QUALITY ASSURANCE PROJECT PLAN

Project No. 14-014

CONSTRAINING NO_X EMISSIONS USING SATELLITE NO_2 MEASUREMENTS OVER THE SOUTHEAST TEXAS

December 2014

PREPARED BY

University of Houston
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PREPARED FOR

Air Quality Research Program (AQRP)

QAPP Category Number: III
Type of Project: Data Evaluation; Research or Development (Modeling)

QAPP Requirements: This QAPP requires descriptions of project description and objectives; organization and responsibilities; scientific approach; quality metrics; data analysis, interpretation, and management; reporting; and references.

QAPP Requirements:

Audits of Data Quality: Cat III = 10% Required
Report of QA Findings: Required in final report

Preface

This Quality Assurance Project Plan is submitted in fulfillment of the following quality assurance project plan requirements of the grant 14-014 from the Air Quality Research Program (AQRP).

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Quality Assurance Project Plan Approval Sheet

Air Quality Research Program (AQRP)

Project Number 14-014

QAPP Title: CONSTRAINING NO_X EMISSIONS USING SATELLITE NO_2 COLUMN MEASUREMENTS OVER THE SOUTHEAST TEXAS

University: University of Houston
Date Submitted: December 18, 2014

Yunsoo Choi___________
Principal Investigator

AQRP Approval to Proceed with QAPP

This QAPP was approved electronically on January 22, 2015 by Vincent M. Torres, The University of Texas at Austin

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

This QAPP was approved electronically on January 22, 2015 by Cyril Durrenberger, The University of Texas at Austin

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Cyril Durrenberger
Quality Assurance Project Plan Officer, Texas Air Quality Research Program

Distribution List

University of Houston – Principal Investigator
Yunsoo Choi

Vincent Torres, Project Manager, Texas Air Quality Research Program
David Westenbarger, Project Liaison, Texas Commission on Environmental Quality
Cyril Durrenberger, Quality Assurance Project Plan Officer, Texas Air Quality Research Program
Chris Owen, Quality Assurance Project Plan Officer, Texas Commission on Environmental Quality
Maria Stanzione, Project Manager, Texas Air Quality Research Program

1. PROJECT DESCRIPTION AND OBJECTIVES

1.1 STUDY PURPOSE

There is a significant presence of petro-chemical facilities, power plants and vehicles in the Houston-Galveston-Brazoria (HGB) region located at southeastern Texas (SETX). The major pollutant in the region is ozone due to the abundant emissions of precursors like nitrogen oxide (NO_X) and Volatile Organic Compounds (VOCs). During the long, hot summer ozone concentrations often rise above the threshold level as stipulated in the National Ambient Air Quality Standards (NAAQS).

The concentration of petrochemical plants is in the Houston Ship Channel (HSC) area, just north of the Galveston Bay. Many of the VOC emissions from the HSC area are highly reactive and have been shown to contribute greatly to the many high ozone episodes in HGB.

Ozone production depends not only on availability of Volatile Organic Compounds (VOCs) and NO_x but also on their relative concentrations, which can be expressed as VOC/NO_x ratio. NO_x is the summation of NO (nitric oxide) and NO_2 (nitrogen dioxide). Misrepresentation of either VOCs or NO_x in an air quality model may change the VOC/NO_x ratio and may lead to inaccurate ozone predictions. In addition to ground and aircraft measurements obtained during the Deriving Information on Surface conditions from Column and Vertically Resolved Observations Relevant to Air Quality (DISCOVER-AQ) campaign, remote sensing data of NO_2 are available to compare with NO_2 values predicted with an air quality models.

Satellite data can be applied in a variety of ways to improve AQ models used to develop State Implementation Plans (SIP). Specifically, they can be used to evaluate the quality of the model-predicted pollutant concentrations and to modify model inputs, such as pollutant emissions (e.g., emissions from wildfires with fire-counts and fire radiative power data), biogenic emissions of VOCs (e.g., with photosynthetically active radiation and leaf area index data), and photolysis rates (e.g., ozone vertical column density data). As a specific example, the NASA Aura Ozone Monitoring Instrument (OMI) NO_2 vertical column density (VCD) data could be used to evaluate the simulation of NO_2, an important ozone precursor, in the Community Air Quality Model (CMAQ). Such an evaluation may reveal inaccuracies of emissions as well as deficiencies in the chemical mechanism.

