QUALITY ASSURANCE PROJECT PLAN

AQRP Project 17-039

Use of Satellite Data to Improve Specifications of Land Surface Parameters

Prepared For

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

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Project Type:

University of Alabama in Huntsville has prepared this QAPP following EPA guidelines for a Quality Assurance (QA) Category III Project: Secondary Data Project and Research or Development (Modeling). It is submitted to the Texas Air Quality Research Program (AQRP) as required in the Work Plan requirements.

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

QA Requirements

Technical Systems Audits: Not Required for the Project
Audits of Data Quality: Cat III = 10% Required
Report of QA findings: Required in final report

Approvals Sheet

This document is a Category III Quality Assurance Project Plan for the ***Use of Satellite Data to Improve Specifications of Land Surface Parameters.*** The Principal Investigator for the project is Richard McNider and Co-PI is Arastoo Pour Biazar.

Electronic Approvals:

This QAPP was approved electronically on 10/18/2016 by Elena McDonald-Buller, The University of Texas at Austin.

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This QAPP was approved electronically on 10/30/2016 by Vincent M. Torres, The University of Texas at Austin.

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This QAPP was approved electronically on 10/28/2016 by Richard T. McNider, The University of Alabama in Huntsville.

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List of Acronyms

AQRP	Texas Air Quality Research Program
ARM	Atmospheric Radiation Measurement
BDSNP	Berkeley-Dalhousie Soil NOx Parameterization
BVOC	Biogenic Volatile Organic Compound
CAMx	Comprehensive Air Quality Model with Extensions
CMAQ	Community Multi-Scale Air Quality model
DISCOVER-AQ	Deriving Information on Surface Conditions from Column and Vertically Resolved Observations Relevant to Air Quality.
GOES	Geostationary Operational Environmental Satellite
GPGS	GOES Product Generation System
IR	Infrared
LU/LC	Land Use/Land Cover
MODIS	Moderate Resolution Imaging Spectroradiometer
MPI	Message Passing Interface
MSFC	Marshall Space Flight Center
NASA	National Aeronautics and Space Administration
PI	Principal Investigator
PM	Particulate Matter
SCAN	Soil Climate Analysis Network
SMOKE	Sparse Matrix Operator Kernel Emissions model
SPoRT	Short-term Prediction Research and Transition Center
SURFRAD	Surface Radiation Network
TCEQ	Texas Commission on Environmental Quality
UMD	University of Maryland
USCRN	U.S. Climate Reference Network
WRF	Weather Research and Forecasting (WRF) model

1 PROJECT DESCRIPTION AND OBJECTIVES

1.1 Purpose of Study

Description: It is the purpose of this project to continue a process to evaluate and improve the performance of the land surface models used in WRF by the use of satellite skin temperatures to better specify physical parameters associated with land use classes. Improved temperature performance impacts biogenic emissions, thermal decomposition (chemical chain lengths and slopes of ozone/NOy curves) and thermally driven winds. Also, land surface parameters control surface deposition, which impacts the efficacy of long-range transport. Physical parameters such as heat capacity, thermal resistance, roughness, surface moisture availability, albedo etc. associated with a land use class are actually used in the land surface model. Many of the land use class associated parameters such as surface moisture availability are dynamic and ill-observed depending on antecedent precipitation and evaporation, soil transport, the phenological state of the vegetation, irrigation applications etc. Other parameters such as heat capacity, thermal resistance or deep soil temperature are not only difficult to observe they are often unknowable *a priori*. Despite the difficulty in specifying these parameters they are incredibly important to model predictions of turbulence, temperature, boundary layer heights and winds.

This proposal is directed toward the Meteorology and Air Quality Modeling and Biogenic Emissions Priority. Biogenic emissions are highly sensitive to temperature. Improvement in temperature predictions in conjunction with improved radiation inputs into a biogenic emission model (MEGAN or BEIS) should increase the quality of biogenic emissions. The project is responsive to three areas in the Meteorology and Air Quality Modeling Priority- (1) boundary layer performance can impact local circulations driven by thermal gradients and the strength of low level jets is controlled by nighttime surface cooling rates; (2) boundary layers can impact clouds both boundary layer topped cumulus and clouds in sea breeze convergence zones; and (3) dry deposition of ozone and nitrogen species is often controlled by stomatal uptake which depends on soil moisture.

