Quality Assurance Project Plan

Project # 20 – 020
New Satellite Tools to Evaluate Emission Inventories: Is a 3-D Model Necessary?

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

Prepared by

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University of Wisconsin – Madison

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Version #2

The University of Wisconsin – Madison has prepared this QAPP following EPA guidelines for a Quality Assurance (QA) Category III Project: Measurement. 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 project titled, New Satellite Tools to Evaluate Emission Inventories: Is a 3-D Model Necessary? The Principal Investigator for the project is Dr. Tracey Holloway and Co-PI is Mr. Jeremiah Johnson.

Electronic Approvals:

This QAPP was approved electronically on 06/10/2020 by

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This QAPP was approved electronically on 6/16/2020

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This QAPP was approved electronically on 06/11/2020 by

Tracey Holloway
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QAPP Distribution List

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University of Wisconsin – Madison
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1.0 Project Description and Objectives

This study will develop best-practice recommendations for the utilization of satellite data for emissions evaluation. Because of their radiative properties, nitrogen dioxide (NO_2) and sulfur dioxide (SO_2) are among of a small group of gas-phase air pollutants that may be reliably detected from space. These gases have short atmospheric lifetimes, such that satellite-based observations are a useful indicator of fuel combustion. Although the characterization of gas-phase emissions has emerged as one of the leading areas for air quality utilization of satellite data, multiple atmospheric processes affect the relationship between satellite-derived column abundance and near surface. We will evaluate two different methods to compare satellite NO_2, and to a limited extent SO_2, with emission inventories developed by the Texas Commission on Environmental Quality (TCEQ).

These methods, using existing, publicly-available models and data, include:

1) Comparison of satellite-derived NO_2 and SO_2 from TROPOspheric Monitoring Instrument (TROPOMI) for summer 2019 with model simulations from a Weather Research and Forecasting (WRF) and Comprehensive Air Quality Model with Extensions (CAMx) modeling system developed for the TCEQ;

2) Simpler approaches to comparing NO_X emissions and TROPOMI data that don't require a photochemical grid model, especially the Exponentially Modified Gaussian (EMG) approach. These simpler methods will be extended to SO_2 as resources and data integrity allow.

1.1 Purpose and Objectives

Although best-practice, the utilization of a photochemical grid model is expensive and time-consuming. Characterizing the value of simpler methods – wherein emissions and satellite data may be directly compared – offers the potential for TCEQ to perform emissions evaluation with satellite data analysis over multiple years and/or considering multiple emission scenarios at a greatly reduced cost.

There are a number of methods that can be used to directly compare emissions and satellite data, even without a model. These range from direct comparison of temporal and spatial emissions patterns [e.g. *Montgomery and Holloway*, 2018], to more sophisticated methods that approximate the effects of meteorology and chemistry, even without the use of a three-dimensional model. As a first step in our analysis, daily TROPOMI NO_2 data will be compared with NO_X emissions, to assess agreement in the absence of meteorological corrections.

This analysis will evaluate methods by which high-resolution satellite data may be compared with emissions inventories, and to assess the necessity of computationally intensive modeling approaches. The specific objectives of this project are:
* Compare satellite data for NO_2 and SO_2 columns with model simulations from the high-resolution WRF-CAMx model

* Evaluate the utility of satellite data for NO_X emissions inventory evaluation, without the use of a high-resolution model

* Evaluate how model-based emissions assessment compares to emissions assessment in the absence of model, finalizing recommendations, software, and algorithms

* Develop best-practice recommendations and software to support future TCEQ utilization of satellite data for emission evaluation

