Quality Assurance Project Plan (QAPP)

Project 22-019

Refining ammonia emissions using inverse modeling and satellite observations over Texas and the Gulf of Mexico and investigating its effect on fine particulate matter

Prepared for

Texas Air Quality Research Program (AQRP)

The University of Texas at Austin

Prepared by

Yunsoo Choi

University of Houston

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Version 1

University of Houston has prepared this QAPP following the Environmental Protection Agency (EPA) guidelines for a Quality Assurance (QA) Category III Project: Research Model Application It is submitted to the Texas Air Quality Research Program (AQRP) as required in the Work Plan requirements.

QAPP Requirements: Project Description and Objectives, Organization and Responsibilities, Specific approach, Model Selection, Model Design, Model Coding, Model Evaluation, Documentation, Reporting as prescribed in the applicable National Risk Management Research Laboratory (NMRL) QAPP Requirements template (https://www.tceq.texas.gov/airquality/airmod/project/quality-assurance).

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 Refining ammonia emissions using inverse modeling and satellite observations over Texas and the Gulf of Mexico and investigating its effect on fine particulate matter project. The Principal Investigator for the project is Yunsoo Choi.

Electronic Approvals:

This QAPP was approved electronically on 09/01/2022 by Elena McDonald-Buller, The University of Texas at Austin.

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

This QAPP was approved electronically on 9/1/2022 by Vincent M. Torres, The University of Texas at Austin.

Vincent M. Torres
Quality Assurance Project Plan Manager, Texas Air Quality Research Program

This QAPP was approved electronically on 9/7/2022 by Khalid Al-Wali, Texas Commission on Environmental Quality.

Khalid Al-Wali
Project Liaison, Texas Commission on Environmental Quality

QAPP Distribution List

Texas Air Quality Research Program
David Allen, Director
Elena McDonald-Buller, Project Manager
Vincent M. Torres, QAPP Manager

Texas Commission on Environmental Quality
Khalid Al-Wali, Project Liaison

University of Houston
Yunsoo Choi, Principal Investigator

1- Project Description and Objectives

In this project we will implement an inverse modeling technique over the state of Texas and the Gulf of Mexico using Community Multiscale Air Quality (CMAQ) models and ammonia (NH_3) remote sensing data from the Cross-track Infrared Sounder (CrIS) for 2019. We will analyze NH_3 emissions from mobile, area, and point sources and emissions from anthropogenic and biogenic sources. By using the inverse modeling, we will leverage satellite observations to update National Emission Inventory (NEI) NH_3 emissions to constrain associated emissions, which are highly uncertain owing to a lack of NH_3 observations, resulting in errors in bottom-up calculated emissions. In the first task, we prepare comprehensive satellite, in situ, and modeling data to run CMAQ model and the iterative Finite Difference Mass Balance (iFDMB) method. In the second task, we will apply the iFDMB inverse modeling technique to revise NH_3 emissions with respect to CrIS observations. Following this method, we will develop adjusting factors to modify NH_3 emissions until they reach an optimum state in which NH_3 concentrations are close to the CrIS observations. We will use a reduced complexity CMAQ model (RCCM) to run the iFDMB. Since running the iFDMB is computationally expensive and requires numerous iterations, using RCCM for simulations will reduce the burden of computations while maintaining the accuracy of predictions. In the third task after updating the emissions inventory, we will investigate the effect of adjusting NH_3 emissions on atmospheric chemistry, including fine particulate matter ($PM_{2.5}$) concentrations, and $PM_{2.5}$ inorganic and organic constituents.