This project will continue and expand activities under a 2015 funded AQRP project using satellite observed skin temperatures. That project was a late selected reduced scope project. Despite some initial issues with a NOAA skin temperature data set, the project ended up showing improvement in model performance for skin temperatures and in wind performance. However, the improvements were not as large as in previous uses of skin temperature data. Part of this may be due to following the Pleim-Xiu air temperature approach in the project, in which absolute differences between model and observed skin temperatures were used rather than skin temperature tendencies. Differences between the model and satellite skin temperatures not related to the boundary layer parameters such as emissivity or atmospheric correction in the satellite product might be an issue. Under this project, skin temperature tendencies will be tested instead, which avoids such problems. The Deriving Information on Surface Conditions from Column and Vertically Resolved Observations Relevant to Air Quality (DISCOVER-AQ) period of 2013 was an unusually cloudy and windy period over most of the Eastern U.S. and not characteristic of the conditions usually associated with ozone episodes in Texas. While significant effort went into QA for the skin temperature data set, cloud contamination in the skin temperatures may still be an issue. Also, in consultation with TCEQ additional periods such as TEXAQS 2006 or the 2012 SIP period will be examined. Finally, the work on the previous project included emphasis on the large 12-km domain. Under, this proposed activity a greater emphasis will be given to fine scale model performance around Houston and Dallas. Particular attention will be given to wind changes due to changes in boundary layer parameters including changes in sea breezes and low level jets.

1.2 Project Objectives

Objectives: Under this project we intend to build on the results of last year's investigation and carry out additional analyses on the impact of the improved land surface model on other model attributes such as wind performance and boundary layer heights. We will carry out additional comparisons with special aircraft observations under the DISCOVER-AQ period. Also, we will continue to refine the techniques for assimilating the satellite data including testing the use of skin temperature tendencies and by adjusting the surface heat capacity. An additional satellite product MODIS Greenness (Case et al. 2014) will be employed. A new calibrated satellite insolation and satellite albedo product will be tested.
The following are listings of sub-objectives for the project. Task descriptions associated with these objectives are given in section 4.0 below.

1. In the present project there will be a focus on small-scale performance around Houston and Dallas and other metrics besides temperature such as wind performance.
2. The use of skin temperature tendencies will be explored rather than absolute value of skin temperature to improve model performance.
3. Adjustments in heat capacity will also be tested for improving model performance.
4. Impact of new satellite derived vegetative fraction to replace the USGS values in WRF will be tested.
5. A new tool for investigating sensitivity of land surface model components will be employed.
6. Impact of new satellite derived insolation and albedo will be tested.
7. An additional model evaluation period will be selected and satellite techniques will be tested.

2 PROJECT ORGANIZATION AND RESPONSIBILITIES

2.1 Responsibilities of Project Participants

The University of Alabama-Huntsville (UAH) will conduct this study under a grant from the Texas Air Quality Research Program (AQRP). The key personnel working on this project and their specific responsibilities are listed below.

PI, Richard T. McNider , University of Alabama in Huntsville, mcnider@nsstc.uah.edu
Responsible for overall project including oversight of QAPP.

Co-PI Arastoo Pour-Biazar, University of Alabama in Huntsville, biazar@nsstc.uah.edu
Responsible for developing and following QAPP. Dr. Pour-Biazar is also responsible for project

direction and schedule including selecting test periods and strategies for model testing and improvement.

Yuling Wu, Research Scientist, wuy@nsstc.uah.edu Responsible for data quality, audits of satellite data, satellite data evaluation, and modeling tasks such as calculating model performance statistics against satellite data. She will also be responsible for the skin temperature data sets and quality assurance.

Kevin Doty, Research Scientists, kevin.doty@nsstc.uah.edu Responsible for over-all model development and testing activities. Including the code changes for the Pleim-Xiu scheme and for over-all evaluation of the model against NWS data.

Elena McDonald-Buller will serve as AQRP Project Manager and Bright Dornblaser as TCEQ Liaison for the project. Vince Torres will serve as the AQRP Quality Assurance Project Plan Manager.

Table 1. Key project participants and their responsibilities.

