Abstract

Project #24-004

Evaluating Updates to CAMx and NOx Emission Inventories using TEMPO Measurements over Texas

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Nitrogen oxide (NOx) emissions are critical to ozone formation in Texas and consequently accurate NOx emission inventories are essential to air quality planning using the Comprehensive Air Quality Model with Extensions (CAMx). Previous work by our team showed that highly resolved (sub 1 km) NO_2 column measurements by the National Aeronautics and Space Administration (NASA) Geostationary Coastal and Air Pollution Events (GEO-CAPE) Airborne Simulator (GCAS) aircraft can constrain the CAMx NOx emission inventory for Houston with source-category specificity. In this project, we will evaluate whether NO_2 column measurements by the new NASA Tropospheric Emissions: Monitoring of Pollution (TEMPO) satellite can constrain CAMx NOx emission inventories as successfully as the GCAS aircraft. At the same time, we will investigate how improving the CAMx NOx chemistry (i.e., particle nitrate photolysis), NO_2 vertical distribution and soil NOx emission inventory influence CAMx agreement with measured NO_2 columns. This project will determine how the new Tropospheric Emissions: Monitoring of Pollution (TEMPO) satellite can be used for NOx emission inventory evaluation. Lessons learned and techniques developed for this project could be applied to other areas in the United States.

Quality Assurance Project Plan (QAPP)

Project 24 – 004
Evaluating Updates to CAMx and NOx Emission Inventories using TEMPO Measurements over Texas

Prepared for
Texas Air Quality Research Program (AQRP)
The University of Texas at Austin

Prepared by

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September 9, 2024
Version #2

Ramboll has prepared this QAPP following the Environmental Protection Agency (EPA) guidelines combining Quality Assurance (QA) Category III: Research Model Development and Applications and Category IV Projects: Secondary Data. It is submitted to the Texas Air Quality Research Program (AQRP) as required in the Work Plan requirements.

QAPP Requirements:

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QA Requirements: Technical Systems Audits - Not Required for the Project
Audits of Data Quality – 10% Required
Report of Findings – Required in Final Report

Approvals Sheet

This document is a Category III Quality Assurance Project Plan for the Evaluating Updates to CAMx and NOx Emission Inventories using TEMPO Measurements over Texas project. The Principal Investigator for the project is Jeremiah Johnson and Co-PIs are Dan Goldberg and Benjamin de Foy.

Electronic Approvals:

This QAPP was approved electronically on 2024-09-22 | 08:05:19 CDT
by Elena McDonald-Buller, The University of Texas at Austin.

Signed by:
Elena McDonald-Buller
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Project Manager, Texas Air Quality Research Program

This QAPP was approved electronically on 2024-09-20 | 12:59:32 PDT
by Vincent M. Torres, The University of Texas at Austin.

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Quality Assurance Project Plan Manager, Texas Air Quality Research Program

This QAPP was approved electronically on 2024-09-20 | 07:56:13 CDT
By Robert Keirstead, Texas Commission on Environmental Quality.

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TCEQ Liaison, Texas Commission on Environmental Quality

This QAPP was approved electronically on 2024-09-20 | 09:39:39 CDT
By Jeremiah Johnson, Ramboll

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QAPP Distribution List

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1.0 Project Description and Objectives

This project will determine how Tropospheric Emissions Monitoring of Pollution (TEMPO) can be used for NOx emissions evaluation. We will use TEMPO NO_2 measurements to evaluate CAMx model updates to NOx chemistry, vertical distribution of NO_2 and the NOx emission inventory. Lessons learned and techniques developed for this project could be applied to other areas in the United States. The project will also demonstrate the capability to estimate NOx emissions using the flux divergence method and multilinear regression model applied to TEMPO NO_2 measurements.

In this project we will use hourly TEMPO NO_2 information (2×4.5 km^2). Complementing the satellite observations, we will run CAMx with 4×4 km^2 spatial resolution and NO_2 sector-based source apportionment over Texas using the 2019 TCEQ emissions inventory. First, we will develop aircraft emissions and enhanced soil NOx emissions and perform an initial CAMx simulation. After developing diurnal NOx emissions estimates from TEMPO, we will then compare CAMx model output with TEMPO data to generate an initial set of baseline NO_2 column comparisons. Following this initial set of baseline comparisons, we will make modifications to the CAMx modeling configuration that include CAMx updates to aerosol nitrate photolysis and vertical distribution of NO_2. We will estimate NOx emissions using the flux divergence method to determine whether TEMPO can help constrain the TCEQ NOx emission inventory over Texas cities. Finally, we will use TEMPO NO_2 measurements and tagged NO_2 columns in a multi-linear regression model to estimate scaling factors for NOx emissions categories.

2.0 Organization and Responsibilities

2.1 Responsibilities of Project Participants

Mr. Jeremiah Johnson will lead the project as PI and coordinate collaboration with Dr. Daniel Goldberg (co-PI), Dr. Daniel Huber and Dr. Benjamin de Foy (co-PI) who will be consultants to Ramboll.

Mr. Jeremiah Johnson will oversee the emissions processing, CAMx model development, WRF and CAMx simulations and lead quality assurance review for all modeling activities. Dr. Daniel Goldberg will process the TEMPO satellite data, create diurnal NO_2 profiles, compare the TEMPO NO_2 columns with CAMx NO_2 columns and perform quality assurance review for all satellite data processing and analysis. Dr. Benjamin de Foy will calculate diurnal NOx emissions by sector from TEMPO satellite measurements applying flux divergence and advanced statistical methods and will perform quality assurance review. Dr. Daniel Huber will modify the default soil NOx parameterization within the MEGAN biogenic emissions model to include an updated soil moisture function and perform quality assurance review for the code updates.

2.2 Project Schedule

The planned duration of the project is 14 months (August 2024 – September 2025). Figure 5 presents the proposed schedule for each task and project deliverable.

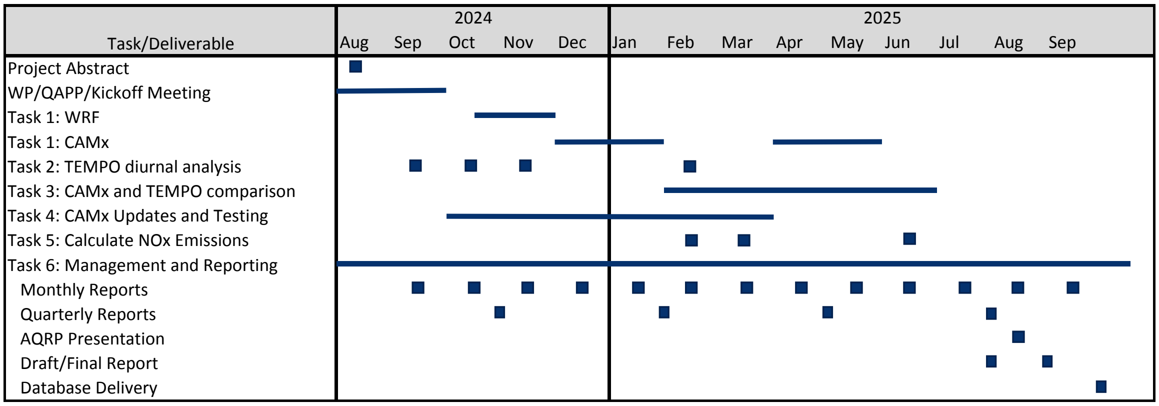

Figure 5. Proposed project schedule.