We propose to perform an analysis of the archived in-situ aircraft and ground measurements, and utilize satellite measurements of NO_2 to improve the bottom-up NO_x emission inputs with an empirical top-down adjustment and study their impact on ozone predictions. In addition, accurate predictions of meteorological variables are crucial to simulate atmospheric chemistry and consequently properly simulate ozone concentrations. We will apply objective analysis (OA) for meteorological simulations to improve predictions of meteorological parameters as well as ozone predictions.

1.2 SITE AND ENVIRONMENTAL SYSTEM TO BE TESTED

In this project, the NO_2 and formaldehyde (HCHO) measurement data from DISCOVER-AQ campaign and/or remote sensing will be used to evaluate model results. The DISCOVER-AQ campaign took place in Houston-Galveston-Brazoria (HGB) in September 2013. Most of the measurement data were collected around city of Houston, ship channel, Galveston Bay and Galveston Island. Our modeling domain will cover southeast Texas (SETX) region. We will also use Continuous Ambient Monitoring Station (CAMS) data in the simulation domain to compare to the model results as additional validation.

1.3 PROJECT OBJECTIVES

Primary Objectives:

- Quantify the posteriori NO_x emissions from a few different a priori surface emissions (e.g., point, area, mobile, and soil sources) using an inverse method with satellite NO_2 columns.
- Evaluate model-simulated HCHO and isoprene concentrations using in-situ ground and/or aircraft measurements.
- Examine how the monthly averaged ratios of NO_2 /HCHO vary spatially.
- Additionally, examine how the in-situ measurement adjusted meteorology improves the meteorological and photochemical model predictions.

1.4 PROJECT TIMELINES

Start Date: January 27, 2015

End date: September 30, 2015

Executive Summary

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

Due Date: Friday, January 9, 2015

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 doc 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 Texas Commission on Environmental Quality (TCEQ).

Due Dates:

Report	Period Covered	Due Date
Quarterly Report #1	January, February 2015	Friday, February 27, 2015
Quarterly Report #2	March, April, May, 2015	Friday, May 29, 2015
Quarterly Report #3	June, July, August, 2015	Monday, August 31, 2015
Quarterly Report #4	September, October, November, 2015	Monday, November 30, 2015

Technical Reports

Technical Reports will be submitted monthly to the Project Manager and TCEQ Liaison as a Word doc using the AQRP FY14-15 MTR Template found on the AQRP website.

Due Dates:

Report	Period Covered	Due Date
Technical Report #1	Project Start – February 28, 2015	Monday, March 9, 2015
Technical Report #2	March 1 - 31, 2015	Wednesday, April 8, 2015
Technical Report #3	April 1 - 28, 2015	Friday, May 8, 2015
Technical Report #4	May 1 - 31, 2015	Monday, June 8, 2015
Technical Report #5	June 1 - 30, 2015	Wednesday, July 8, 2015
Technical Report #6	July 1 - 31, 2015	Monday, August 10, 2015
Technical Report #7	August 1 - 31, 2015	Tuesday, September 8, 2015

Financial Status Reports

Financial Status Reports will be submitted monthly to the AQRP Grant Manager (Maria Stanzione) by each institution on the project using the AQRP FY14-15 FSR Template found on the AQRP website.

Due Dates:

Report	Period Covered	Due Date
FSR #1	Project Start – February 28, 2015	Monday, March 16, 2015
FSR #2	March 1 - 31, 2015	Wednesday, April 15, 2015
FSR #3	April 1 - 28, 2015	Friday, May 15, 2015
FSR #4	May 1 - 31, 2015	Monday, June 15, 2015
FSR #5	June 1 - 30, 2015	Wednesday, July 15, 2015
FSR #6	July 1 - 31, 2015	Monday, August 17, 2015
FSR #7	August 1 - 31, 2015	Tuesday, September 15, 2015
FSR #8	September 1 - 30, 2015	Thursday, October 15, 2015
FSR #9	Final FSR	Monday, November 16, 2015

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.

Due Date: Tuesday, August 18, 2015

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.

Due Date: Wednesday, September 30, 2015

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 June 2015.