The objectives of this project are:

1. Updating NH_3 emissions inventory over Texas and the Gulf of Mexico
2. The contribution of updated NH_3 emissions on $PM_{2.5}$ concentrations
3. The investigation of the effect of adjusting NH_3 emissions on atmospheric chemistry

2- Organization and Responsibilities

2-1- Key Personnel and Tasks

This project is being conducted by University of Houston under a grant from the Texas Air Quality Research Program (AQRP). The project Principal Investigator (PI) is Dr. Yunsoo Choi, who will oversee the progress and quality of the project. Mr. Mahmoudreza (Semko) Momeni will develop and use the inverse modeling system for NH_3 emissions (Tasks 2 & 3), and he also will be involved in collecting in-situ and remote sensing data and carrying out quality control (Task 1). Mr. Arash Kashfi Yeganeh will be involved in collecting in-situ data, carrying out quality control, and providing the meteorological and emissions inventory (Task 1), and he will provide feedback on the updated inventory $PM_{2.5}$ concentrations (Task 3). Mr. Hadi Zanganeh Kia will be involved in collecting in-situ data and carrying out quality control, and running meteorological modeling (Task 1). Mr. Ali Mousavinezhad will be involved in collecting in-situ data and carrying out quality control, and running emissions modeling (Task 1).

2-2- Progress schedule

Task	Sep 2022	Oct 2022	Nov 2022	Dec 2022	Jan 2023	Feb 2023	Mar 2023	Apr 2023	May 2023	Jun 2023	July 2023	Aug 2023
Preparing met data	■											
Running met model (WRF)	■	■										
Evaluating met model result			■									
Preparing emissions data		■										
Running emissions model (SMOKE)		■	■									
Preparing satellite and in-situ data	■	■	■	■								
Running framework (iFDMB)				■	■	■						
Running standard CMAQ with a-priori and a-posteriori emissions							■	■	■			
Evaluating a-priori and a-posteriori NH_3concentrations									■	■		
Evaluating a-priori and a-posteriori NH_3concentrations										■	■	
Investigating $PM_{2.5}$ concentrations using updated emissions											■	
Comparing model output using a-priori emissions with those using a-posteriori emissions										■	■	

Technical Reports	■	■	■	■	■	■	■	■	■	■		
Financial Reports	■	■	■	■	■	■	■	■	■	■	■	■
Quarterly Reports		■			■			■			■	
Draft Final Report											■	
Final Report												■
AQRP Workshop												■

3- Scientific approach

3-1- Weather Research and Forecasting (WRF)

We will start the project by obtaining meteorological data for chemical transport modeling simulations. We will perform WRF simulations to obtain various parameters, including air temperature, specific humidity, surface pressure, the U/V components of wind speed, longwave/shortwave radiation flux downwards, and precipitation at 12 km spatial resolution over the Texas. Meteorological inputs for running WRF will be obtained from the North American Mesoscale Forecast System (NAM) reanalysis datasets. The NAM data has a horizontal resolution of 12-km with a 6-hour temporal resolution and generates reanalyzed data for temperature, wind, moisture soil, and dozens of other parameters.

3-2- Sparse Matrix Operator Kernel Emissions (SMOKE)

Emissions input for running the Chemical Transport Model (CTM) will be obtained from the National Emissions Inventory (NEI) (Eyth et al., 2022). The United States Environmental Protection Agency (US EPA) provides information on the emissions of pollutants in the atmosphere through the National Emissions Inventory (NEI), which is a comprehensive and detailed estimate of air emissions of criteria pollutants, criteria precursors, and hazardous air pollutants from different air emissions sources such as NEI point sources, NEI nonpoint sources, NEI onroad sources, and NEI nonroad sources. We will use the NEI modeling platform that uses NEI emissions inventory and Sparse Matrix Operator Kernel Emissions (SMOKE) to spatially and temporally allocate the emission values to modeling grids. NEI modeling platform 2017 will be used to produce emissions at 12km spatial resolution for Texas for the whole year of 2019.

3-3- Satellite

In this project, we use the Cross-track Infrared Sounder (CRIS) satellite observations to constrain the emissions. The CrIS instrument is an infrared sounder onboard the sun-synchronous satellite Suomi National Polar-orbiting Partnership (SNPP) (Shephard & Cady-Pereira, 2015) mission, launched in October 2011, with a mean local daytime overpass time of 13:30 and a mean local nighttime overpass time of 01:30. CrIS provides an across-track scanning swath width of 2,200 km and a nadir spatial resolution of 14 km (Dammers et al., 2017). For the preparation of the CrIS satellite observations for this project, we will employ a CrIS observation operator.