2.0 Organization and Responsibilities

2.1 Responsibilities of Project Participants

Dr. Tracey Holloway will lead the project as Principal Investigator, coordinate collaboration with Ramboll, and supervise the University of Wisconsin – Madison research team. Mr. Jeremiah Johnson and Dr. Greg Yarwood of Ramboll will conduct WRF-CAMx modeling. Dr. Daniel Goldberg will apply the EMG technique to TROPOMI to estimate NO_X emissions. Dr. Monica Harkey will support the comparison of gridded TROPOMI data for summer 2019 with the WRF-CAMx model results from Ramboll. A Research Intern will grid satellite data for comparison with CAMx and work with Ramboll and Dr. Goldberg on all TROPOMI data processing. The Information Processing Consultant will support data transfer, file sharing, data archiving, and advanced software needs. An undergraduate or post-undergraduate intern will support the gridding of TROPOMI for comparison with CAMx.

2.2 Project Schedule

A schedule of project deliverables is shown below, assuming a start date during June 2020.

Deliverable	**2020**							**2021**									
	J	**J**	**A**	**S**	**O**	**N**	**D**	**J**	**F**	**M**	**A**	**M**	**J**	**J**	**A**	**S**	**O**
Modeling	X	X	X	X	X	X											
Satellite data		X	X	X	X	X	X										
Model analysis						X	X	X	X								
Emissions data processing	X	X	X														
Direct satellite comparison		X	X	X													
EMG satellite comparison					X	X	X	X									
Optional SO_2 analysis								X	X	X	X	X					
Mobile Inventory Methods			X	X													
Final modeling									X	X	X	X					
Methods Recommendation											X	X	X				
Technical Reports	X	X	X	X	X	X	X	X	X	X	X	X	X	X			
Financial Reports		X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
Quarterly Reports		X			X			X			X			X			X
Draft Final Report														X			
Final Report															X		
AQRP Workshop															X		

3.0 Scientific Approach

This work will develop best-practice recommendations for the utilization of satellite data for emissions evaluation. We will develop methods to leverage remote sensing capabilities to improve emission inventories, without undermining the process-based nature of the inventories, essential for their use in air quality management.

3.1 Satellite-based observations

Satellites measure the column abundance of NO_2 and SO_2, known as the vertical column density (VCD). All analysis will utilize data from the Tropospheric Ozone Monitoring Instrument (TROPOMI). TROPOMI is polar-orbiting with daily global coverage at a nadir resolution of 7 km × 3.5 km, launched in 2017. The spatial resolution offered by TROPOMI is over 10x higher than any previous gas-monitoring satellite, with the Ozone Monitoring Instrument (OMI; nadir resolution of 13 km × 24 km) offering the next-highest capability. As a polar-orbiting satellite with an afternoon overpass, care must be taken in the interpretation of TROPOMI column retrievals as an indicator of near-surface emissions [*Streets et al.*, 2013; *Goldberg et al.*, 2019b; *Penn and Holloway*, 2020]. TROPOMI provides "snapshots" at the same time each day, except as limited by cloud cover, surface albedo, or instrument errors.

We will grid the TROPOMI data for comparison with CAMx output. This will be performed with the Wisconsin Horizontal Interpolation Program for Satellites (WHIPS). WHIPS was developed by the Holloway Group at the University of Wisconsin—Madison, with NASA Applied Sciences support, and allows users to reformat multiple data products from the Ozone Monitoring Instrument (OMI), as well as gas and aerosol products from other satellite platforms. Satellite data may be mapped to any grid, for direct comparison with model data. TROPOMI data will be gridded for the data analysis period: March 1 through October 15, 2019.

3.2 CAMx simulations

Model simulations will be conducted by Ramboll, using an existing high-resolution WRF-CAMx model for 2019 developed for TCEQ (Near Real-Time Exceptional Event Model; NRTEEM) described in *Johnson et al.* [2019]. WRF and CAMx modeling domains at 36, 12, and 4 km are used for the NRTEEM system. The 36 km modeling domain includes all of the continental US and large areas of Central America and Canada; The 12 and 4 km domains are the TCEQ State Implementation Plan (SIP) domains, which are used for other modeling efforts by the TCEQ and Ramboll.

