Quality Assurance Project Plan

Project 20 – 011
Improving Estimates of Wind-Blown Dust from Natural and Agricultural Sources

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

Prepared by

Chris Emery (Principal Investigator)
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Novato, California

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Version 4

Ramboll has prepared this QAPP following EPA guidelines for a Quality Assurance (QA) Category III Project: Research Model Development and 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, Model Selection, Model Design, Model Coding, Model Calibration, Model Verification and Evaluation, Model Documentation, Reporting, References.

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 Improving Estimates of Wind-Blown Dust from Natural and Agricultural Sources project. The Principal Investigator for the project is Chris Emery.

Electronic Approvals:

This QAPP was approved electronically on 05/22/2020 by

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

This QAPP was approved electronically on 7/17/2020 by

Vincent M. Torres
Quality Assurance Project Plan Manager, Texas Air Quality Research Program
The University of Texas at Austin

This QAPP was approved electronically on 7/17/2020 by

Chris Emery
Principal Investigator, Ramboll

QAPP Distribution List

Texas Air Quality Research Program
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Texas Commission on Environmental Quality
Barry Exum, Project Liaison

Ramboll
Chris Emery, Principal Investigator

1.0 Project Description and Objectives

Ramboll has recently developed the "WBDUST" emission model, which is an adaptation of the dust emission scheme and global soil properties compiled by Klingmueller et al. (2017). The Texas Commission on Environmental Quality's (TCEQ) visibility modeling using WBDUST in combination with the Comprehensive Air quality Model with extensions (CAMx; Ramboll, 2018) indicates a need to improve emission estimates from dust sources because the model consistently under predicts soil-derived particulate matter (PM), especially in the coarse mode, according to speciated monitoring within federally protected Class I Wilderness Areas and National Parks (Ramboll, 2019). Ramboll has also consistently noted insufficient dust emissions estimates from WBDUST for several modeling applications over regional, continental and hemispheric scales. Our implementation of minor updates to WBDUST that relax certain restrictions on the numerous criteria that must align to emit dust have resulted in limited improvements. Further improvements require refined vegetative and soil datasets and emission modeling approaches. Visibility simulations will benefit from enhanced WBD modeling and the explicit treatment of elemental species (Iron [Fe], Magnesium [Mg], Manganese [Mn], Calcium [Ca], Potassium [K], Aluminum [Al], Silicon [Si], Titanium [Ti]), which explicitly influence certain secondary PM chemistry pathways and better align with current speciated monitoring.

The CAMx WBDUST emission model provides an existing framework that will be improved in this project with updated parameterizations and enhanced, more locally specific and more temporally resolved landcover and soil data. Our project will review and evaluate current windblown dust (WBD) models, adapt alternative methods, identify/incorporate improved datasets characterizing soil types and vegetative cover, and reevaluate WBD results using CAMx to quantify performance improvements in Class I areas throughout the south-central US.

The project objectives include:

1. Review the current CAMx WBDUST algorithm with respect to methodology, soil/landcover input data, speciation, and CAMx performance against measurements;
2. Compare the CAMx WBD algorithm to techniques employed within other models (e.g., CMAQ, WRF-Chem), consider advantages and disadvantages among each, and adapt best approaches for an improved CAMx emission model for speciated WBD;
3. Review available landcover, cropland/agricultural activity, and speciation datasets to further improve characterization of WBD from the agricultural sector, and develop a methodology to process such data for direct use in the updated WBD emissions processor;
4. Document changes in CAMx performance for dust species, especially in the coarse mode, using an existing national modeling dataset.

2.0 Organization and Responsibilities

This project is being conducted by Ramboll under a grant from the Texas Air Quality Research Program (AQRP). The project Principal Investigator (PI) is Mr. Chris Emery, who will assume overall responsibility for the research and overall responsibility for quality assurance. Dr. Greg Yarwood will serve as a tchenical advisor for all tasks. Mr. Emery will be assisted by Mr. Tejas Shah, who will lead the review and development of landcover and agricultural datasets, and by Dr. Uarporn Nopmongcol, who will lead all modeling activities and performance evaluation. The personnel working on this project and their specific responsibilities are listed in Table 1.