3-4- The evaluation of updated emissions inventory

We will evaluate adjusted emissions by the comparison of in-situ and satellite observations with concentrations modeled by a-priori emissions and a-posteriori emissions.

3-5- CMAQ

CMAQ is a chemical transport model developed and maintained by the US EPA that comprehensively predicts the most important processes affecting the chemistry of the atmosphere. Emissions from different sources such as anthropogenic, biogenic and wildfires could be represented within this model. Also processes such as advection, diffusion, and wet and dry deposition and chemical reactions are represented within this model. By using an extensive database of atmospheric chemical reactions CMAQ predicts the chemical production and loss of hundreds of pollutants to demonstrate the chemistry of the atmosphere.

3-6- iFDMB

In this project, we apply the iFDMB inverse modeling to refine the NH_3 emissions inventories implemented by Mahmoudreza (Semko) Momeni in the University of Houston Air Quality Forecasting (UHAQF) group under supervision of Dr. Yunsoo Choi. The iFDMB will progress until the normalized mean error (NME) of new emissions with respect to the emissions calculated from the last iteration is less than 1% or 2%.

3-7- RCCM

The iFDMB technique performs multiple model simulations to be converged to the final results. To reduce the computational cost, a Reduced-Complexity CMAQ Model (RCCM) is employed to simulate NH_3.

3-8- Evaluation of the updated NH_3 emissions

After adjusting the emissions, the standard CMAQ model will be run with a-priori emissions (emissions before updating) and a-posteriori emissions (updated emissions) in 2019. We will evaluate adjusted emissions by the comparison of in-situ and satellite observations with concentrations modeled by a-priori emissions and a-posteriori emissions. Over the Gulf of Mexico, we consider only NH_3 species and will compare the NH_3 vertical column density modeled using the a-posteriori and a-priori emissions with those obtained from CrIS satellite observations.

3-9- Investigation of $PM_{2.5}$ concentrations

We will explore changes in $PM_{2.5}$ concentrations after adjusting the NH_3 emissions inventory and calculating the contribution of inorganic $PM_{2.5}$ in total $PM_{2.5}$. To address this uncertainty, we will compare the NH_3, ammonium (NH_4^+), sulfate (SO_4^{-2}), and nitrate (NO_3^-) species modeled using the a-posteriori and a-priori emissions with those measured by surface stations and then we will analyze the spatial distribution of the species.

4- Model Selection

WRF-SMOKE-CMAQ modeling system is a state-of-the-art numerical method to simulate air pollution used for both regulatory and research purposes. We opt to use WRF-SMOKE-CMAQ modeling system because the UH-AQFS has already developed several inverse modeling systems to improve emissions inventories using this modeling setup. In this project we will use the iFDMB framework developed in Mahmoudreza (Semko) Momeni in the UHAQF group under supervision of Dr. Yunsoo Choi to improve NH_3 emissions using satellite data. Meteorological and emissions input for 2019 will be prepared using WRF and SMOKE for the state of Texas.

5- Model Design

5-1- iFDMB

In the iFDMB, a-priori concentrations retrieved using the CMAQ model (In this project we use RCCM to make the run faster) are used to linearize the sensitivity of the column density (Ω) to NH_3 emissions (E) at every grid point. Then, top-down emissions (E_t) are calculated at each iteration as follows (Cooper et al., 2017b; Lamsal et al., 2011):

$$E_t = E_a(1 + \frac{1}{\beta}\frac{\Omega_o - \Omega_a}{\Omega_a})$$

where E_a presents a-priori emissions from the previous iteration, Ω_o the observed column from the observation operator, Ω_a the simulated column from the observation operator, and β the initial sensitivity given as:

$$\beta = \frac{\Delta\Omega/\Omega}{\Delta E/E}$$

A perturbation of 20% to the a-priori emissions, E, is applied in each grid to determine the initial sensitivity. The iteration process is repeated until the normalized mean error (NME) of new emissions with respect to the emissions calculated from the last iteration is less than 1% or 2% (Momeni et al 2022). For this project, we will use a python-based iFDMB developed by Mahmoudreza (Semko) Momeni in the UHAQF group under supervision of Dr. Yunsoo Choi.