The NRTEEM modeling platform covers a simulation period of March 1 through October 15, 2019 (the first full year for which TROPOMI data are available). Chemical analysis is performed by CAMx v6.50 with the CB6r4 chemical mechanism, with input meteorology calculated by WRF version 3.9.1.1 with GFS 0.25 degree analysis data for initial/boundary conditions. We will update the WRF-CAMx emissions inventory to incorporate anthropogenic emissions from the 2020 TCEQ projection (closest to 2019 available), and 2019 hourly CEMS data for power plants that are a focus of our analysis. Biogenic emissions for 2019 are calculated from Model of Emissions of Gases and Aerosols from Nature v. 3.1 developed by Ramboll in AQRP project 18-005; (MEGAN; [*Guenther et al.*, 2006]), and fire emissions are from the near- real-time Fire INventory of NCAR (FINN) version 2 (if available from AQRP project 18-022).

3.3 EMG analysis

Beirle et al. [2011] proposed estimating NO_X emissions using a statistical fitting of satellite-observed NO_2 plumes to an exponentially modified Gaussian function (EMG). We will apply a modification of this approach, as presented in *Goldberg et al.* [2019]. This methodology will be implemented by Dr. Goldberg as a consultant to our study, wherein daily plumes from TROPOMI will be mapped onto an x-y grid and then rotated based on the daily wind-direction. As a result, all plumes will be superimposed, increasing the signal-to-noise ratio and generating a more robust fit [*Valin et al.*, 2013; *Lu et al.*, 2015; *Goldberg et al.*, 2019b, 2019a, 2019c] NO_X emissions associated with plumes will be calculated using the following equation:

$$NO_X\ emissions = 1.33\ (\alpha / \tau_{\mathrm{effective}}),\ \ where\ \ \tau_{\mathrm{effective}} = x_o / w$$

In this equation, w represents the wind speed, $\tau_{\mathrm{effective}}$ represents the mean effective NO_2 lifetime; x_o represents the fitted decay distance; and α represents total burden obtained by the exponentially modified Gaussian fit. NO_2 is converted to NO_X by multiplying by a factor of 1.33 which is typical of the mean column-averaged NO_X/NO_2 ratio in an urban area during the mid-afternoon.

The wind speed and direction needed for these calculations will be taken from the Ramboll WRF simulations at 4 km, and compared with more widely available re-analysis data (such as the fifth generation European Medium-Range Weather Forecasting ReAnalysis data, ERA-5). Mean near-surface wind speed over all days with valid satellite data will be included.

4.0 Quality Metrics

TROPOMI VCDs will be gridded retaining original quality flags, along with information about the averaging kernel, solar zenith angle, and cloud cover. Satellite data may then be screened for quality flags, sun angle, and cloud cover in accordance with best practices recommended by the satellite product team.

We will calculate VCDs from WRF-CAMx in a manner appropriate for comparison with satellite data (vertical integration using TROPOMI averaging kernel; filtering for cloud cover to ensure comparable data availability).

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 9.

5.2 Data Validation

Data validation procedures are discussed under Sections 6.3 and 7.3.

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 SO_2 as observed from satellites. This procedure includes: a) comparing TROPOMI data with NRTEEM emissions directly; b) comparing TROPOMI data with WRF-CAMx model output; c) comparing EMG 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 data associated with this project will be backed up to an external hard drive and stored for 3 years following the completion of the project. Where appropriate, files will also be stored online via the UW-Madison Box system; publicly available data will be put on UW servers for distribution. Any paper documents will be scanned and stored electronically.

6.0 Discussion of WRF-CAMx

6.1 Selection

WRF-CAMx is a state-of-the-science modeling system, under regular review and development, used in both regulatory and research applications. We select to use the WRF-CAMx modeling system for the availability of the NRTEEM modeling platform and database available for our area of interest. Additionally, WRF-CAMx and NRTEEM inputs are available with a high spatial resolution during a timeframe of TROPOMI data availability. WRF-CAMx has also been employed previously for comparison with other satellite products, from OMI [*Kemball-Cook et al*., 2015].