2. PROJECT ORGANIZATION

2.1 KEY POINTS OF CONTACT

- University of Houston
  - Yunsoo Choi – Principal Investigator
- AQRP
  - Mr. Vincent Torres, Project Manager

2.2 QA MANAGER

Dr. Xiangshang Li, Research Scientist,

Department of Earth and Atmospheric Sciences, University of Houston

2.3 PROJECT PARTICIPANTS AND RESPONSIBILITIES

2.3.1 Air Quality Research Program

AQRP Project Manager: Mr. Vincent Torres
AQRP Quality Assurance Project Plan Officer: Dr. Cyril Durrenberger

2.3.2 University of Houston

Overall project coordination [Yunsoo Choi]

- Coordinates overall contract, budget and planning issues

Modeling research activities [Yunsoo Choi]

- Supervises NO_x emission establishment from inverse modeling, Weather and Research Forecasting (WRF) - Sparse Matrix Operator Kernel Emissions (SMOKE) -CMAQ modeling, and the analysis of model results
- Manages personnel involved in modeling work
- Coordinates the validation and modeling according to the QAPP requirements
- Leads scientific exploitation
- Contributes to reports and journal articles

3. EXPERIMENTAL APPROACH

This project does not involve any experiments although it will use measurements which have been through rigorous quality checking.

Using satellite data entails a good understanding of the data, such as what do the measurements stand for, the spatial resolution, time latency, level of processing, spectral uncertainties, vertical column density (VCD) creation uncertainties etc. The PI and another team member have extensive experiences working with remote sensing, including satellite data.

NASA OMI tropospheric NO_2 (Level 2, V2.1) will be used for this project. NASA OMI product is more consistent and has been through validation studies (e.g., Bucsela et al., 2013). For OMI, the crossing of the equator occurs at 13:45 local time. The size of the ground footprint varies across the swath from 13×24 km^2 at nadir (direct from above) to ~40×160 km^2 for the edge of the orbit due to the optical aberrations and asymmetric alignment (i.e., panoramic effect). The uncertainties of the product vary from location to location and under different meteorological conditions. The overall error on the tropospheric vertical column density is <30% under clear-sky conditions and typical polluted conditions (>10^{15} molecules cm^{-2}) (Bucsela et al., 2013).

DISCOVER-AQ aircraft measurements are available online for the National Oceanic and Atmospheric Administration (NOAA) aircraft P-3B, part of the rich datasets collected during DISCOVER-AQ campaign. The latest version of P-3B data have over 100 parameters, merged from measurements from a number of instruments on board. The data files are dated October 2014. There are 10 days flight data available during the DISCOVER-AQ campaign period.

Surface observational data consist of regular measurements from CAMS, operated by the Texas Commission on Environmental Quality (TCEQ). The CAMS measurement network collects real-time meteorology data and air pollution concentration data. The measured parameters differ from station to station. The station density at southeast Texas is relatively high. The number of sites having meteorological, ozone and NO_x measurements are 63, 52 and 30, respectively, in the 4-km domain during DISCOVER-AQ time period.

All above observations are obtained from well established agencies.

4. SAMPLING PROCEDURES

This project focuses on the modeling and analysis. How sampling or measurements are conducted are not within the scope of study.

5. TESTING AND MEASUREMENT PROTOCOLS

Not in the scope of this study.

6. QA/QC CHECKS

This project does not involve any QA/QC checks on measurements. The measurement data used in this project are from reliable sources and have been through QA/QC checks before they were made public.

7. QUALITY ASSURANCE FOR THE NUMERICAL MODELING

7.1 QUALITY OBJECTIVES

The quality objectives of this project are to ensure that the 1) measurement data are correctly retrieved, interpreted and their uncertainties clearly documented, 2) modeling practices will be reliable in activities such as: (a) installing and testing the necessary modeling components; (b) conducting meteorological and air quality simulations; (c) evaluating and analyzing the model results with measurements and (d) supporting EPA's Community Modeling and Analysis System (CMAS).

Since we have experience in modeling and are familiar with model behavior, we should be able to detect any abnormality during the upcoming modeling study. We have tools to check the each model's output and can ensure only valid output are passed to the next stage. For each work assignment will be developed as a cooperative effort between the PI and personnel responsible for the research tasks.

To assess the model output, the results will be plotted against available observed data and statistics will be calculated. The general steps are 1) Extract model data using tools in section 7.6 2) Pre-process raw in-situ or remote sensing data 3) Compare model predictions with observations 4) Create graphics to visualize model and observation data using tools in section 7.6 5) Calculate statistics using metrics in section 7.3.

Quality assurance of meteorological and AQM simulation results will be performed by evaluating modeled data against measured values using available observed air quality measurements. This will be performed in accordance with EPA guidelines regarding model evaluation (available at http://www.epa.gov/crem/library/cred_guidance_0309.pdf).