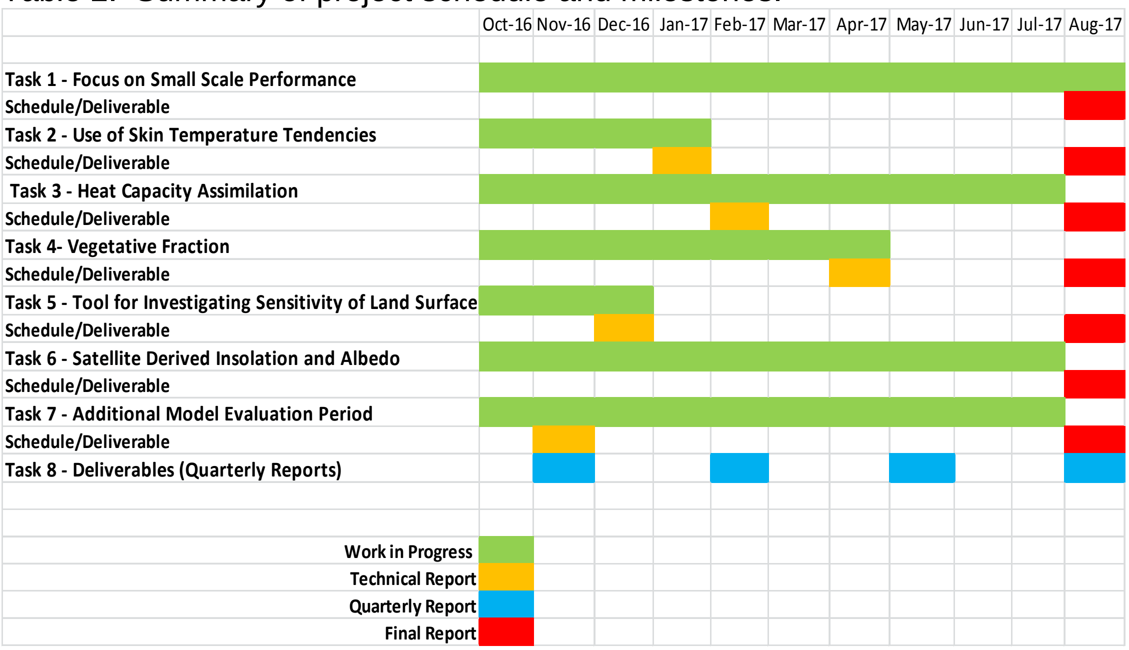
Participant	Organization	Project Responsibility
Richard T. McNider	UAH	Responsible for overall project management including oversight of QAPP.
Arastoo Pour Biazar	UAH	Responsible for identifying case studies and model evaluation.
Yuling Wu	UAH	Responsible for data quality and audits of satellite data.
Kevin Doty	UAH	Responsible for model data QAPP.

In addition, we will be working closely with AQRP scientists and TCEQ staff to ensure the successful transition of data, models, and tools for their regulatory activities. TCEQ staff will participate in the review of the technical documentation generated during this project.

2.2 Project Schedule and Deliverables

The project is divided into seven major tasks: (1) Small scale performance; (2) Use of skin temperature tendencies; (3) Heat capacity assimilation; (4) Vegetative fraction specification; (5) Investigating sensitivity of land surface; (6) Satellite-derived insolation and albedo; and (7) Additional model evaluation. The table below shows the overall schedule for completion of major tasks in this project including interim milestones and deliverables. A more detailed schedule for deliverables, including responsibilities and timeline for interim reports is presented in section 8 under "Project Deliverables" sub-section. While the final report will include a comprehensive report of the project and findings from all of the activities under this project, we will be including a more extensive technical report detailing the progress and findings of each task as an appendix to appropriate monthly or quarterly reports. The delivery dates for these technical reports (in addition to monthly reports indicated under section 8) are marked as yellow in Table 2. For example, a technical report detailing the results from task 2 will be included as an appendix to the January 2017 monthly report. Similarly, the technical report for task 3 will be included in February monthly report and for task 4 in April. Note that the technical reports listed in Table 2 as deliverables are summation reports on the topic and are not the same as the monthly technical report (MTR) required by AQRP. The MTRs will be provided monthly per the AQRP schedule as indicated in section 8.

Table 2. Summary of project schedule and milestones.