3.0 Scientific Approach

3.1 Satellite-based observations

Satellites measure the column abundance of NO_2, known as the vertical column density (VCD). All analysis will utilize data from the Tropospheric Emissions: Monitoring of POllution (TEMPO) instrument and the Tropospheric Monitoring Instrument (TROPOMI). TEMPO was launched in April 2023 and has been acquiring measurements over North America since August 2, 2023 at a spatial resolution of 4.5 km x 2 km at its center of field of regard. TEMPO is a geostationary instrument and typically acquires measurements once per hour during daylight hours. However, the instrument has the capability to enter a "rapid scan" mode, acquiring more than one observation per hour at the same spatial resolution. TROPOMI is a polar-orbiting instrument with once per day coverage in the extratropics at 13:30 local time with a nadir resolution of 5.5 km × 3.5 km. TROPOMI was launched in October 2017 and has been acquiring measurements since April 30, 2018. While TEMPO has better temporal and spatial coverage over North America than TROPOMI, the TEMPO NO_2 algorithm is nascent compared to the more mature TROPOMI NO_2 algorithm which has been more thoroughly evaluated.

We will screen the TEMPO NO_2 data for clouds and erroneous data using a cloud fraction filter of <0.15 and a non-zero "qa_flag" which screens out erroneous measurements, as recommended by the TEMPO Users' Guide[1]. We will screen the TROPOMI data for clouds and erroneous data using the recommended qa_flag > 0.75 filter. All TEMPO and TROPOMI NO_2 data are publicly available on NASA Earthdata (https://search.earthdata.nasa.gov/). Care must be taken in the interpretation of satellite column retrievals as an indicator of near-surface emissions (Streets et al., 2013).

We will grid the TEMPO and TROPOMI data for comparison with CAMx output. This will be performed with publicly available IDL code (Goldberg et al., 2021) and allows users to reformat data on to any grid type, including that of a model simulation. TEMPO and TROPOMI data will be gridded for the data analysis period: August - October 2023 with a focus on September 2023.

3.2 CAMx simulations

Model simulations will be conducted by Ramboll, by adapting TCEQ's 2019 State Implementation Plan (SIP) WRF and CAMx modeling platforms for the August 25 – September 30, 2023 modeling period. The WRF and CAMx modeling domains at 36, 12, and 4 km are the same as those used in the AQRP 22-023 project. The 36 km, 12 km and 4 km domains are the TCEQ SIP domains, which are used for other modeling efforts by the TCEQ and Ramboll. Chemical analysis is performed by CAMx v7.30 with input meteorology calculated by WRF version 4.6 with Global Forecast System (GFS) 0.25° × 0.25° analysis data for initial/boundary conditions.

We will use anthropogenic emissions from the 2019 TCEQ modeling inventory (closest to 2023 available) and August – September 2023 hourly CEMS data for power plants. Anthropogenic emissions will be from the 2019 TCEQ modeling inventory (closest to 2023 available) with addition of aircraft climb-out (above 1 km) and cruise emissions based on the Emissions Database for Global Atmospheric Research (EDGAR) 0.1° global database (Crippa et al., 2023). Lightning NOx (LNOx) emissions will be developed using Ramboll's LNOx processor. Biogenic emissions will be developed using our WRF simulation and the Model of Emissions of Gases and Aerosols from Nature (MEGAN) version 3.2 developed by Ramboll in AQRP project 18-005 (Guenther et al., 2012). We will update the soil NOx (SNOx) parameterization within MEGAN v3.2 from the standard BDSNP algorithm to use the soil moisture function of Huber et al. (2023).

The modeling team will create grids of source-apportioned NO_2 concentrations between the surface and the top of the troposphere. We will then calculate the vertical column between the surface and ~13 km to match the TEMPO and TROPOMI satellite observations.

[1] https://asdc.larc.nasa.gov/documents/tempo/guide/TEMPO_Level-2-3_trace_gas_clouds_user_guide_V1.0.pdf

3.3 Flux divergence NO_X emissions quantification method

NO_X emission rates can be inferred from NO_2 using a combination of spatially continuous NO_2 airshed measurements, wind data, and statistical inversion techniques. By tracking the NO_2 plume decay since origination, the NO_X emissions at the source can be back-calculated. For this project, we will estimate NOx emissions using the flux divergence method (Beirle et al., 2019):

$$NO_x\ Emissions = 1.32\big(\nabla \cdot (VCD \cdot \mathrm{u})\big) \quad (1)$$

Fluxes of NO_2 are obtained by multiplying NO_2 vertical column densities (VCDs) with wind speeds (u) in orthogonal directions. The divergence of the fluxes yields an emission estimate in units of mol m^{-2} s^{-1}. The fluxes can then be integrated across the 2-D urban area to get emission rates. Estimates of NOx emissions are obtained by multiplying the estimates by the ratio of NOx to NO_2, which is the same 1.32 value as the Exponentially Modified Gaussian (EMG) method (Beirle et al., 2021). We will use the same 100 m ERA5 wind product as used in the literature (Beirle et al., 2021).

3.4 Multi-Linear Regression analysis

We will build a Multiple Linear Regression Model (MLR) to find the optimal combination of the sectoral emissions simulated by CAMx that match the TEMPO retrievals, following the method described in Goldberg et al. (2023).

The MLR model applies a scaling factor to each source sector that is simulated independently in the CAMx source apportionment runs in order to obtain an optimum match between the TEMPO retrievals and the total CAMx NO_2 vertical column densities. The model will produce adjustment factors for NO_X emissions from each sector, which will be used to develop an optimized emission inventory. A second set of CAMx simulations will be conducted to test the level of improvement obtained by the procedure. The MLR method was developed and validated over Houston using the GCAS measurements (Goldberg et al., 2023; 2024).

4.0 Quality Metrics

TEMPO and TROPOMI measurements will be gridded to the CAMx 4.0 x 4.0 km^2 domain retaining original quality flags, along with information about the averaging kernel, solar zenith angle, and cloud cover. Satellite data will be screened for quality assurance flags in accordance with best practices recommended by the satellite product team, as discussed in Section 3.1.

We will calculate NO_2 vertical columns from CAMx in a manner appropriate for comparison with TEMPO and TROPOMI satellite data (between surface and ~13 km).

5.0 Data Analysis, Interpretation and Management

5.1 Data Reporting

Data reporting procedures will be documented in the project final report as discussed under Section 10. Data reduction procedures for satellite-based measurements are described in Section 3.1.

5.2 Data Validation

Data validation procedures are discussed under Sections 7.3 and 8.3.

5.3 Data Analysis Procedures

Qualitative and quantitative analysis will be performed to identify the role of emissions in contributing to column abundance of NO_2 and as observed from satellites. This procedure includes: a) comparing TEMPO and TROPOMI data with ground measurements (Pandora instruments); b) comparing TEMPO and TROPOMI data with CAMx model output; c) comparing remote sensing derived NOx emissions with known power plant emissions; d) using all sources of data to explain and evaluate agreement and disagreement among these data sources.

5.4 Data Storage

All modeling and measurement data associated with this project will be stored on a local computer and backed up to an external hard drive and transferred to AQRP following the completion of the project.

6.0 Discussion of WRF and CAMx

6.1 Selection

WRF and CAMx are state-of-the-science modeling systems, under regular review and development, used in both regulatory and research applications. We select to use the WRF CAMx models for the availability of the 2019 TCEQ SIP modeling platform and database available for our area of interest. Our project team has employed WRF and CAMx successfully for comparison with TROPOMI as part of AQRP project 22-023 (Goldberg et al. 2023; 2024; Nawaz et al., 2024) and AQRP project 20-020 (Goldberg et al., 2022; Holloway et al., 2021).

6.2 Calibration

We will calibrate the WRF and CAMx models by comparing CAMx output concentrations to available NO_2 and ozone air quality measurements using ground-based TCEQ Continuous Ambient Monitoring Stations (CAMS) across Texas and assessing whether agreement falls within accepted ranges (e.g., Emery et al., 2017). As part of this project, we will make updates to the CAMx model intended to improve agreement with TEMPO and TROPOMI satellite measurements, but we will also evaluate the impacts of these updates to surface measurements using statistical measures including normalized mean bias and error (NMB and NME), root mean squared error (RMSE) and correlation coefficient (r). WRF meteorological outputs will be evaluated against available surface weather stations using Ramboll's METSTAT software if resources permit.