The specific modeling quality assurance activities are described below for the following three areas:

<u>Model input/output</u>

The input data associated with the modeling study are either collected or processed by various agencies such as National Center for Environmental Prediction (NCEP), NOAA, and TCEQ etc. Normally the data have been through QA/QC checks within the agencies and considered very reliable. CMAQ simulation results will be evaluated with the Continuous Air Monitoring Station (CAMS) data, aircraft data from DISCOVER-AQ, and satellite data from

OMI. During evaluation process, we first match the model output to the observation data as described in the “Scope of Work” document. Next we plot time series and spatial contours wherever appropriate to visually examine the data. Finally, we will compute statistics, monthly or daily wherever proper, to check how model and observation match. The statistics include correlation coefficient, index of agreement, biases, mean absolute error, etc. as described in section 7.3.

Modeling codes

This project does not involve new code developments as we simply apply the latest models to simulate the chemistry at SE Texas. No attempts will be directed to modify the source code. Although there are codes written in-house for post-processing and analyses, most of them have been well tested before. One example is the Visual Basic (VB) and Interactive Data Language (IDL) codes used for extracting model output and generating matching model data points corresponding to the aircraft measurements. The code has been repetitively used in previous model/aircraft data comparison studies.

Reconciliation with User Requirements

The input data are either measured by our group or gathered through reliable sources. These observation data supposedly have passed strict QA/QC checks. Output data in every step will be checked to ensure the simulations are performed correctly. In the case of suspected output, an investigation will be carried out to determine the causes - either modeling errors or inadequate input data. Then, after the corrective actions are taken the problematic process will be re-done. UH will provide data from any stage of modeling as requested by AQRP for quality assurance.

7.2 MODELING PROTOCOLS

For emission processing, we will use the SMOKE model. For meteorological simulations, we will utilize the WRF model and for air quality, we will employ CMAQ.

Case selection and episode description

Air quality episodes are selected from the DISCOVER-AQ campaign period. There are a total of 12 P3-B and 14 B200 aircraft flights throughout September 2013. Therefore, we will simulate the whole September 2013, i.e., 09-01 to 09-30.

Modeling domain

We expect that the CMAQ modeling domain will be, 150×134 cells at 12-km, and 84×66 cells at 4-km domains, respectively. The WRF domains are slightly larger as seen in Figure 7.1.

Both WRF and CMAQ share the same vertical structure since no layer collapsing has been employed in Meteorology-Chemistry Interface Processor (MCIP). The vertical structure is listed in Table 7.1.