3 MODEL SELECTION: FUNCTIONAL REQUIREMENTS

3.1 Model: Required Functions

The functional requirements of the model to be used in this project are its relevance and viability for science investigation as well as SIP applications. The primary model to be employed in this investigation is the WRF Model http://www2.mmm.ucar.edu/wrf/users/. It has become a standard tool for creating the physical atmosphere in air quality studies. It is the model that has been used by TCEQ in both science investigations and in recent SIP applications.

The model chosen for this study must have a modular structure coupling the land-surface physics to the atmospheric boundary layer parameterization. In particular, the model must include Pleim-Xiu surface layer and PBL options. Since WRF model satisfies these requirements, it was chosen for this study.

3.2 Attributes: Functionality, Interfacing, Performance, and Constraints

The major attributes in the WRF model are the land surface model and the Planetary Boundary Layer (PBL) parameterization. This project will primarily work with the Pleim-Xiu surface layer and PBL options. However, the NOAH land surface model may also be employed for testing and evaluation.

It is planned to use the WRF 3.8 version in this investigation as compared to the 3.6 version in the previous activity.

The WRF model is a community research and operational model jointly sponsored by NCAR and the NWS. It has become the prime weather model used by the U.S. EPA research activities and NOAA air quality forecast system. It is a deterministic model depending on initial states of the atmosphere and boundary conditions. In the present activity, these initial states will be provided by NOAA reanalysis products.

The model domain will cover most all the continental U.S. at a grid resolution of 12km. A smaller domain of 4km will also likely be employed over Texas.

We expect to run all codes and scripts on a multi-core Linux cluster and supporting MPI (message Passing Interface) parallel processing directives. Model code will be compiled using Portland Group compiler for 64-bit architecture.

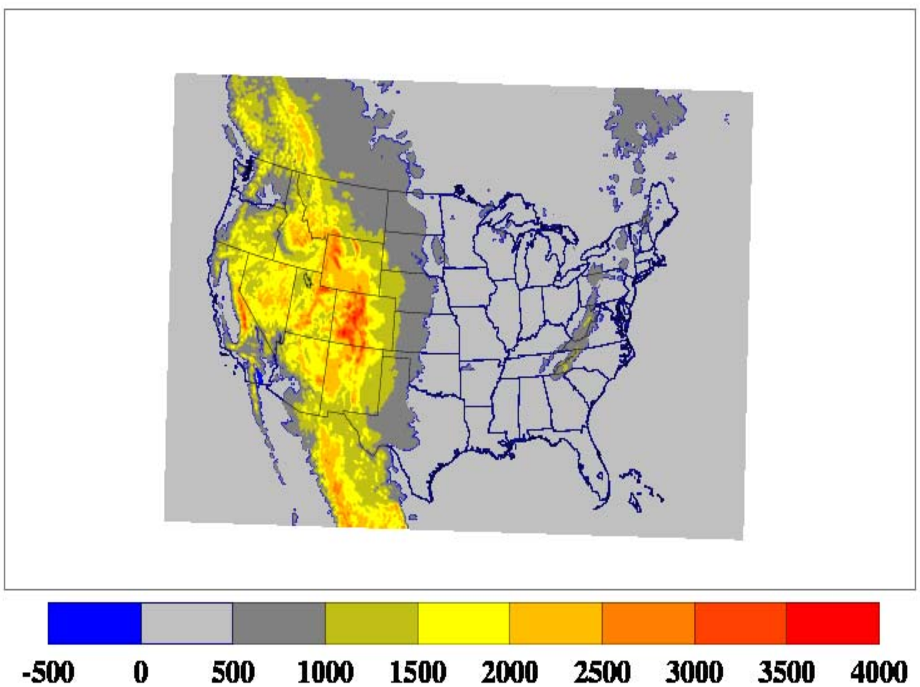


Figure 1. *Illustration of 12 km domain to be used in the project. As time permits a smaller 4 km grid will be used consistent with recommendations of TCEQ on the domain extent.*

To remain consistent with WRF model code, all the codes will be written in the Fortran90 standard with extensions compatible with today's most widely used FORTRAN compiler in WRF user's community (i.e., Portland Group for Linux operating systems). Since this project comprises many complex components and functionalities, it is not possible to have the entire code contained in a single module. Shell scripts will be written to manage the processes, manage the flow of the data, and perform the calculations properly. The scripts for each major component will be constructed in a way that a single script will serve as the main script that manages the overall performance of the system, so that the users do not have to deal with multiple parts of the code separately. The codes and scripts will adhere to the WRF coding/format style, including the use of appropriate in-code documentation (comment statements), loop indentation, and memory management techniques. The requirement for memory should be minimized. All variables will be type-declared using the FORTRAN “implicit none” statement at the top of each routine.