The project will be overseen by AQRP Project Manager Dr. Elena McDonald-Buller and TCEQ Project Liaison Barry Exum. They will review the project deliverables and documentation.

Table 1. Project participants and their key responsibilities.

Participant	**Key Responsibilities**
Chris Emery	Principal investigator, responsible for providing technical guidance, contribute to model development, develop and review reports and presentations, and overall quality assurance.
Greg Yarwood	Project technical advisor
Tejas Shah	Lead review of alternative landcover and agricultural activity datasets, their processing to support the development of model-ready WBD emission estimates, dataset quality assurance, and contribute to reporting.
Uarporn Nopmoncol	Lead all modeling activities, model performance evaluation against monitoring data, modeling quality assurance, and contribute to reporting.
Fiona Jiang	Assist with developing software to process raw landcover and agricultural data to useable formats for the WBD emissions model.
Yuge Shi	Assist with developing software to process raw landcover and agricultural data to useable formats for the WBD emissions model.
Sai Sreedhar Varada	Perform emission processing for photochemical model inputs.
Chao-Jung Chien	Assist with various modeling and data analysis tasks.
Marco Rodriguez	Assist with various modeling and data analysis tasks.
Pradeepa Vennam	Assist with various modeling and data analysis tasks.
Jean Guo	Assist with various modeling and data analysis tasks.

An overall schedule of project activities by task is shown in Table 2. The schedule assumes a start date during June 2020 and end date of August 31, 2019.

Table 2. Schedule of project activities.

ID	Task	2020							2021							
		J	J	A	S	O	N	D	J	F	M	A	M	J	J	A
	Kickoff Meeting	X														
1	Review WBDUST Estimates		X	X	X											
2.1	Alternative Emission Methods				X	X	X									
2.2	Alternative Landcover Data						X	X	X							
3	Update WBDUST & Evaluation									X	X	X	X			
4	Monthly Progress Reports	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
4	Quarterly Progress Reports		X			X			X			X			X	
4	Draft Final														X	
4	Final															X
	AQRP Workshop															X

3.0 Model Selection

The existing program WBDUST will be updated in this project. Estimated dust emissions are typically estimated on an hourly basis for use in regional and global photochemical transport models ranging in spatial resolution from 1-100+ km. Like several other emission models (e.g., biogenic and nitrogen oxide [NOx] from lightning), WBDUST is designed to operate on a stand-alone basis on Linux systems. The program will not depend directly on other software platforms such as GIS applications, but will ingest gridded data generated by such applications. The program is not designed for Windows computers.

4.0 Model Design

WBDUST is based on a set of parameterizations (Klingmueller et al., 2017) that estimate wind-blown dust from emissive areas as a function of input gridded meteorological data (winds, soil moisture) for a given modeling domain and resolution, a global gridded barren land mask, global gridded leaf area index (LAI), global gridded soil clay fraction, and global gridded elemental component distributions. The global data allow for WBDUST to be applied anywhere in the world but spatial and temporal limitations in those datasets are less applicable for smaller-scale domains where local contributions from unresolved activities such as seasonal tilling play a larger role in dust emission rates. The updates will allow WDBUST to ingest more localized data from monthly to seasonal agricultural activities.

Ramboll will review the current WBDUST algorithm and tabulate key strengths/ weaknesses. Ramboll will conduct a literature review of WBD emission models employed in other modeling systems, such as the Weather Research and Forecasting model with chemistry (WRF-Chem; NCAR, 2019) and the Community Multi-scale Air Quality (CMAQ) model (EPA, 2019). Specifically, details of each methodology and sources of soil/vegetative cover and other key inputs will be compared to the current CAMx WBDUST modeling system. Key differences in methodology and input data will be noted and advantages and disadvantages of each approach will be tabulated as consistently as possible to the WBDUST review. We will conduct a literature review of scientific publications that assess each of the candidate methods in terms of performance in replicating measured dust concentrations. Based on this evaluation, we will select specific updates to the WBDUST parameterization or a full adaptation of a chosen alternative method into the WBDUST modeling system that will continue to operate using CAMx-ready meteorological input files.