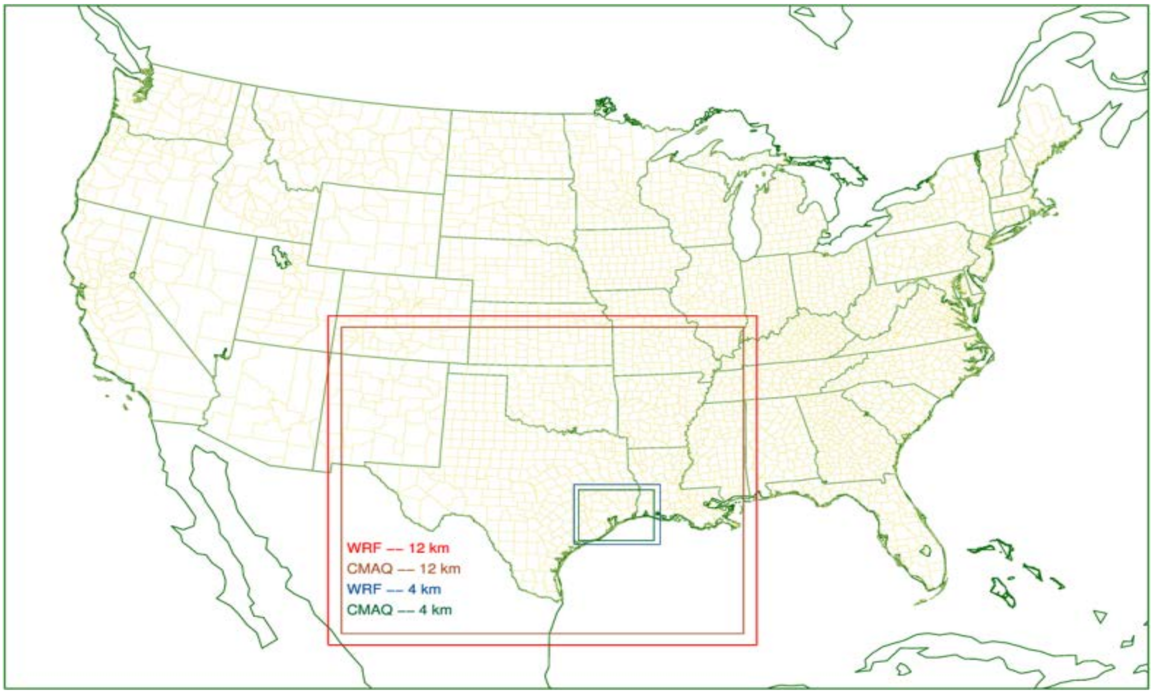

Figure 7.1: WRF (thick lines) and CMAQ (thin lines) used for the UH Air Quality Forecasting (AQF) System. There are two domains: the 12-km Texas domain and the 4-km Houston-Galveston-Brazoria (HGB) domain.

CMAQ and corresponding WRF vertical layer structures are presented in the following table:

Table 7.1. Vertical layer structures of WRF and CMAQ used for the modeling.

Layer	AGL (m)	Layer	AGL (m)
1	32.4	15	1517.8
2	81.2	16	1751.4
3	163.1	17	1990
4	245.9	18	2233.9
5	329.5	19	2534.7
6	413.7	20	3164.8
7	498.4	21	4193.1
8	583.8	22	5415.3
9	669.7	23	6964.2
10	756.2	24	9083.3
11	887.2	25	11444.6
12	1019.6	26	14549.2
13	1153.4	27	16540.7
14	1288.8		

Emissions Inventory

Model-ready emissions are to be prepared using the Sparse Matrix Operator Kernel Emissions (SMOKE) model. The 2011 National Emission Inventory (NEI) generated by the Environmental Protection Agency (EPA) is used to estimate hourly emission rates from anthropogenic sources for the continental U.S. and South East domains. In addition, emissions from natural sources were estimated with Biogenic Emissions Inventory System (BEIS3). For the part of the Mexico in our 12-km domain, US NEI2011 contains the latest Mexico inventories. If NEI2011 is used, the Mexico emissions will be automatically included.

Meteorological model set up

WRF will be our meteorological model. The physics options are shown in table 7.2 below. The analysis input will be North American Regional Reanalysis (NARR) dataset. The NARR data are based on an Eta 221 grid at 29 pressure levels. Its horizontal resolution is 32-km and the frequency is 3-hourly. The initial and boundary conditions will be generated from the NCEP NARR input by WRF model.

Observational nudging is regarded as a low-cost and effective method in improving meteorological model performance, but it requires additional observational data. In this study, we acquire the input observation data and generating files in little_r format using UH in-house developed codes. Observational data come from the Meteorological Assimilation Data Ingest System (MADIS) and Continuous Ambient Monitoring Station (CAMS). MADIS is a National Oceanic and Atmospheric Administration (NOAA) program that collects, integrates, performs quality checks, and distributes observations from NOAA and non-NOAA organizations. The four MADIS datasets used for the obs-nudging are NOAA Profiler Network (NPN), Cooperative Agency Profilers (CAP), Aviation Routine Weather Report (METAR) and NOAA Radiosonde (RAOB). CAMS is a surface based monitor network measuring air pollutants, meteorological data, and other parameters. It is maintained by Texas Commission on Environmental Quality (TCEQ).

Table 7.2. WRF physics options to be used

WRF Version	V3.6.1, latest
Microphysics	Lin et al. Scheme
Long-wave Radiation	Rapid Radiative Transfer Model for GCMs (RRTMG)
Short-wave Radiation	New Goddard scheme
Surface Layer Option	Monin-Obukhov with Carslon-Boland viscous sublayer scheme
Land-Surface Option	Unified Noah LSM (Land Surface Model)
Urban Physics	None
Boundary Layer Scheme	Yonsei University (YSU)
Cumulus Cloud Option	Kain-Fritsch
Four Dimensional Data Assimilation	Grid and observation-nudging

Photochemical model setup

i. Domain setup

We expect that the CMAQ modeling domain will be, 150×134 cells at 12-km, and 84×66 cells at 4-km domains, respectively.

The CMAQ domains are also shown in Figure 1, as brown and green boxes.

ii. Emission processing

Model-ready emissions are to be prepared using the Sparse Matrix Operator Kernel Emissions (SMOKE) model. For emission inventory sources other than mobile sources, we will use the 2011 National Emission Inventory (NEI2011) generated by the Environmental Protection Agency (EPA) or latest Texas Emission Inventory (TEI) if either is officially released and adapted to CMAQ. Emissions from natural sources were estimated with BEIS3. The mobile emissions were processed with 2014 Motor Vehicle Emission Simulator (MOVES) using an updated inventory.