6.3 Verification

Model verification will be performed by processing NO_2 and ozone concentrations and using visualization software to ensure that the results are in a reasonable range. The review of concentration output fields will be performed independently by Ramboll staff who did not conduct the CAMx modeling. A minimum of 10% of the data generated in this study will be audited for data quality through visualization of outputs of the CAMx photochemical modeling.

6.4 Evaluation

Evaluation of WRF and CAMx modeling for AQRP project 20-023 is described by Goldberg et al., (2023) and Nawaz et al. (2024). Ambient NO_2 and O_3 concentrations simulated by CAMx will be compared to ground-based observations of NO_2 and O_3 at TCEQ CAMS across Texas during the modeling time period. We will evaluate the chemistry updates by examining NO_2 columns oxidant concentrations in continental and marine environments (especially over the Gulf of Mexico). We will evaluate the vertical mixing updates by examining surface NO_2 concentrations, NO_2 vertical profiles and NO_2 columns for urban and rural areas of Texas.

6.5 Documentation

The CAMx User's Guide is available online (http://camx-wp.azurewebsites.net/Files/CAMxUsersGuide_v7.30.pdf). Namelist files used to run CAMx will be included in appropriate technical and final reporting. Documentation for WRF is provided in Skamarock (2021) and in the user's guide (https://www2.mmm.ucar.edu/wrf/users/wrf_users_guide/build/html/index.html).

7.0 Discussion of Flux Divergence

7.1 Selection

The flux divergence technique used in AQRP Project 22-023 and documented in Goldberg et al. (2023; 2024) was selected for its ability to produce emission estimates directly from TROPOMI data without information from a model simulation.

7.2 Calibration

Calculation of parameters in the flux divergence approach (Goldberg et al., 2019a; 2019b; 2019c) are based on wind speed and direction, which will be taken from the Ramboll WRF simulation at 4 km. We will compare the meteorology from WRF to widely available re-analysis data (such as the ECMWF ERA-5) for the purpose of anticipating how using re-analysis data (rather than WRF simulations) may influence the flux divergence analysis. In AQRP Project 22-023, we found reduced noise when using CAMx air mass factors in addition to WRF meteorology (Goldberg et al., 2023; 2024).

7.3 Validation

Emissions estimates from the flux divergence technique will be compared to emissions from the WA Parish Generating Station, which is large and a relatively isolated point source that has well-constrained emissions measured by CEMS.

7.4 Documentation

The flux divergence method is described in Beirle et al. (2019; 2023).

8.0 Discussion of MLR

8.1 Selection

The MLR model can identify the contributions of individual emission source sectors to the total NO_2 VCDs. The MLR method is an inverse method that identifies scalar adjustment factors for each source sector to improve the overall match of the CAMx simulations. This method was developed for Houston using GCAS measurements and CAMx simulations (Goldberg et al., 2023; 2024).

8.2 Calibration

Calibration entails comparing the MLR source adjustment factors to improvements in air quality measurements and assessing whether agreement falls within accepted ranges, and determining whether action must be taken to recalibrate the model. If the model falls outside an accepted range, the method will identify sectors that could be simulated separately in future analysis to improve model performance.

8.3 Validation

To test the quality of the method, we will apply the MLR to evaluate scaling factors on modeled sectors compared with total modeled columns (rather than compared with TEMPO columns). Since the model results are the combination of all sectors without scaling factors, the MLR method should return adjustment factors close to 1. Any departure will indicate the presence of uncertainty in the method.
To evaluate the uncertainty in the method we will use a double bootstrap procedure. The retrieval times used in the analysis will be selected at random (with replacement). Within each scene, the pixels selected will also be selected at random (with replacement). This procedure is carried out 100 times for each level of bootstrapping, leading to 10,000 simulations. The resulting scaling factors will therefore include both mean values and standard deviation of the uncertainty.

8.4 Documentation

The method is described in detail in Goldberg et al. (2023; 2024).

9.0 Audits of Data Quality

Per requirements for Category III projects, we will audit a minimum 10% of the input data used in all aspects of the project.

A member of the research team not involved with the creation of a dataset will review 10% or more of the dataset for quality assurance purposes. A report of the findings from these Audits of Data Quality will be included in the draft and final report. This independent review will entail data visualization and discussion of qualitative and quantitative metrics.

10.0 Reporting

As required, we will provide regular and timely submission of monthly technical reports, monthly financial status reports, and quarterly reports as well as an abstract at project initiation and, near the end of the project, submission of the draft final and final reports, according to the schedules given below.

Mr. Johnson, or his designee, will electronically submit each required report to both the AQRP and TCEQ liaisons and will follow the State of Texas accessibility requirements as set forth by the Texas State Department of Information Resources per https://aqrp.ceer.utexas.edu/. All drafts of planned presentations (such as at technical conferences), or manuscripts to be submitted for publication resulting from this project, will be provided to both the AQRP and TCEQ liaisons per the Publication/Publicity Guidelines included in Attachment G of the subaward.

Mr. Johnson will lead reporting activities with assistance from co-PIs and his team at Ramboll. Project data to be submitted to the AQRP archive will include all gridded NO_2 data from TEMPO, TROPOMI and CAMx over the study domain and period.

Abstract: At the beginning of the project, an Abstract will be submitted to the Project Manager for use on the AQRP website. The Abstract will provide a brief description of the planned project activities, and will be written for a non-technical audience.

Abstract Due Date: Friday, August 23, 2024

Quarterly Reports: The Quarterly Report will provide a summary of the project status for each reporting period. It will be submitted to the Project Manager as a Word document file. It will not exceed 3 pages and will be text only. No cover page is required. This document will be inserted into an AQRP compiled report to the TCEQ.

Quarterly Report Due Dates:

Report	Period Covered	Due Date
Quarterly Report #1	August, September, October 2024	Thursday, October 31, 2024
Quarterly Report #2	November, December 2024, January 2025	Friday, January 31, 2025
Quarterly Report #3	February, March, April 2025	Wednesday, April 30, 2025
Quarterly Report #4	May, June, July 2025	Thursday, July 31, 2025

Monthly Technical Reports (MTRs): Technical Reports will be submitted monthly to the Project Manager and TCEQ Liaison in Microsoft Word format using the AQRP FY24-25 MTR Template found on the AQRP website.

MTR Due Dates:

Report	Period Covered	Due Date
Technical Report #1	Project Start – August 31, 2024	Tuesday, September 10, 2024
Technical Report #2	September 1 – 30, 2024	Thursday, October 10, 2024
Technical Report #3	October 1 - 31, 2024	Sunday, November 10, 2024
Technical Report #4	November 1 - 30, 2024	Tuesday, December 10, 2024
Technical Report #5	December 1 - 31, 2024	Friday, January 10, 2025
Technical Report #6	January 1 - 31, 2025	Monday, February 10, 2025
Technical Report #7	February 1 - 28, 2025	Monday, March 10, 2025
Technical Report #8	March 1 - 31, 2025	Thursday, April 10, 2025
Technical Report #9	April 1 - 30, 2025	Saturday, May 10, 2025
Technical Report #10	May 1 - 31, 2025	Tuesday, June 10, 2025
Technical Report #11	June 1 - 30, 2025	Thursday, July 10, 2025
Technical Report #12	July 1 - 31, 2025	Sunday, August 10, 2025

DUE TO PROJECT MANAGER

Financial Status Reports (FSRs): Financial Status Reports will be submitted monthly to the AQRP Grant Manager (RoseAnna Goewey) by each institution on the project using the AQRP 22-23 FSR Template found on the AQRP website.