5-2- RCCM

The iFDMB technique requires multiple model simulations to be converged to the final results. To reduce the computational cost, a Reduced-Complexity CMAQ Model (RCCM) is applied instead of the standard CMAQ to simulate NH_3. In the RCCM, NH_3 and NH_4^+ considered as two tracer pollutants of the model and all of the chemical processes of other species are turned off (Momeni et al, 2022). The developed RCCM included dry and wet deposition, the transport of NH_3 and NH_4^+, and NH_x partitioning; the subroutine of ISORROPIA-II (Fountoukis & Nenes, 2007) in the aerosol module calculates the gas-particle partitioning of NH_3 and NH_4^+. For this project, we will employ a RCCM designed for NH_3 that was developed by Mahmoudreza (Semko) Momeni in the UHAQF group under supervision of Dr. Yunsoo Choi.

5-3- Observation Operator

As explained, in order to apply the iFDMB technique to improve NH_3 emissions, satellite data from the CRIS satellite observations will be used. Since the space of CrIS does not match the space of CMAQ and the CrIS data has the averaging kernel, for the preparation of the CrIS satellite observations, we will employ a CrIS observation operator developed by Mahmoudreza (Semko) Momeni in the UHAQF group under supervision of Dr. Yunsoo Choi. To reduce the error of applying the satellite observations, only valid pixels with quality flag values exceeding 3 or 5 will be selected.

6- Model Coding

To perform this project, we use a python-based data assimilation framework developed by Mahmoudreza (Semko) Momeni in the UHAQF group under supervision of Dr. Yunsoo Choi. This framework will be open source and is user friendly. The framework includes iFDMB approach and calculates observation operators for some satellite observations to be used in the iFDMB approach. Also, the framework can automatically download satellite data over the modeling domain to be used by related observation operator.

7- Model Evaluation

For several tasks in this project, model simulations will be conducted, and the results will be plotted against observed data to validate the meteorological and air quality simulations over Texas. The following metrics will be assessed for the comparison:

- Correlation (r) between model values and observed values:

$$r = \frac{\sum_{t=1}^{n}[(x_t - \bar{x})(y_t - \bar{y})]}{\sqrt{\sum_{t=1}^{n}(x_t - \bar{x})^2 * \sum_{t=1}^{n}(y_t - \bar{y})^2}}$$

Where, n is number of data points, x is observed values, and y is model values. Noting that over-bar “-“ is the mean of a variable.

- Index of Agreement (IOA) between model values and observed values:

$$IOA = 1 - \frac{\sum_{t=1}^{n} {e_t}^2}{\sum_{t=1}^{n}(|y_t - \bar{x}| + |x_t - \bar{x}|)^2}$$

Where, n is Number of data points, e_t is y_t-x_t, x is observed values, y is model values. Noting that over-bar “-“ is the mean of a variable.

- Root Mean Square Error (RMSE):

$$RMSE = \sqrt{\frac{1}{n}\sum_{t=1}^{n} {e_t}^2}$$

Where, n is number of data points, e_t is y_t-x_t, x is observed values, and y is model values.

- Mean Absolute Error (MAE):

$$MAE = \frac{1}{n}\sum_{t=1}^{n} |e_t|$$

Where, n is number of data points, e_t is y_t-x_t, x – observed values, and y is model values.

- Mean Bias (MB):

$$MB = \frac{1}{n}\sum_{t=1}^{n} e_t$$

Where, n is number of data points, e_t is y_t-x_t, x is observed values, and y is model values.