There have been several significant changes made in NEI2011. Especially, on-road mobile emissions have been updated from MOVES2011 to MOVES2014. To support these changes in MOVES2014, the UH forecasting system needs to update the current SMOKE system to the latest SMOKE version 3.6 released in November 2014. Because of the new Source Category Codes (SCC) and activity input data updates, proper evaluation processes are required to prepare accurate emissions input files for CMAQ modeling system.

iii. Generating meteorological input using MCIP

Meteorological input for CMAQ will be processed using the UH-modified MCIP with the WRF output. The UH-modified MCIP corrected a few bugs such as a bug in layer collapsing and has minor enhancements such as improved mass-conservation formulation over the default MCIP. Traditionally, UH has contributed to the EPA MCIP code development.

iv. Proposed major CMAQ configurations

Proposed major CMAQ configurations are shown in Table 7.3. All of these options have been tested by our group.

Table 7.3 Major CMAQ options

CMAQ version	V5.0.1, latest is v5.0.2
Chemical Mechanism	**Carbon-Bond version 5 (CB05) gas-phase mechanism** with active chlorine chemistry, updated toluene mechanism, fifth-generation CMAQ aerosol mechanism with sea salt, aqueous/cloud chemistry
Lightning NOx emission	Included by using inline code
Horizontal advection	Yamartino Scheme (YAMO)
Vertical advection	WRF omega formula
Horizontal mixing/diffusion	Multiscale (multiscale)
Vertical mixing/diffusion	Asymmetric Convective Model version 2 (acm2)
Chemistry solver	Euler Backward Iterative (EBI) optimized for the Carbon Bond-05 mechanism
Aerosol	Aerosol module version 5 (AERO5) for sea salt and thermodynamics
Cloud Option	Asymmetric Convective Model (ACM)
Initial Condition (IC) / Boundary Condition (BC)	Default static profiles

7.3 MODEL PERFORMANCE EVALUATION

For several tasks in this project, model simulations will be performed and the results will be plotted against observed data to validate the NO_x emissions in southeast Texas. Additionally, we will validate model results at surface level through CAMS observations.

The following standard statistics will be calculated for the comparison:

1) Correlation (r) between model values and observed values

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

n – number of data points, x – observed values, y - model values, over-bar - mean

2) Index of Agreement (IOA) between model values and observed values

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

n – number of data points, $e_t = y_t - x_t$, x – observed values, y - model values, over-bar - mean

3) Root Mean Square Error (RMSE)

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

n – number of data points, $e_t = y_t - x_t$, x – observed values, y - model values

4) Mean Absolute Error (MAE)

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

n – number of data points, $e_t = y_t - x_t$, x – observed values, y - model values

5) Mean Bias (MB)

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

n – number of data points, $e_t = y_t - x_t$, x – observed values, y - model values

It is also possible to analyze the models' performance through graphics, such as scatter plots and time series of observed versus predicted hourly pollutant concentrations.

7.4 TRAINING

This project requires staff scientists with experience in remote sensing, data processing, air quality modeling and model development.

For the project, the project personnel are experienced researchers who have either the required expertise or the ability to acquire necessary skills. Base on time/cost restraint, we will determine the necessity of the attendance of certain training workshops, such as; NCAR WRF Workshop, EPA's Emissions Workshops, and the Models-3 CMAS workshop.

7.5 MODEL OUTPUT ARCHIVE

We will rely on a powerful Linux server with over 100 TB data storage. When these are filled up, they can be physically archived away for offline storage and new batch of replacements will be installed. Offline storages will be labeled and cataloged. We will add storage to the server when necessary to support the archiving and analyzing need.

7.6 TOOLS VALIDATING MODEL OUTPUT

Tools used for extracting data:

1. IDL programs extracting WRF, MCIP and CMAQ data
2. Visual Basic (VB) programs extracting WRF, MCIP and CMAQ data are:
   - 1A_Extract_CMAQ_MCIP_3D_Data, (example shown below)
   - 1D_Extract_MCIP_2D
   - 1E_Extract_WRF_3D
   - 1F_Extract_WRF_2D