FSR Due Dates:

Report	Period Covered	Due Date
FSR #1	Project Start – August 31, 2024	Sunday, September 15, 2024
FSR #2	September 1 - 30 2024	Tuesday, October 15, 2024
FSR #3	October 1 - 31, 2024	Friday, November 15, 2024
FSR #4	November 1 - 31, 2024	Sunday, December 15, 2024
FSR #5	December 1 - 31, 2024	Wednesday, January 15, 2025
FSR #6	January 1 - 31, 2025	Saturday, February 15, 2025
FSR #7	February 1 - 28, 2025	Saturday, March 15, 2025
FSR #8	March 1 - 31, 2025	Tuesday, April 15, 2025
FSR #9	April 1 - 30, 2025	Thursday, May 15, 2025
FSR #10	May 1 - 31, 2025	Sunday, June 15, 2025
FSR #11	June 1 - 30, 2025	Tuesday, July 15, 2025
FSR #12	July 1 - 31, 2025	Friday, August 15, 2025
FSR #13	August 1 - 31, 2025	Monday, September 15, 2025
FSR #14	Final FSR	Wednesday, October 15, 2025

DUE TO GRANT MANAGER

Draft Final Report: A Draft Final Report will be submitted to the Project Manager and the TCEQ Liaison. It will include an Executive Summary and a report of the findings from the Audits of Data Quality. It will be written in third person and will follow the State of Texas accessibility requirements as set forth by the Texas State Department of Information Resources.

Draft Final Report Due Date: Friday, August 1, 2025

Final Report: A Final Report incorporating comments from the AQRP and TCEQ review of the Draft Final Report will be submitted to the Project Manager and the TCEQ Liaison. It will be written in third person and will follow the State of Texas accessibility requirements as set forth by the Texas State Department of Information Resources.

Final Report Due Date: Sunday, August 31, 2023

Project Data: All project data including but not limited to QA/QC measurement data, databases, modeling inputs and outputs, etc., will be submitted to the AQRP Project Manager within 30 days of project completion. The data will be submitted in a format that will allow AQRP or TCEQ or other outside parties to utilize the information.

AQRP Workshop: A representative from the project will present at the AQRP Workshop in the first half of August 2025. The selected date will be updated.

11.0 References

Beirle, S., Borger, C., Dörner, S., Eskes, H., Kumar, V., de Laat, A., and Wagner, T. Catalog of NOx emissions from point sources as derived from the divergence of the NO_2 flux for TROPOMI, Earth Syst. Sci. Data, 13, 2995–3012, https://doi.org/10.5194/essd-13-2995-2021, 2021.

Beirle, S., Borger, C., Dörner, S., Li, A., Hu, Z., Liu, F., Wang, Y. and Wagner, T. 2019. Pinpointing nitrogen oxide emissions from space. Science advances, 5(11), p.eaax9800.

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Emery, C.E., Z. Liu, A.G. Russell, M.T. Odman, G. Yarwood and N. Kumar. 2016. Recommendations on statistics and benchmarks to assess photochemical model performance. J. of the Air and Waste Management Assoc., Vol. 67, Issue 5. DOI: 10.1080/10962247.2016.1265027. (https://www.tandfonline.com/doi/full/10.1080/10962247.2016.1265027).

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Goldberg, D. L., Saide, P. E., Lamsal, L. N., de Foy, B., Lu, Z., Woo, J.-H., Kim, Y., Kim, J., Gao, M., Carmichael, G., and Streets, D. G.: A top-down assessment using OMI NO_2 suggests an underestimate in the NOx emissions inventory in Seoul, South Korea, during KORUS-AQ, Atmos. Chem. Phys., 19, 1801–1818, https://doi.org/10.5194/acp-19-1801-2019, 2019c.

Goldberg, D.L., Anenberg, S.C., Lu, Z., Streets, D.G., Lamsal, L.N., E McDuffie, E., Smith, S.J., 2021. Urban NOx emissions around the world declined faster than anticipated between 2005 and 2019. Environ. Res. Lett. 16, 115004. https://doi.org/10.1088/1748-9326/ac2c34

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Scope of Work

Project #24-004
Evaluating Updates to CAMx and NOx Emission Inventories using TEMPO Measurements over Texas

Prepared for

Air Quality Research Program (AQRP)
The University of Texas at Austin

By

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September 9, 2024
Version #2

QA Requirements: Audits of Data Quality: 10% Required
Report of QA Findings: Required in Final Report

NOTE: The Workplan package consists of three independent documents: Scope of Work, Quality Assurance Project Plan (QAPP), and budget and justification. Please deliver each document (as well as all subsequent documents submitted to AQRP) in Microsoft Word format.

Approvals

This Scope of Work was approved electronically on 2024-09-22 | 08:05:19 CDT
by Elena McDonald-Buller, The University of Texas at Austin

Signed by:
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Elena McDonald-Buller
Project Manager, Texas Air Quality Research Program

This Scope of Work was approved electronically on 2024-09-20 | 07:56:13 CDT
by Robert Keirstead, Texas Commission on Environmental Quality

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Robert Keirstead
Project Liaison, Texas Commission on Environmental Quality

Contents

1.0 Abstract

Nitrogen oxide (NOx) emissions are critical to ozone formation in Texas. Our previous Air Quality Research Program (AQRP) project (22-023) showed that highly resolved NO_2 columns (sub 1 km) can constrain the Houston NOx emission inventory with source-category specificity. However, our Comprehensive Air quality Model with extensions (CAMx) air quality model suffered a region-wide low-bias in NO_2 columns similar to biases found by other models that have been attributed to deficits in background tropospheric NO_2. Therefore, we will make several improvements to the NOx emission inventory and the CAMx model that aim to reduce this low bias. We will then test whether NO_2 columns from the new Tropospheric Emissions: Monitoring of Pollution (TEMPO) satellite can similarly constrain the Houston NOx emission inventory with source-category specificity. A challenge will be that TEMPO provides coarser spatial resolution (2 x 4.5 km^2) than available to our previous work which used aircraft column NO_2 measurements at 250 x 560 m^2 spatial resolution, but TEMPO also provides hourly data resolution over more days which may compensate for less spatial resolution. We will also conduct several other analyses to directly investigate TEMPO NO_2 column data. This project is among the first to compare TEMPO NO_2 measurements with air quality model results and evaluate how TEMPO can be used for NOx emissions evaluation. We will again exploit the ability of CAMx to tag NO_2 concentrations (and columns) by source sector.

This project maps to at least three Research Priority Areas of the Texas AQRP, as shown in Table 1 below.

Table 1. How this project will respond to the AQRP Research Priority Areas.

Research Priority Area	How this project addresses the Research Priority
Improve accuracy of photochemical grid models	Evaluate whether adding particle nitrate photolysis (renoxification) and revising vertical mixing in CAMx improves comparisons of modeled NO_2 to satellite NO_2 columns and surface measurements.
Improve emissions inventories	Improve the modeling emission inventories by adding aircraft emissions and updating the soil NOx algorithm in Model of Emissions of Gases and Aerosols from Nature (MEGAN) to adjust to soil moisture more dynamically. Evaluate NOx emission inventories using TEMPO satellite measurements by applying the flux divergence method. Test whether TEMPO data can constrain Houston NOx emissions by source category similarly to AQRP project 22-023.
Use of satellite and other remote sensing data	Utilize TEMPO satellite to better understand diurnal patterns of NO_2 and its relationship to NO_X emissions. Apply TEMPO satellite data as mentioned in the priority areas above. Tropospheric Monitoring Instrument (TROPOMI) data will also be utilized in comparison to TEMPO when there is temporal overlap in the afternoon.