Ramboll will develop a Task Technical Memorandum containing description of current WBDUST program, summary of literature review, and list of specific WBDUST updates.

Ramboll will review publicly available landuse datasets that can be adapted to improve spatial landcover characterization in the US. A leading data source is the recent US Geological Survey (USGS) 2016 National Landcover Database (NLCD) (USGS, 2019). NLCD provides a nation-wide dataset (48 conterminous states) at 30-meter resolution and contains spatial reference and descriptive data for characteristics of the land surface such as thematic class (e.g., urban, agriculture, and forest), percent impervious surface, and percent tree canopy cover. This same dataset is used in the Model of Emissions of Gases and Aerosols from Nature (MEGAN, Guenther et al., 2012), and so provides consistency between biogenic and WBD emission estimates. The 30-m resolution data will be aggregated to a national 1 km resolution database. WBDUST will be updated to alternatively read these data, map to the CAMx grid, and generate an alternative CAMx input landcover file for consistency in air quality simulations.

Correctly representing the spatial and temporal variations in surface vegetation is also important due to its various effects on dust generation including drag partitioning, local wind acceleration, near-source removal, and protective coverage. Global LAI products are available from the Moderate Resolution Imaging Spectroradiometer (MODIS) that can be used to develop high-resolution (1 km) time-varying (8-day) vegetation coverage. Ramboll will adapt this global MODIS LAI data product as an alternative input to the WBDUST model.

Agricultural tilling exposes land tracts to seasonal wind erosion, and except through the current LAI input, this type of WBD source is not well resolved temporally or spatially. We will review the National Agricultural Statistics Service (NASS) “CropScape” mapping tool (NASS, 2012) and crop calendar data. CropScape provides detailed land use data by crop type. From our review, Ramboll will develop a methodology to use these valuable sources of data in WBDUST to improve the characterization of agricultural land cover types and particularly the specific areas and times that croplands are exposed for wind erosion.

Ramboll will develop a Task Technical Memorandum describing our review of available landcover, LAI and agricultural datasets for use in WBDUST, and approaches and programs developed to ingest new datasets into the WBDUST model. The memo will document our review and evaluation of these datasets, including dataset versions and development dates, and refer to how their product quality is assessed from their sources.

5.0 Model Coding

WBDUST is written in Fortran90 following modern coding practices. All updates will continue to be Fortran90 for consistency. WBDUST will be run on workstations with Linux operating systems (the specific choice of Linux brand or distribution is not material). The computer should have a modern installation of a common Fortran compiler (Portland Group, Intel, or Gnu). WBDUST is compiled using a "makefile" script that is distributed with the source code.

Ramboll will enhance the CAMx WBDUST framework to ingest alternative landcover/vegetation, soil and/or agricultural activity datasets and to update the emission parameterization. Ramboll anticipates that alternative geographic-based datasets will be available in Geographic Information System (GIS) shapefile or various raster formats. We will develop new GIS or Python scripts as needed to prepare raw datasets in Network Common Data Form (NetCDF) input/output (I/O) structures for direct ingestion into the updated WBDUST program.

The new system will be functionally evaluated and quality-assured in an idealized testbed simulation, through a technique often referred to as code tracing, to ensure all algorithms and updates are working appropriately and giving correct results for the given input test dataset. This is the same approach used by Ramboll's CAMx developers when implementing and testing any code updates to the model. This quality-assurance step will be conducted by the lead coder and reviewed by the project manager.