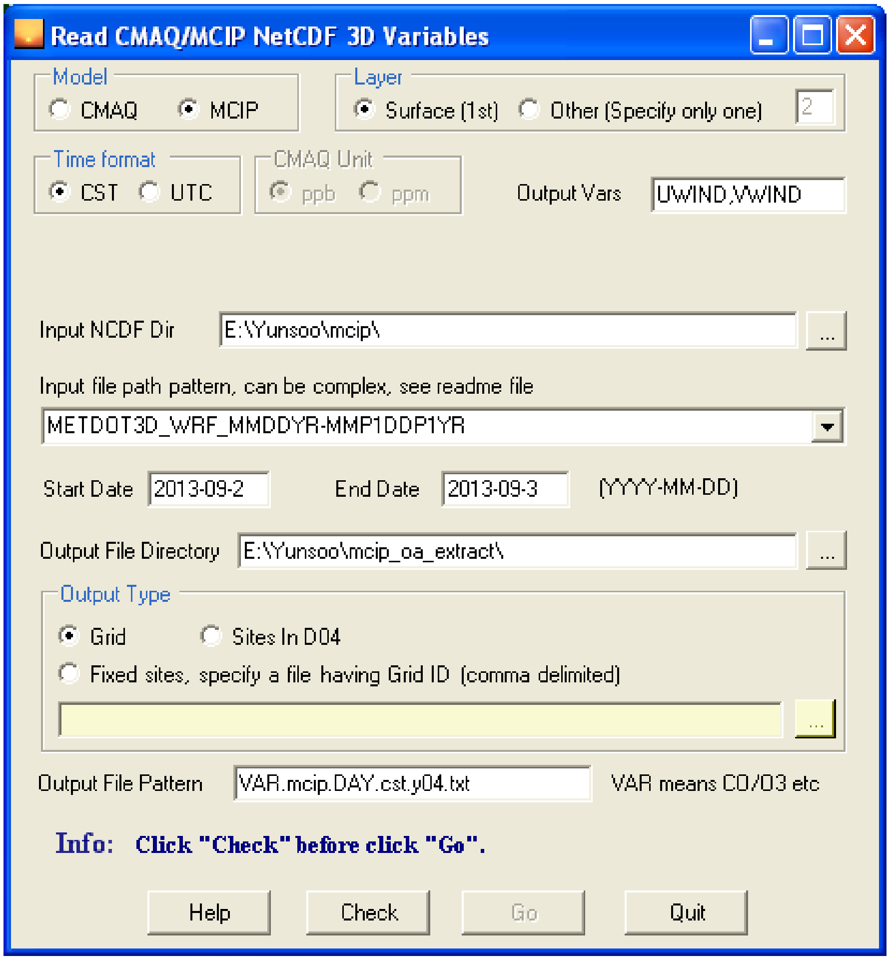

Figure 7.2. VB program extracting MCIP and CMAQ 3-Dimensional data

Tools visualizing both model and observation data:

We have VB programs for plotting WRF, MCIP and CMAQ output:

- Plotting spatial wind vectors
- Plotting spatial temperature contours
- Plotting O_3, NO_2, NO, CO, HCHO spatial contours, shown below
- Plotting temperature, O_3, NO_2 concentration vertical profiles

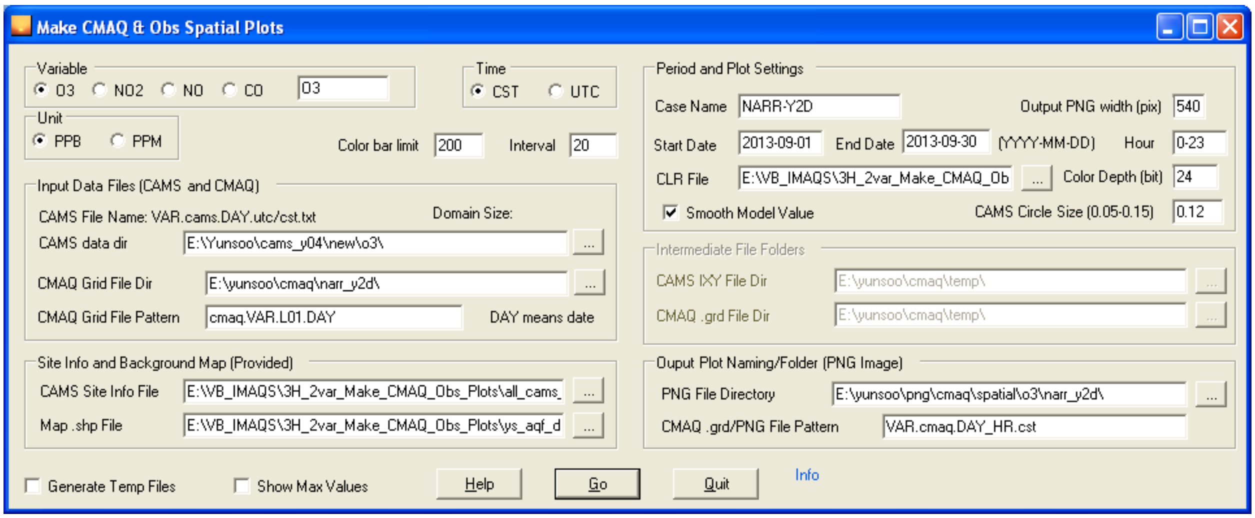

Figure 7.3. VB program plotting CMAQ output and observation spatial contour plots

A combined ozone spatial contour and wind spatial vector plot is shown below.