2.0 Background

Previous studies have shown the unique benefit of using spatially continuous satellite data to evaluate NO_X emissions in regional chemical transport model simulations (e.g., Canty et al., 2015; Curier et al., 2014; Harkey et al., 2015; Kemball-Cook et al., 2015; Souri et al., 2016; Travis et al., 2016). These studies compared satellite NO_2 columns to model simulations accounting for the vertical sensitivity of the satellite measurement. Results were mixed, but generally found that satellite NO_2 was larger than the model in rural areas and smaller in urban areas. These studies suggested a potential overestimate of NO_X emissions in U.S. urban areas and demonstrated the importance of stratospheric transport, lightning NO_X emissions, soil NO_X emissions, and NO_2 chemical recycling. Prior work by scientists on this team, sponsored by AQRP (project 20-020), demonstrated the capability to estimate NO_X emissions for the Dallas/Fort Worth metropolitan region for the summer of 2019 using the Tropospheric Monitoring Instrument (TROPOMI; Holloway et al., 2021). Agreement between satellite and modeled column NO_2 was within 20%. In a follow-up project focused on Houston (Goldberg et al., 2023; 2024a; Nawaz et al., 2024), the team was able to gain evidence for a low bias in the satellite instrument, that led to artificial agreement between satellite and model, and therefore modelled urban NOx emissions are now biased low (a model rural low bias still persisted as with previous studies). The latter project was also able to quantify neighborhood-scale and sector-by-sector NOx emission biases using a combination of satellite data, aircraft data, and sub-kilometer chemical transport models. Outside of Texas, the team has conducted similar analyses for other North American cities (Goldberg et al., 2019a, 2019b, 2024b), power plants (de Foy et al., 2015), South Asia (de Foy and Schauer, 2022), and global megacities (Goldberg et al., 2021) using TROPOMI and a complementary satellite instrument, the Ozone Monitoring Instrument (OMI).

Comparison of satellite and modeled NO_2 columns often reveals a widespread and persistent low model bias, often attributed to the free troposphere. In this project, we will evaluate whether TEMPO NO_2 columns can constrain NOx emissions as successfully as the Geostationary Coastal and Air Pollution Events (GEO-CAPE) Airborne Simulator (GCAS) aircraft and determine whether updates to NOx chemistry (particle nitrate photolysis), NO_2 vertical distribution and the NOx emissions inventory in the CAMx model can improve agreement with measured NO_2 columns.

Recently, Shah et al. (2023) comprehensively evaluated free troposphere NOx (FT-NOx) measurements over the Continental United States (CONUS), agreement between the Goddard Earth Observing System with Chemistry (GEOS-chem) model and these measurements, emission source contributions to FT-NOx in GEOS-chem, the potential influence of particulate nitrate (pNO3) photolysis to FT-NOx, and overall implications for comparing modeled to observed NO_2 columns. Findings of Shah et al. guide our approach to improving CAMx simulations of FT-NOx.

Figure 1, adapted from Shah et al., shows vertically resolved source contributions to NOx over the contiguous US in summer (August). Lightning and aircraft NOx emissions in the FT are important above the planetary boundary layer (PBL) and particularly important to column NO_2 measurements because instrument sensitivity is greater above the PBL. Upward transport of near-ground NOx emissions makes these emissions important throughout the tropospheric column. We will (1) add aircraft emissions above 1,000 ft above ground level (agl) because they are usually omitted from regulatory modeling databases, including Texas Commission on Environmental Quality (TCEQ's) modeling platform (2) improve estimation of soil NOx emissions by updating the Berkeley Dalhousie Soil NOx Parameterization (BDSNP; Hudman et al., 2012) algorithm in MEGAN3 (3) improve the Weather Research and Forecasting (WRF)-CAMx treatment of vertical diffusion in the FT which can impact vertical transport of NOx. We will also implement in CAMx a scheme for pNO3 photolysis similar to Shah et al. while preserving the integrity of the CAMx tools for source apportionment (Ozone Source Apportionment Technology and Particulate Source Apportionment Technology; OSAT and PSAT) and sensitivity analysis (Direct Decoupled Method; DDM).

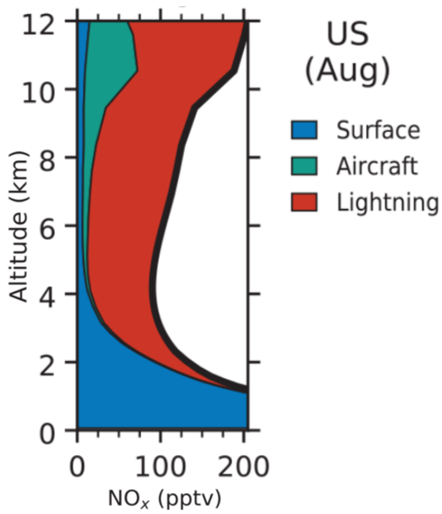

Figure 1. Vertically resolved source contributions to NOx over the contiguous US in summer modeled by GEOS-chem (adapted from Shah et al., 2023).

3.0 Objectives

This project will determine how TEMPO can be used for NOx emissions evaluation. We will use TEMPO NO_2 measurements to evaluate CAMx model updates to NOx chemistry, vertical distribution of NO_2 and the NOx emission inventory. Lessons learned and techniques developed for this project could be applied to other areas in the United States. The project will also demonstrate the capability to estimate NOx emissions using the flux divergence method and multilinear regression model applied to TEMPO NO_2 measurements.

4.0 Task Descriptions

In this project we will use hourly TEMPO NO_2 information (2 × 4.5 km^2). Complementing the satellite observations, we will run CAMx with 4 × 4 km^2 spatial resolution and NO_2 sector-based source apportionment over Texas using the 2019 TCEQ emissions inventory. Task 1 will add aircraft emissions and enhanced soil NOx emissions and perform an initial CAMx simulation. After developing diurnal NOx emissions estimates from TEMPO (Task 2), we will then compare CAMx model output with TEMPO data to generate an initial set of baseline NO_2 column comparisons (Task 3). Following this initial set of baseline comparisons, we will make modifications to the CAMx modeling configuration that include CAMx updates to aerosol nitrate photolysis and vertical distribution of NO_2 (Task 4). We will estimate NOx emissions using the flux divergence method to determine whether TEMPO can help constrain the TCEQ NOx emission inventory over Texas cities. Finally, we will use TEMPO NO_2 measurements and tagged NO_2 columns in a multi-linear regression model to estimate scaling factors for NOx emissions categories (Task 5).

Task 1: Texas 4 km CAMx baseline simulation for NO_2 and Ozone

We will run WRF and CAMx with 4 km grid resolution over Texas for August 25 – September 30, 2023 using emission inventory data from the TCEQ. Ramboll will perform the model simulations and is experienced working with these models and TCEQ emission data. We will follow TCEQ's 2019 State Implementation Plan (SIP) WRF and CAMx configurations to the extent possible for consistency and to enable use of TCEQ emission data.

Anthropogenic emissions will be from the 2019 TCEQ modeling inventory (closest to 2023 available) with addition of aircraft climb-out (above 1 km) and cruise emissions based on the Emissions Database for Global Atmospheric Research (EDGAR) 0.1° global database (Crippa et al., 2023). Lightning NOx (LNOx) emissions will be developed using Ramboll's LNOx processor. Biogenic emissions will be developed using our WRF simulation and the MEGAN version 3.2 developed by Ramboll in AQRP project 18-005 (Guenther et al., 2012).

We will update the soil NOx (S_{NOx}) parameterization within MEGAN v3.2 from the standard BDSNP algorithm to use the soil moisture function of Huber et al. (2023). The standard BDSNP produces peak soil NOx emissions at 30% water-filled pore space (WFPS) for all grid cells, whereas the updated version produces peak emissions at the median WFPS for each grid cell producing a more dynamic emissions parameterization. In the central/eastern U.S., where WFPS from WRF typically exceeds 30% depending on the land surface model used, the updated parameterization tends to increase April-July soil NOx emissions and decrease July-September soil NOx emissions. Preliminary evaluation of the updated scheme for 2019 using WRF-Chem found improved seasonal variation in NO_2 columns relative to TROPOMI over agricultural regions of the Midwest (Figure 2).