6.0 Model Calibration

Ramboll will be implementing existing algorithms and parameterizations selected from the literature review based on data requirements, speed of execution, and performance against ambient measurements. It will be assumed that various coefficients and tuning parameters within the chosen functions have been calibrated by the original authors. Therefore, no additional calibration to the algorithms is anticipated once installed in WBDUST. The lead coder will conduct functional QA/QC tests as described in Section 5 to ensure the new algorithms are working correctly with the given input data. Testing will include an audit of data quality on at least 10% of the input and model output data by the emissions and modeling leads by means of code tracing and other functional tests of the program in an idealized testbed simulation to ensure all algorithms and updates are working appropriately and giving correct results for the given input test dataset.

7.0 Model Verification and Evaluation

Ramboll will generate hourly, gridded, speciated WBD emission estimates for the EPA's 2016 Modeling Platform using the new algorithms and input datasets. Additional CAMx simulations will be performed with the new dust emission estimates and model results will be compared graphically and statistically to CAMx results using the original dust estimates. In all cases, an audit of data quality will be performed on at least 10% of the input and model output data by the emissions and modeling leads. This quality assurance step will be performed graphically by plotting and reviewing input and output datasets to ensure reasonable and consistent results. Differences between original and updated WBDUST results will be tabulated; any improvements and remaining performance issues will be documented. The results of the audits of data quality will be included in the project final report.

In both cases, model results will be compared directly to 2016 speciated PM data collected at monitoring sites as part of the Interagency Monitoring of Protected Visual Environments (IMPROVE) network. Standard statistical measures such as normalized and fractional mean bias, gross error, and correlation will be calculated to quantify model-measurement agreement (Table 3). Performance statistics will be compared to model performance benchmarks recently developed by Emery et al. (2016).

Ramboll will test WBDUST sensitivity with alternative or various combination of inputs, including alternative meteorological, LAI, landcover and agricultural activity datasets and/or input variability across seasons. Results from each sensitivity will be compared and evaluated against measurements. Sensitivity will be characterized quantitatively using statistical metrics as described above.

All qualitative and quantitative evaluations results will be fully documented in the project final report. Ramboll will send the WBDUST program and attendant documentation to TCEQ for additional testing and evaluation with their visibility modeling platform.

Table 3. Definition of performance metrics for evaluating CAMx modeling.

Metric	**Definition**[1]
Mean Bias (MB)	$\frac{1}{N}\sum_{i=1}^{N}(P_i - O_i)$
Mean Error (ME)	$\frac{1}{N}\sum_{i=1}^{N}\lvert P_i - O_i\rvert$
Root Mean Squared Error (RMSE)	$\sqrt{\frac{\sum_{i=1}^{N}(P_i - O_i)^2}{N}}$
Normalized Mean Bias (NMB) (-100% to +∞)	$\frac{\sum_{i=1}^{N}(P_i - O_i)}{\sum_{i=1}^{N} O_i}$
Normalized Mean Error (NME) (0% to +∞)	$\frac{\sum_{i=1}^{N}\lvert P_i - O_i\rvert}{\sum_{i=1}^{N} O_i}$
Coefficient of Determination (r^2) (0 to 1)	$\left(\frac{\sum_{i=1}^{N}(P_i - \overline{P})(O_i - \overline{O})}{\sqrt{\sum_{i=1}^{N}(P_i - \overline{P})^2 \sum_{i=1}^{N}(O_i - \overline{O})^2}}\right)^2$

8.0 Model Documentation

Ramboll will document the WBDUST formulation, assumptions, input datasets and their sources, quality assurance review results, and model verification/evaluation results in the Task 3 technical memorandum and in the project final report. The final report will include a User's Guide including hardware and software requirements and user instructions on installation, use and input file development steps. The report will also enumerate recommendations to address remaining performance issues or the need for additional improvements.

The WBDUST source code will also include sample job scripts and attended text files that describe the program, literature references to all algorithms implemented in the model, programmer's instructions, the required and optional input datasets, and basic user instructions.

The new WBDUST modeling system and supporting datasets will be delivered to the AQRP and TCEQ along with all documentation as listed under Section 9. Ultimately, the new WBDUST program will be distributed by Ramboll from the CAMx web site (www.camx.com).