6.2 Calibration

WRF-CAMx modeling calibration with the NRTEEM platform is described by *Johnson et al.* [2019].: "This calibration entails comparing CAMx output concentrations to air quality measurements, assessing whether agreement falls within accepted ranges (e.g., Emery et al., 2017), and determining whether action must be taken to recalibrate the model. If the model falls outside an accepted range, we might consider making some adjustment (change emissions, meteorology) to bring the model within range which can be viewed as calibration."

6.3 Validation

Validation of WRF-CAMx modeling with the NRTEEM platform is described by *Johnson et al.* [2019]. Ambient NO_X concentrations simulated by the final WRF-CAMx modeling with adjusted emissions will be compared with all available ground-based observations of NO_X during the modeling time period.

6.4 Documentation

The CAMx User's Guide is available online (http://www.camx.com/files/camxusersguide_v6-50.pdf). Namelist files used to run CAMx will be included in appropriate technical and final reporting.

7.0 Discussion of EMG

7.1 Selection

The EMG technique presented by *Goldberg et al.* [2019a, 2019b, 2019c] was selected for its ability to produce emission estimates directly from TROPOMI data with minimal additional data.

7.2 Calibration

Calculation of parameters in the EMG approach [*Goldberg et al.,* 2019a; 2019b; 2019c] are based on wind speed and direction, which will be taken from the Ramboll WRF simulations at 4km. 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 EMG analysis in the future if WRF simulations are not available. The comparison will focus on the meteorological parameter that EMG uses, namely wind speed. These will be compared at the commencement of the EMG analysis.

7.3 Validation

Emissions estimates from the EMG technique will be compared to emissions from five power plants in Texas, which are large and relatively isolated point sources that have well-constrained emissions measured by CEMS. These power plants will have differing spatial isolation, surrounding emissions, and fuel. Additionally, we will compare EMG emissions estimates with emissions from five cities in Texas with significant on-road vehicle contributions to NO_X. These cities have been selected to represent three different methodologies for developing mobile source emission inventories: i) link-based travel demand model within Texas (Dallas/Fort Worth and San Antonio); ii) non link-based within Texas (Austin and College Station); iii) default travel demand from the EPA MOtor Vehicle Emissions Simulator (MOVES) (Shreveport).

7.4 Documentation

8.0 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. This independent review will entail data visualization and discussion of qualitative and quantitative metrics.

9.0 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.

Dr. Holloway, or her 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 http://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.

Dr. Holloway will lead reporting activities with assistance from Ramboll and her team at the University of Wisconsin – Madison. Project data to be submitted to the AQRP archive will include all gridded NO_2 data from TROPOMI over the study domain and period. Updated WHIPS software to support future model-satellite comparisons will be made available on a public Python distribution platform (e.g. github).

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, July 31, 2020

Quarterly Reports: Each Quarterly Report will provide a summary of the project status for each reporting period. It will be submitted to the Project Manager as a Microsoft Word file. It will not exceed 2 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	May, June, July 2020	Friday, July 31, 2020

Quarterly Report #2	August, September, October 2020	Friday, October 30, 2020
Quarterly Report #3	November, December 2020, January 2021	Friday, January 29, 2021
Quarterly Report #4	February, March, April 2021	Friday, April 30, 2021
Quarterly Report #5	May, June, July 2021	Friday, July 30, 2021
Quarterly Report #6	August, September, October 2021	Friday, October 29, 2021

Quarterly Report Due Dates:

Report	Period Covered	Due Date
Quarterly Report #1	May, June, July 2020	Friday, July 31, 2020
Quarterly Report #2	August, September, October 2020	Friday, October 30, 2020
Quarterly Report #3	November, December 2020, January 2021	Friday, January 29, 2021
Quarterly Report #4	February, March, April 2021	Friday, April 30, 2021
Quarterly Report #5	May, June, July 2021	Friday, July 30, 2021
Quarterly Report #6	August, September, October 2021	Friday, October 29, 2021

Monthly Technical Reports (MTRs): Technical Reports will be submitted monthly to the Project Manager and TCEQ Liaison in Microsoft Word format using the AQRP FY20-21 MTR Template found on the AQRP website.