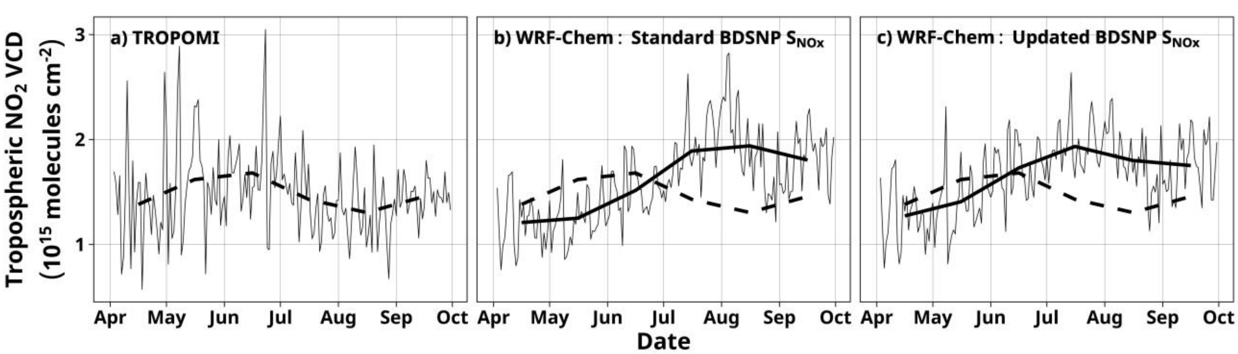

Figure 2. Tropospheric NO_2 Vertical Column Densities (VCDs) for April–September 2019 averaged for the Midwest Corn Belt region determined from (a) TROPOMI observations, (b) WRF-Chem with standard BDSNP and (c) WRF-Chem with Huber et al. (2023) updated BDSNP S_{NOx} schemes. Lines show daily average (thin lines), monthly average simulated (solid thick lines) and monthly average TROPOMI VCDs (dashed thick lines). Adapted from Huber et al. (2024).

We will use the CAMx OSAT source apportionment tool to tag NO_2 from 8 sectors (Table 2). We provide sample spatial maps of surface layer tagged NO_2 contributions from on-road mobile (left) and shipping (right) emissions over Houston as part of AQRP 22-023 in Figure 3. We will evaluate CAMx NO_2 and ozone surface concentrations using data collected at TCEQ Continuous Air Monitoring Stations (CAMS) within the 4 km CAMx domain. We will compute tropospheric column NO_2 (including source tagging; Table 2) from CAMx layers between the surface and ~13 km as discussed in Task 3.

Table 2. Source sectors for NO_2 tagging in CAMx.

No.	Source Sector	No.	Source Sector
1	Biogenic (soil NOx)	5	Off-road mobile including shipping
2	Lightning NOx	6	Electric Generating Units (EGUs)
3	Aircraft climb-out and cruise	7	Oil and Gas
4	On-road mobile	8	Other

Once preliminary results from model/satellite intercomparison are available (Task 3), the model will be re-run for short periods to test and potentially refine the CAMx updates to particulate nitrate chemistry and vertical distribution of NO_2 described under Task 4. The final CAMx simulation will be compared to the initial baseline simulation as well as surface observations and TEMPO NO_2 columns.

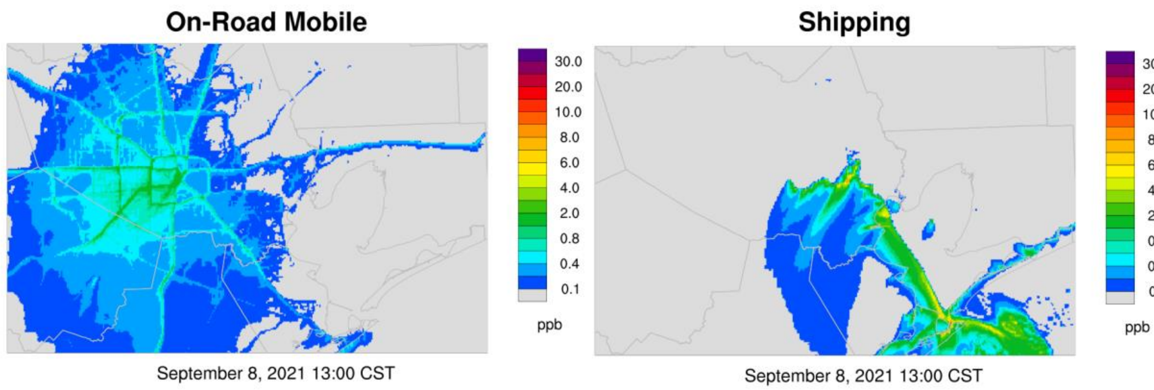

Figure 3. Surface layer tagged NO_2 contributions from on-road mobile (left) and shipping (right) emissions for September 8, 2021 13:00 CST over Houston as part of AQRP 22-023.

Task 2: Create TEMPO NO_2 Diurnal Profiles and Compare to Diurnal NOx Emission Maps

TEMPO is the first remote sensing instrument to continuously gather information on column NO_2 during all daylight hours over the continental United States. Before 2023, low earth orbiting instruments, such as OMI and TROPOMI, were able to gather column NO_2 information only in the early afternoon. Prior remote sensing instruments were informative, but assumptions were needed to translate the early afternoon measurement to a different hour of the day or a full-day average. The new capability provided by TEMPO allows us to evaluate the NOx emission inventories during individual hours separately, and target times of days when emission patterns vary. The key capability is being able to compare hours individually within a single day. For example, NOx emissions from on-road vehicles have a bimodal emission pattern peaking in the evening, while having a secondary peak in the morning. Measurements from TEMPO in the morning (~9 AM), early afternoon (~1 PM) and early evening (~5 PM) may be compared to each other, after accounting for meteorological and NO_2 lifetime differences at each hour, to understand relative emission patterns at each hour.

For this task, we will process TEMPO NO_2 data to a 0.01°× 0.01° grid, and then plot the diurnal NO_2 patterns during August 1 – October 31, 2023, centered on September 2023, for seven ~50 x 50 km regions: Dallas-Fort Worth, Houston, San Antonio, Austin, a power plant (Martin Lake), and rural areas (with low NOx emissions) in East Texas and West Texas. Measurements within the full region of interest will be averaged together to create a single value representative of the region, rather than any specific location within the region. TEMPO NO_2 measurements in the early afternoon will be compared to coincident TROPOMI NO_2 measurements at approximately 13:30 local time to understand potential differences between the two instruments.

During September 2023, there were, on average, 14 TEMPO NO_2 observations per day, with only two days fully missing (September 5th & 8th). The September 2023 timeframe also had several instances of TEMPO "special operations" (more frequent scans) over eastern Texas when there were up to 35 scans per day. These special operations occurred on September 11 – 12, 2023 and September 17 – 19, 2023, and instead of one TEMPO measurement per hour, there were five measurements per hour for several hours. The rapid scans will allow us to increase the instrument's signal to noise ratio and oversample to finer spatial resolution (~1 km) within each hour.

We will then process additional variables to convert *diurnal column NO_2* patterns into *diurnal NOx emissions* patterns. First, we will need to subtract out a background/inflow value to calculate a localized NO_2 enhancement; this will be individually done for each hour by calculating the values at the inflow boundary of the target domain. Then we will need to assume an NO_2 lifetime at the individual hour to convert NO_2 enhancements into a NOx enhancement. At first, an NO_2 lifetime will be approximated, and then when the CAMx simulation is complete, a more informed NO_2 lifetime can be used. Finally, we will need to account for meteorological variables, such as boundary layer depth and wind speed. European Centre for Medium-Range Weather Forecasts (ECMWF) Reanalysis v5 (ERA5) data will be used, and WRF data will be incorporated if we see major differences between the two datasets. The ultimate goal of this task to develop a method to generate diurnal NOx emissions patterns without the use of a chemical transport model that could then be used to evaluate diurnal patterns assumptions of NOx emissions input into chemical transport models such as CAMx.

Task 3: Comparison of NO_2 Columns between CAMx and TEMPO

To elucidate how CAMx baseline (Task 1) and with updates for nitrogen chemistry and vertical transport (Task 4) is performing, we will also compare the model output to TEMPO. TEMPO has the advantage of having spatially continuous measurements across Texas during cloud-free daylight hours and allows an evaluation of NO_2 in areas without ground monitors.

For this task, we will re-grid the TEMPO NO_2 columns onto the CAMx 4 km grid and re-calculate the NO_2 vertical columns using the simulated NO_2 column information from the CAMx simulation. Once re-gridded to the CAMx 4 km grid, the data can be averaged over multiple days to obtain gridded TEMPO NO_2 averages during each individual daylight hour.