WRF preprocessor will be modified to accept satellite-derived skin temperature and insolation input data. All data and scripts will be provided to the AQRP and TCEQ scientists.

3.3 Hardware and Operating System Requirements

We expect to run all codes and scripts on a multi-core Linux cluster and supporting MPI (message Passing Interface) parallel processing directives. Model code will be compiled using Portland Group compiler for 64-bit architecture.

4 MODEL DESIGN

4.1 Model Development

The main model development will involve modifications to the Pleim-Xiu 2003 land surface model, which has been one of the preferred models in air quality studies especially by EPA. In last year’s project the assimilation scheme to adjust soil moisture was modified to use satellite skin temperature rather than NWS observed 2-m temperatures.

Pleim-Xiu technique: Pleim and Xiu 2003 noted that since surface moisture is not a direct observable that use of auxiliary information is needed. They have used observed NWS surface temperatures to nudge moisture. Here they adjust surface layer moisture w_G using the difference between model daytime temperatures (T^F) and analyses of observed temperatures (T^A) and model and observed relative humidity.

$$\Delta w_G = \alpha_1\left(T^A - T^F\right) + \alpha_2\left(RH^A - RH^F\right)_{\text{Daytime}} \qquad (1)$$

The Pleim-Xiu approach has been widely used and in recent California inter-comparisons performed better than the NOAH complex land surface scheme (Fovell 2013). In the past project because observed NWS observations are coarse, the NWS observed temperatures were replaced with satellite skin temperatures, i.e.

$$\Delta w_G = \beta_1\left(T_s^{Sat} - T_s^{Mod}\right)_{Morning} \qquad (2)$$

The final project report (McNider et al. 2015) - http://aqrp.ceer.utexas.edu/projectinfoFY14_15%5C14-022%5C14-022%20Final%20Report.pdf) provides details of the implementation of the satellite skin temperature assimilation including the recovery of a radiating skin temperature in the Pleim-Xiu scheme.

4.2 Component Description: New Model Data Sets

New model data sets to be used in this investigation are:

(1) **Satellite derived insolation**: One of the key factors in land surface temperatures is the correct specification of incoming solar radiation into the land surface. Models often

have clouds at the wrong place a wrong time. Under this task we will use satellite-derived insolation in the WRF model in place of the modeled insolation. Data has been processed at UAH for September 2013 and also for 2012, which is likely to encompass the new model test period. UAH/NASA insolation data is a near real-time operational retrieval from GOES Imager produced by Short-term Prediction Research and Transition Center (http://weather.msfc.nasa.gov/sport/goes_imager/descriptions.html) and then archived at UAH. The data has been used in previous air quality studies (Pour-Biazar et al., 2007; Tang et al., 2014; Ngan et al., 2012). The algorithm was revised recently to increase its accuracy by including a dynamic precipitable water field and performing bias correction (Pour-Biazar et al., 2015). The improved retrievals for September 2013 were used in a previous AQRP project (Pour-Biazar et al., 2015) and have been thoroughly examined for quality. The 2012 data will be examined in the same manner for quality assurance.

(2) **Satellite Skin Temperature**: Under this task we will provide GOES and MODIS skin temperature data sets to evaluate the spatial and temporal performance of the WRF model (and other models) in Texas. These data have been provided for the DISCOVER-AQ for September 1-30, 2013. Data sources and QA/QC procedures have been explained in previous AQRP reports (http://aqrp.ceer.utexas.edu/viewprojectsFY14-15.cfm?Prop_Num=14-022). While satellite data can infer a land surface temperature (LST) it is not always a direct clean observable in that cloud contamination and atmospheric intereference may alter the direct radiometric . Adjustments to remove contamination in the surface radiation from the intervening atmosphere and also emissivity assumptions have to be made. To examine the observed error in skin temperatures we will use two skin temperature products for the 12 km WRF domain. The NOAA ALEXI skin temperature product, which was employed in last year's project, and the MODIS operational LST product (see Wan and Dozier 1996 and updates). While we expect some differences in the actual values of the different satellite LST, we expect anomalies across land uses to be more invariant. One caveat which may cause a delay in providing the quality of data needed for model verification in task 4 and task 5 are cloud contamination in the skin temperatures. Cloud contamination yields a skin temperature that is much cooler than the neighboring cloud free pixels. The fact that temperature difference between a pixel with cloud contamination and a neighboring cell is usually much larger (more than 1.5 standard deviation) than what can be expected (mean) from LU/LC changes is used to filter out cloud contaminated data. This procedure has been explained in McNider et al., 2015 (http://aqrp.ceer.utexas.edu/projectinfoFY14_15/14-022/14-022%20Final%20Report.pdf).