9.0 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. Mr. Yarwood 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/). Mr. Emery anticipates attending and presenting at the AQRP data 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.

Abstract: At the beginning of the project, an Abstract will be submitted to the AQRP 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 AQRP 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

Monthly Technical Reports (MTRs): Technical Reports will be submitted monthly to the AQRP 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	Friday, July 10, 2020
Technical Report #2	July 1 - 31, 2020	Monday, August 10, 2020
Technical Report #3	August 1 - 31, 2020	Thursday, September 10, 2020
Technical Report #4	September 1 - 30 2020	Friday, October 9, 2020
Technical Report #5	October 1 - 31, 2020	Tuesday, November 10, 2020
Technical Report #6	November 1 - 30, 2020	Thursday, December 10, 2020
Technical Report #7	December 1 - 31, 2020	Friday, January 8, 2021
Technical Report #8	January 1 - 31, 2021	Wednesday, February 10, 2021
Technical Report #9	February 1 - 28, 2021	Wednesday, March 10, 2021
Technical Report #10	March 1 - 31, 2021	Friday, April 9, 2021
Technical Report #11	April 1 - 30, 2021	Monday, May 10, 2021
Technical Report #12	May 1 - 31, 2021	Thursday, June 10, 2021
Technical Report #13	June 1 - 30, 2021	Friday, July 9, 2021

Financial Status Reports (FSRs): Financial Status Reports will be submitted monthly to the AQRP Grant Manager (RoseAnna Goewey) 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

Draft Final Report: A Draft Final Report will be submitted to the AQRP 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 report the results of the audits of data quality.

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.

Presentations and Publications/Posters: All data and other information developed under this project which is included in **published papers, symposia, presentations, press releases, websites and/or other publications** shall be submitted to the AQRP Project Manager and the TCEQ Liaison per the Publication/Publicity Guidelines included in Attachment G of the Subaward.

10.0 References

Klingmueller K., S. Metzger, M. Abdelkader, V.A. Karydis, G.L. Stenchikov, A. Pozzer, J. Lelieveld, 2017. Revised mineral dust emissions in the atmospheric chemistry-climate model EMAC (based on MESSy 2.52). *Geosci. Model Dev. Discuss.*, https://doi.org/10.5194/gmd-2017-160.

Emery, C., Z. Liu, A.G. Russell, M.T. Odman, G. Yarwood, N. Kumar, 2016. Recommendations on statistics and benchmarks to assess photochemical model performance, *J. Air & Waste Management Association*, http://dx.doi.org/10.1080/10962247.2016.1265027.

EPA, 2019. Community Multiscale Air Quality (CMAQ) model web page: https://www.epa.gov/cmaq.

Guenther, A. B., X. Jiang, C. L. Heald, T. Sakulyanontvittaya, T. Duhl, L. K. Emmons, and X. Wang, 2012. The Model of Emissions of Gases and Aerosols from Nature version 2.1 (MEGAN2.1): an extended and updated framework for modeling biogenic emissions, *Geosci. Model Dev*., 5(6), 1471-1492.

NASS, 2012. "CropScape-cropland data layer." USDA National Agricultural Statistics Service: Washington, DC, USA (2012).

NCAR, 2019. National Center for Atmospheric Research, WRF-Chem Modeling page: https://www2.acom.ucar.edu/wrf-chem.

Ramboll, 2018. User's Guide: Comprehensive Air quality Model with extensions, Version 6.50 (April, 2018). www.camx.com.

Ramboll, 2019. Regional haze modeling to evaluate progress in visibility in and near Texas. Draft Final Report prepared by Ramboll, Novato, CA; submitted to the Texas Commission on Environmental Quality, Austin, TX (December, 2019).

USGS, 2019. Multi-Resolution Land Characteristics Consortium Project, URL: https://www.mrlc.gov/national-land-cover-database-nlcd-2016.