Once the satellite observations and model simulation are on the same model grid, then an intercomparison between the datasets can be performed. As a prerequisite to this, we will need to process the satellite observations using the NO_2 vertical profile information from CAMx. Without this step, TEMPO satellite observations would be subject to artifacts related to their original a priori assumptions provided by the National Aeronautics and Space Administration (NASA) GEOS Composition Forecasting (GEOS-CF) model. After this re-processing is completed, it is appropriate to directly compare NO_2 from model and satellite to each other. TEMPO, in comparison to low earth orbiters such as OMI and TROPOMI, is acquiring measurements when the sun angle is lower (i.e., when the visible light pathway through the troposphere is longer), so it is probable that NO_2 profile information from CAMx will yield larger changes for TEMPO NO_2 column measurements than TROPOMI, especially during the morning and evening hours.

The analysis will compare NO_2 on a county-level scale for seven representative locations in the domain (Dallas-Fort Worth, Houston, San Antonio, Austin, the Martin Lake power plant, and rural areas (with low NOx emissions) in East Texas and West Texas) and on a day-to-day basis when the two datasets (model and satellite) are collocated in time and space. We will then perform this analysis successively to evaluate impacts of the CAMx model updates.

Task 4: CAMx Updates and Testing

Following the baseline CAMx simulation and subsequent model performance evaluation (Task 1) and comparison to TEMPO NO_2 columns (Task 3), we will perform several updates to NOx chemistry and vertical mixing described below. We will then perform short CAMx sensitivity tests without source apportionment and compare with TEMPO NO_2 columns to determine the impact of these changes.

Chemistry Updates

Many studies report that the photolysis frequency of particulate-phase nitrate ion (pNO3) is enhanced relative to gas-phase HNO3 photolysis by a factor of 10-500, as summarized by Shah et al. (2023). The process is potentially important to NOx availability where direct NOx emissions are small because the products of pNO3 photolysis are NO_2 and/or HONO (termed renoxification). However, details of pNO3 photolysis remain uncertain. We will adopt the parametrization of pNO3 photolysis developed by Shah et al. (2023) which was constrained by measurements and their global GEOS-chem simulation. Their parameterization focuses on pNO3 associated with sea-salt aerosol and therefore has most impact over oceanic regions, especially at tropical latitudes. We will evaluate how introducing pNO3 photolysis in CAMx influences NO_2-columns and oxidant concentrations in continental and marine environments, and especially over the Gulf of Mexico. Several air quality models, including CAMx, tend to overestimate ozone over the Gulf (AQRP project 22-008) which may be exacerbated by adding pNO3 photolysis (Shah et al., 2023). We would update the CAMx source apportionment (OSAT and PSAT) to account for pNO3 photolysis and also update the DDM sensitivity analysis if resources allow.

Vertical Mixing

As an off-line model, CAMx receives gridded meteorological input data that is usually created from WRF by the WRFCAMx processor. WRFCAMx must be flexible to work with the variety of PBL parameterization schemes available with WRF, e.g., vertical mixing described by a turbulent kinetic energy (TKE) scheme vs. bulk boundary layer mixing schemes. Within CAMx, vertical mixing is modeled using K-theory and relies on turbulent mixing coefficients (Kv) diagnosed by WRFCAMx using parameters available in WRF output files. We will investigate potential updates to the Kv diagnosis in WRFCAMx by intercomparing existing Kv parameterizations, noting strengths and weaknesses among all schemes in generating turbulent mixing fields in time and space (including the FT) for short periods. For urban areas, the existing parameterization optionally adjusts Kv to account for urban roughness and heat-island effects not represented by standard WRF simulations and we will reevaluate the magnitude and height range of this adjustment. We will evaluate these updates by running CAMx and examining surface NO_2 concentrations, NO_2 vertical profiles and NO_2 columns for urban and rural areas of Texas.

Task 5: Estimating NOx Emissions by Sector and by Time of Day using CAMx Source Apportionment and TEMPO Retrievals

The flux divergence method can provide high resolution maps of NOx emissions using spatial remote sensing data. The method has been used to identify point sources and intra-urban variations using

TROPOMI retrievals over Houston (Goldberg et al., 2022), cities in South Asia (de Foy and Schauer, 2022) and elsewhere around the world (Beirle et al., 2023). We also applied this method to GCAS retrievals over Houston in AQRP 22-023 and it was able to identify major highways, shipping lanes in Galveston Bay and large point sources in the greater Houston area.

In this project, we will apply the flux divergence method for the first time to TEMPO data. The main advantage of TEMPO over other satellite products such as TROPOMI is hourly resolution during daylight hours. We will therefore be able to carry out the flux divergence method by time of day to estimate the diurnal variability in emissions for the model domain.

In AQRP 22-023, we applied a Multi-Linear Regression model to obtain an optimal match between the CAMx columns by source sectors and the GCAS NO_2 columns. This analysis revealed that the mobile source emissions were potentially underestimated in the inventory, while the ship emissions were possibly overestimated, as shown in Figure 4. For this project, we will use a similar algorithm to optimize the match between the CAMx NO_2 columns and the TEMPO retrievals. This will be done individually by time of day so that we can estimate diurnal profiles of emissions for distinct source sectors. Large point sources have known diurnal profiles that will be used to evaluate the method. These profiles will be compared with diurnal profiles of emissions in urban areas. As in the previous project, we will perform an uncertainty analysis using multi-level bootstrapping, using scenes to be included in the analysis as well as the pixels within each scene. This combination was found to give a robust estimate of both the adjustment factors and their uncertainty. We expect that using this method with TEMPO results will have a reduced spatial resolution compared with GCAS, but an improved temporal resolution: we will be able to determine differences by time of day as well as by day of the week. There will also be many more scenes available thereby reducing noise and the uncertainty in the results.

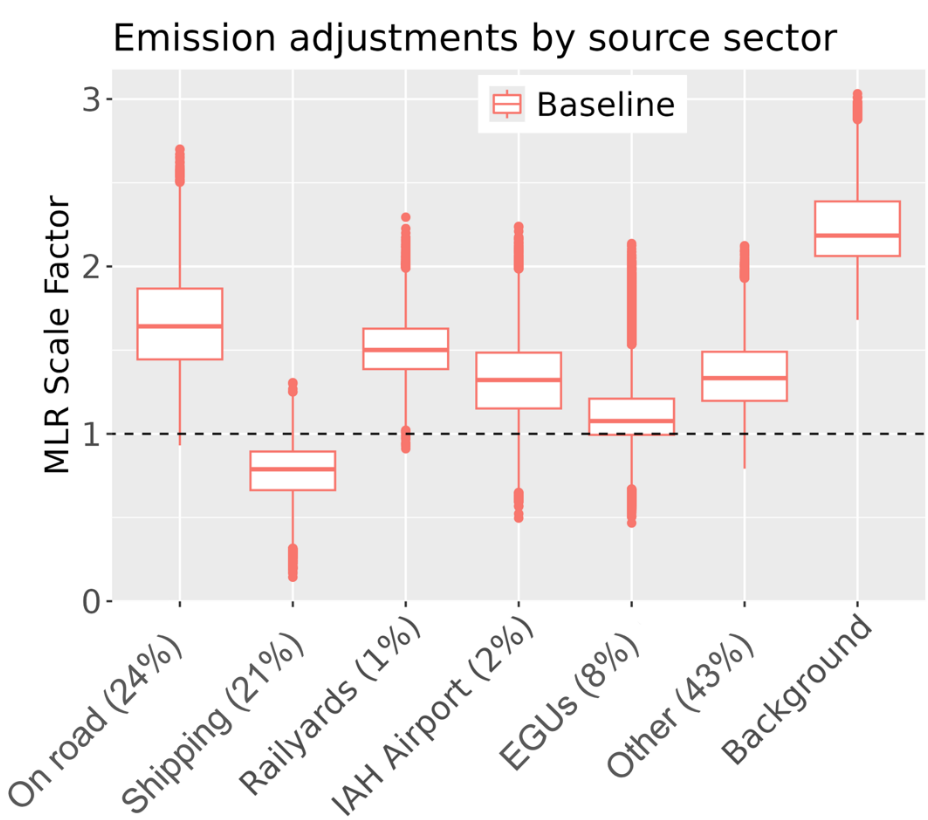

Figure 4. Box-and-whisker plot of scaling factors obtained from the Multi Linear Regression Model with 100 bootstrapped selection of rasters each consisting of 100 bootstrapped selection of grid blocks included in the analysis. Percentages show the fraction of domain-wide NOx emissions from each sector. Adapted from Goldberg et al. (2024a).