We will also analyze model performance through graphics such as scatter plots and time series of observed versus predicted hourly pollutant concentrations. More specifically, we will analyze how iFDMB changes NH_3 emissions, and $PM_{2.5}$ concentrations, before the update (priori) and after the update (posteriori). We will investigate $PM_{2.5}$ organic and inorganic constituents in priori and posteriori with respect to observations available.

8- 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 QA/QC purposes. This independent review will involve data visualization and discussion of qualitative and quantitative metrics.

9- Reporting

As required, monthly technical, monthly financial status, and quarterly reports as well as an abstract at project initiation and, near the end of the project, the draft final and final reports will be submitted according to the schedule below. Dr. Choi or his designee will electronically submit each report to both the AQRP project manager and the TCEQ liaisons and will follow the State of Texas accessibility requirements as set forth by the Texas State Department of Information Resources (http://aqrp.ceer.utexas.edu/). A representative from the project will present at the AQRP Workshop. Draft copies of any 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. Final project data and associated metadata will be prepared and submitted to the AQRP archive. Each deliverable and required deadline for submission are presented below.

9-1- 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: **September 1, 2022**

9-2- 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	September-October 2022	October 31, 2022
Quarterly Report #2	November 2022-January 2023	January 31, 2023
Quarterly Report #3	February-April 2023	April 30, 2023
Quarterly Report #4	May-July 2023	July 31, 2023

9-3- Monthly Technical Reports (MTRs)

Technical Reports will be submitted monthly to the Project Manager and TCEQ Liaison in Microsoft Word format using the AQRP Template found on the AQRP website.

MTR Due Dates:

Report	Period Covered	Due Date
Technical Report #1	September 1-30, 2022	October 10, 2022
Technical Report #2	October 1-31, 2022	November 10, 2022
Technical Report #3	November 1-30, 2022	December 10, 2022
Technical Report #4	December 1-31, 2022	January 15, 2023
Technical Report #5	January 1-31, 2023	February 10, 2023
Technical Report #6	February 1-28, 2023	March 10, 2023
Technical Report #7	March 1-31, 2023	April 10, 2023
Technical Report #8	April 1-30, 2023	May 10, 2023
Technical Report #9	May 1-31, 2023	June 10, 2023
Technical Report #10	June 1-30, 2023	July 10, 2023

9-4- 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 FSR Template found on the AQRP website.

FSR Due Dates:

Report	Period Covered	Due Date
Financial Report #1	September 1-30, 2022	October 10, 2022
Financial Report #2	October 1-31, 2022	November 10, 2022
Financial Report #3	November 1-30, 2022	December 10, 2022
Financial Report #4	December 1-31, 2022	January 15, 2023
Financial Report #5	January 1-31, 2023	February 10, 2023
Financial Report #6	February 1-28, 2023	March 10, 2023
Financial Report #7	March 1-31, 2023	April 10, 2023
Financial Report #8	April 1-30, 2023	May 10, 2023
Financial Report #9	May 1-31, 2023	June 10, 2023
Financial Report #10	June 1-30, 2023	July 10, 2023
Financial Report #11	July 1-31, 2023	August 10, 2023
Financial Report #12	August 1-31, 2023	August 31, 2023

9-5- 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: **July 31, 2023**

9-6- 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: **August 31, 2023**

9-7- 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 August 31, 2023. 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 **August 15, 2022**.

10- References

Cooper, M., Martin, R. v., Padmanabhan, A., & Henze, D. K. (2017). Comparing mass balance and adjoint methods for inverse modeling of nitrogen dioxide columns for global nitrogen oxide emissions. *Journal of Geophysical Research*, *122*(8), 4718–4734. https://doi.org/10.1002/2016JD025985

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Shephard, M. W., & Cady-Pereira, K. E. (2015). Cross-track Infrared Sounder (CrIS) satellite observations of tropospheric ammonia. *Atmos. Meas. Tech*, *8*, 1323–1336.

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