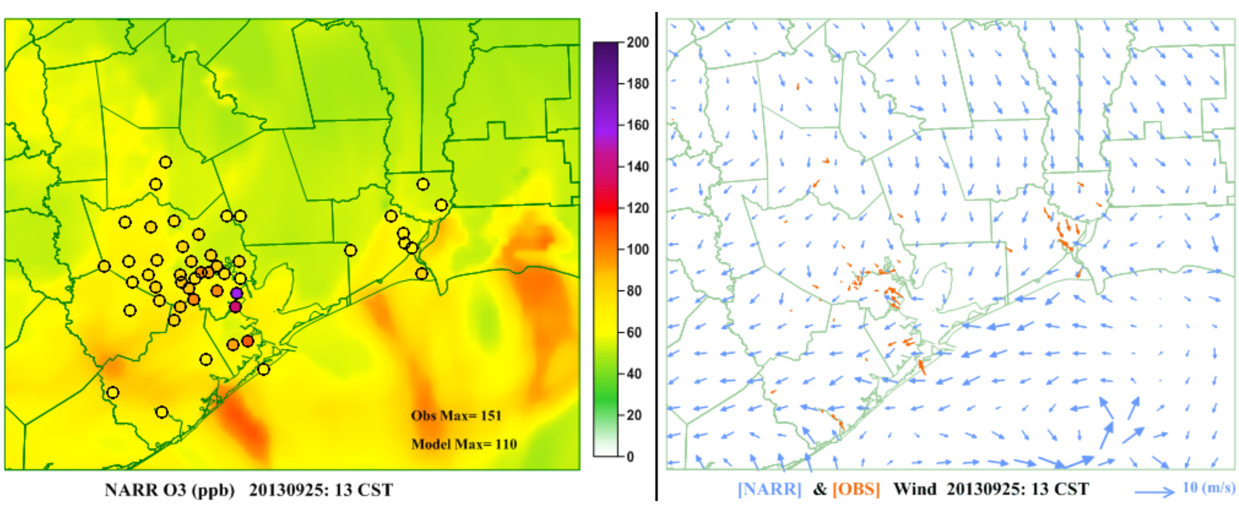

Figure 7.4. Spatial ozone contour and wind vector plot, both model and observation are shown

8. DATA STORAGE, REPORTING

8.1 DATA STORAGE

A large amount data will be generated from this project. Model data and observation data will be archived at our server, which has over 100 TB storage. In addition, two backups of all data will be made using external hard drives. The data will be stored for 5-years. The data will be sent to AQRP if requested.

8.2 REPORTING REQUIREMENTS

Records produced by this project will consist of data files in several stages of modeling. Model input and output inventory will be recorded. Progress reports on modeling and analysis will be submitted as requested.

8.3 DELIVERABLES

A final report that summarizes the project and results will be delivered to AQRP.

9. AUDITS OF DATA QUALITY

9.1 AUDIT PERSONELL

Dr. Xiangshang Li, research scientist, University of Houston

9.2 DATA TO BE AUDITED

Model simulation period covers 30 days. We plan to audit 10% data, i.e., a 3-day period.

The ozone concentration reached maximum in HGB on September 25, 2013. We plan to audit 3 days: from 09/24 to 09/26. All the model input files and output files during the 3-day period will be examined.

9.3 AUDIT PROCEDURES

These include the WRF input, which are NARR files, and WRF output which are "wrfout" files. Important parameters such as wind and temperature simulations will be plotted to see if they are reasonable. The inputs for CMAQ are emission files and MCIP output. Again, important parameters such as NO_2 emissions will be plotted. Important output parameters such as O_3, HCHO, NO_2 and NO will be plotted.

For observation data (including remote sensing), model and observation comparison plots will be created and statistical evaluation (see section 7.3) for the 3-day period will be performed.

The results of audit will be included in the final report.

10. REFERENCES

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