MTR Due Dates:

Report	Period Covered	Due Date
Technical Report #1	Project Start - June 30, 2020	Wednesday, June 10, 2020
Technical Report #2	July 1 - 31, 2020	Friday, July 10, 2020
Technical Report #3	August 1 - 31, 2020	Monday, August 10, 2020
Technical Report #4	September 1 - 30 2020	Thursday, September 10, 2020
Technical Report #5	October 1 - 31, 2020	Friday, October 9, 2020
Technical Report #6	November 1 - 30, 2020	Tuesday, November 10, 2020
Technical Report #7	December 1 - 31, 2020	Thursday, December 10, 2020
Technical Report #8	January 1 - 31, 2021	Friday, January 8, 2021
Technical Report #9	February 1 - 28, 2021	Wednesday, February 10, 2021
Technical Report #10	March 1 - 31, 2021	Wednesday, March 10, 2021
Technical Report #11	April 1 - 30, 2021	Friday, April 9, 2021
Technical Report #12	May 1 - 31, 2021	Monday, May 10, 2021
Technical Report #13	June 1 - 30, 2021	Thursday, June 10, 2021
Technical Report #14	July 1 - 31, 2021	Friday, July 9, 2021

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 20-21 FSR Template found on the AQRP website.

FSR Due Dates:

Report	Period Covered	Due Date
FSR #1	Project Start - June 30	Wednesday, July 15, 2020
FSR #2	July 1 - 31, 2020	Friday, August 14, 2020

FSR #3	August 1 - 31, 2020	Tuesday, September 15, 2020
FSR #4	September 1 - 30 2020	Thursday, October 15, 2020
FSR #5	October 1 - 31, 2020	Friday, November 13, 2020
FSR #6	November 1 - 31, 2020	Tuesday, December 15, 2020
FSR #7	December 1 - 31, 2020	Friday, January 15, 2021
FSR #8	January 1 - 31, 2021	Monday, February 15, 2021
FSR #9	February 1 - 28, 2021	Monday, March 15, 2021
FSR #10	March 1 - 31, 2021	Thursday, April 15, 2021
FSR #11	April 1 - 30, 2021	Friday, May 14, 2021
FSR #12	May 1 - 31, 2021	Tuesday, June 15, 2021
FSR #13	June 1 - 30, 2021	Thursday, July 15, 2021
FSR #14	July 1 - 31, 2021	Friday, August 13, 2021
FSR #15	August 1 - 31, 2021	Wednesday, September 14, 2021
FSR #16	Final FSR	Friday, October 15, 2021

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. 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. It will also include a report of the QA findings.

Draft Final Report Due Date: Monday, August 2, 2021

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: Tuesday, August 31, 2021

Project Data: All project data including but not limited to QA/QC measurement data, metadata, databases, modeling inputs and outputs, etc., will be submitted to the AQRP Project Manager within 30 days of project completion (September 20, 2021). The data will be submitted in a format that will allow AQRP or TCEQ or other outside parties to utilize the information. It will also include a report of the QA findings.

AQRP Workshop: A representative from the project will present at the AQRP Workshop in the first half of August 2021.

10.0 References

Beirle, S., K. F. Boersma, U. Platt, M. G. Lawrence, and T. Wagner (2011), Megacity emissions and lifetimes of nitrogen oxides probed from space, *Science, 333*(6050), 1737-1739, doi:10.1126/science.1207824.

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