 5pm on GCAS flight days. Redder colors indicate higher NO_2 columns contributed by emissions from W A Parish in CAMx simulation while bluer colors indicate lower NO_2 columns. The x and y axes correspond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

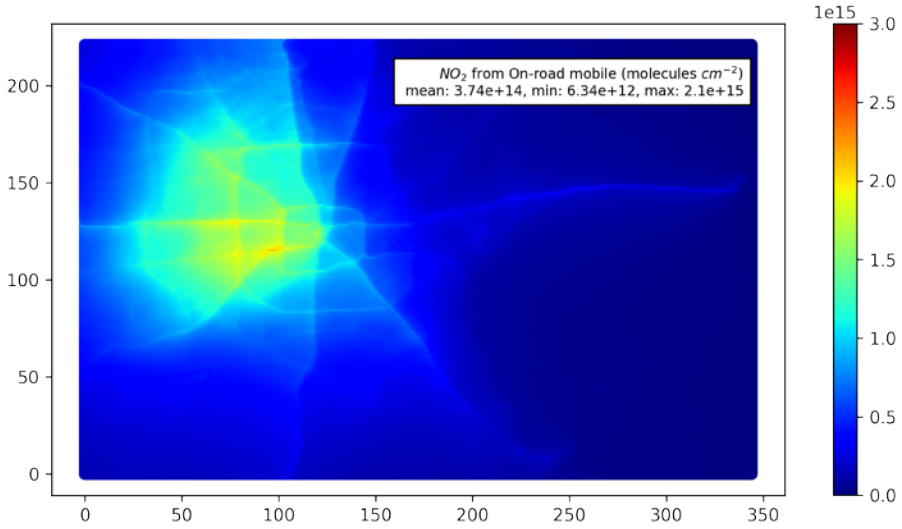

Figure 7. CAMx simulated source apportioned NO_2 columns from on-road vehicle emissions from between 8am and 5pm on GCAS flight days. Redder colors indicate higher NO_2 columns contributed by emissions from on-road vehicles in CAMx simulation while bluer colors indicate lower NO_2 columns. The x and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

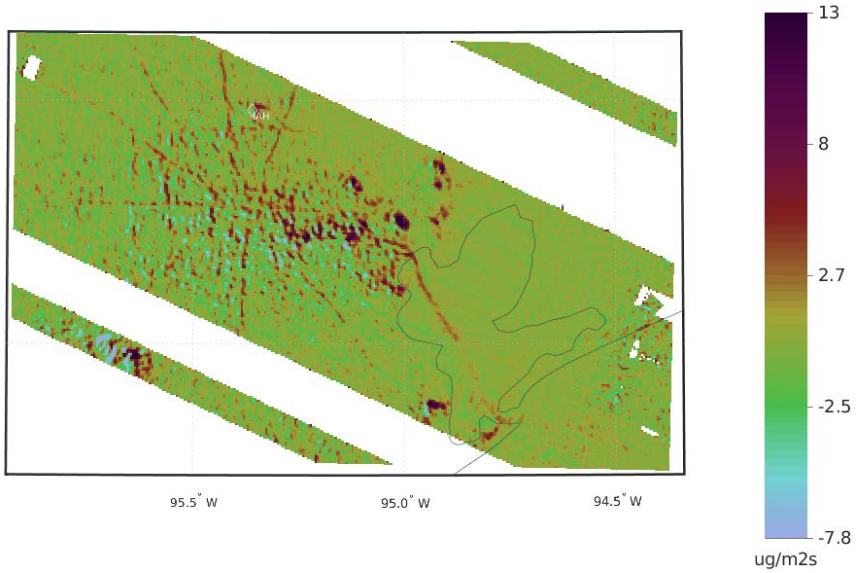

Figure 8. Flux divergence field using GCAS retrievals with CAMx Air Mass Factors. Point sources can be clearly seen, as well as the emissions from ship traffic through the bay and the signature from highways.

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. While we were able to re-run the simulation with a small NO_X emissions change to two power plants, we had hoped to be able to make additional changes to the NO_X emissions, but our team ran out of time. We do not expect the lack of a more substantial change to the NO_X emissions in the simulation to alter project conclusions, but it would have helped solidify some of our findings.

Two new TROPOMI NO_2 algoirthms were released during this project (NASA MINDS version 1.1 in Fall 2022 and ESA version 2.4 in Spring 2023), which could not be incorporated into this project. The new algorithms appear to have a small increase in NO_2 values across the United States, but this has not yet been validated by our team for the Houston metropolitan area. Future work will utilize these newer algorithms. The new TROPOMI algorithms do not affect the GCAS vs. CAMx vs. Pandora intercomparison.

The TEMPO launch was delayed to April 2023, and data is not expected to be made available to Early Adopters until Fall 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 – Completed

Task 2 – Completed

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.

Task 5 – The NO_2 portion of this task is complete. A qualitative comparison will occur for HCHO in July 2023.

Task 6 – Development of the machine learning model will continue using the source apportionment information from the CAMx simulation. Preliminary results will be available end of July 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 Daniel Goldberg

Principal Investigator Daniel Goldberg