Task 6: Project Management and Reporting

At the start of the project, the team will develop and submit to the AQRP a work plan that includes scope of work (this document), detailed budget, and a Quality Assurance Project Plan (QAPP). The QAPP will conform to Category III projects and with Environmental Protection Agency (EPA 2001) QA/R-5 guidance. Once approved, the team will hold a kickoff call with AQRP and TCEQ representatives to discuss the work plan and specific details of the project, answer questions, and address anticipated issues. During the project, we will submit monthly technical and financial reports, and quarterly progress reports, adhering to AQRP requirements.

At the close of the project, we will develop a final project presentation to be delivered at the 2025 AQRP workshop at the University of Texas in Austin. The team will also produce a draft final report and a final report documenting all activities performed for the study, summarizing project findings and recommendations for future research, and emphasizing those findings of interest to modelers and planners at TCEQ. All reports developed during this project will conform to AQRP accessibility requirements and formats. The team will make available all datasets developed during the project to the AQRP and TCEQ at the end of the project.

5.0 Schedule

The planned duration of the project is 14 months (August 2024 – September 2025). Figure 5 presents the schedule for each task and project deliverable.

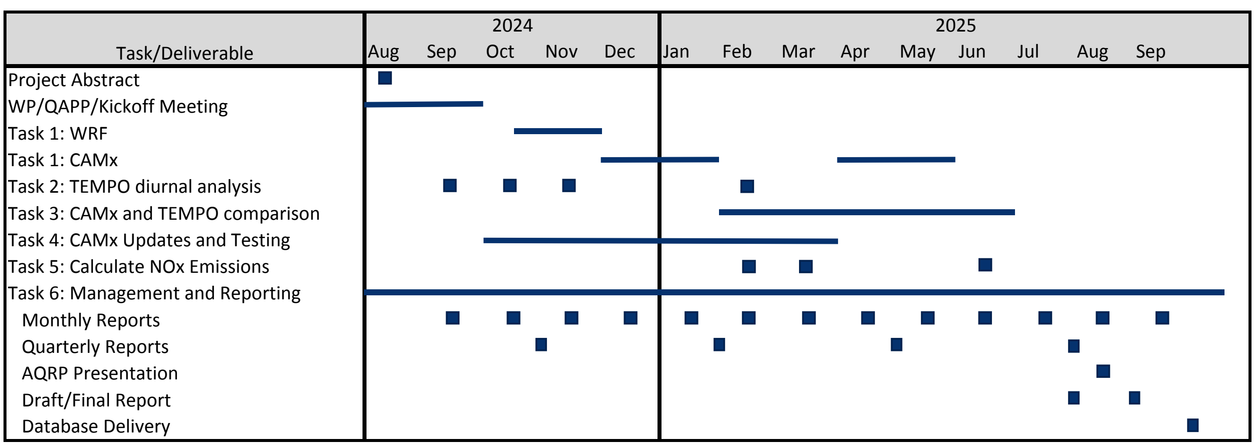

Figure 5. Planned project schedule.

6.0 Project Participants and Responsibilities

Mr. Jeremiah Johnson will lead the project as PI and coordinate collaboration with Dr. Daniel Goldberg (co-PI), Dr. Daniel Huber and Dr. Benjamin de Foy (co-PI) who will be consultants to Ramboll.

Mr. Jeremiah Johnson will oversee the emissions processing, CAMx model development, WRF and CAMx simulations. Dr. Daniel Goldberg will process the TEMPO satellite data, create diurnal NO_2 profiles, and compare the TEMPO NO_2 columns with CAMx NO_2 columns. Dr. Benjamin de Foy will calculate diurnal NOx emissions by sector from TEMPO satellite measurements applying flux divergence and advanced statistical methods. Dr. Daniel Huber will modify the default soil NOx parameterization within the MEGAN biogenic emissions model to include an updated soil moisture function.

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Budget and Budget Justification

Project #24-004
Evaluating Updates to CAMx and NOx Emission Inventories using TEMPO Measurements over Texas

Prepared for

Air Quality Research Program (AQRP)
The University of Texas at Austin

By

Jeremiah Johnson (Principal Investigator)
Ramboll
Novato, CA

Dr. Dan Goldberg (co-Principal Investigator)
George Washington University
Washington, D.C.

Dr. Benjamin de Foy (co-Principal Investigator)
Saint Louis University
Saint Louis, MO

August 22, 2024
Version #1

QA Requirements: Audits of Data Quality: 10% Required
Report of QA Findings: Required in Final Report

NOTE: The Workplan package consists of three independent documents: Scope of Work, Quality Assurance Project Plan (QAPP), and budget and justification. Please deliver each document (as well as all subsequent documents submitted to AQRP) in Microsoft Word format.

Approvals

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RoseAnna Goewey
Program Manager, Texas Air Quality Research Program

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Elena McDonald-Buller
Project Manager, Texas Air Quality Research Program

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Robert Keirstead
Project Liaison, Texas Commission on Environmental Quality

Budget and Budget Justification

Lbr Classification/Name	Loaded Hourly Labor Rate	Total Hrs	Total Dollars
P4			
Chris Emery	249.00	66	16,434
Gary Wilson	249.00	12	2,988
Greg Yarwood	249.00	94	23,406
Jeremiah Johnson	249.00	120	29,880
P3			
Jung Chien	214.00	28	5,992
Pradeepa Vennam	214.00	94	20,116
P2			
Trang Tran	183.00	84	15,372
Liji David	183.00	40	7,320
P1			
Blake Himes	139.00	94	13,066
Fianna Li	139.00	156	21,684
Support	107.00	19	2,033
Ramboll Labor Subtotal		807	158,291
Daniel Goldberg			30,000
Daniel Huber			10,000
Benjamin de Foy			30,000
Travel			1,000
Equipment			400
ODCs Subtotal			1,400
GRAND TOTAL		807	229,691

The team's proposed total budget is $229,691, of which $228,291 is allocated to labor charges and $1,400 to other direct costs. Ramboll's labor rates are based on current fully loaded rates agreed between the TCEQ and Ramboll. Dr. Greg Yarwood will update the CB7 chemical mechanism and source apportionment schemes in CAMx to include aerosol nitrate photolysis. Mr. Chris Emery will update the vertical mixing scheme in the WRFCAMx processor. The budget includes $30,000 for Dr. Daniel Goldberg, $10,000 for Dr. Daniel Huber and $30,000 for Dr. Benjamin De Foy, all as direct consultants to Ramboll. Ramboll will not add any additional fees to consultant costs. Roles for key personnel are provided above.

Direct costs include a travel budget of $1,000 for the project Principal Investigator to attend the AQRP workshop in Austin, Texas. Direct costs also include expenses for high-volume disk drives for the data transfer at the end of the project.

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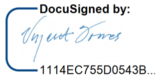
Vincent Torres vmtorres@eid.utexas.edu Associate Director The University of Texas at Austin, Center for Energy & Environmental Resources Security Level: Email, Account Authentication (None) **Electronic Record and Signature Disclosure:** Not Offered via DocuSign	 Signature Adoption: Uploaded Signature Image Using IP Address: 128.62.227.73	Sent: 9/20/2024 7:52:28 AM Viewed: 9/20/2024 2:59:02 PM Signed: 9/20/2024 2:59:32 PM

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