(3) **Satellite Derived Greenness**: In last year's project we found that the seasonally adjusted USGS vegetation used in the Pleim-Xiu scheme was producing erroneous values especially in the Western U.S. We communicated directly with Jon Pleim and he agreed and said that a new paper by Ran et al. (2015) found similar results. Because of the importance of vegetative fraction and in view of Ran et al. (2015), we will employ a MODIS derived vegetative fraction in the land surface model. Case et al. (2014) has developed a MODIS-derived 1-km CONUS Green Vegetation Fraction (GVF) dataset which extends back to June 2011. We plan to use this dataset to replace the USGS values in the WRF model to assess its impact on the September 2013 simulation.

As noted in the previous project, we found considerable deficiencies in the seasonal adjustments to the USGS data employed by the Pleim-Xiu scheme. Since that time we have found (personal communication Jon Pleim) that EPA will likely drop this seasonal adjustment and go to a satellite derived greenness fraction. Thus, we believe that our approach is consistent and perhaps ahead of EPA. We inherently believe that not only are seasonal adjustments needed but that these can depend on specific years. For example the Texas greenness is likely much different for the drought years 2010 and 2011 from 2013. We will make a control case simulation using USGS data and then using the satellite greenness values and use the performance statistics in Table 3 to assess the impact of the new data set on the model near surface air temperature predictions.

4.3 Rationale for Selected Software/Hardware Tools

The software and hardware selected for this project are consistent with WRF ARW 3.8.1 (http://www2.mmm.ucar.edu/wrf/users/downloads.html) programming code, compilers and platforms used to develop, build and run this model, respectively. This will ensure compatibility with TCEQ's current computer system.

5 IMPLEMENTATION (MODEL CODING)

5.1 Software System Development: Model Coding

To remain consistent with WRF/CAMx code, all the codes will be written in the Fortran90 standard with extensions compatible with today's most widely used FORTRAN compiler in WRF user's community (i.e., Portland Group for Linux operating systems). Since this project comprises many complex components and functionalities, it is not possible to have the entire code contained in a single module. Shell scripts will be written to manage the processes, manage the flow of the data, and perform the calculations properly. The scripts for each major component will be constructed in a way that a single script will serve as the main script that manages the overall performance of the system, so that the users do not have to deal with multiple parts of the code separately. The codes and scripts will adhere to the WRFcoding/format style, including the use of appropriate in-code documentation (comment statements), loop indentation, and memory management techniques. The requirement for memory should be minimized. All variables will be type-declared using the FORTRAN "implicit none" statement at the top of each routine.

5.2 Data Input to WRF

The regridding and subsetting of the skin temperature data will be carried out as a stand-alone preprocessing system to WRF. The code and documentation of this regridding software will be provided as part of the deliverables of the skin temperature system. While this regridding software will be provided, other general subsetting codes that may be familiar to the user can also be employed.

We expect to develop the skin temperature retrieval system as a stand-alone process accessing the NOAA Comprehensive Large Array-data Stewardship System (CLASS) web site (http://www.nsof.class.noaa.gov/saa/products/welcome). The process will retrieve the skin temperature data from NOAA public server and a regridding/subsetting code will be used to put the data into the user defined WRF grid. This process will be described in the interim and/or final reports. Code for reading the skin temperature into WRF will be added. There are several approaches to importing data into WRF from non-standard sources. In the past we have imported hourly GOES data into the WRF system by writing it out in the so-called 'WPS intermediate format (see ARW, Version 3 Modeling System User's Guide July 2014, p 3-33)' and along with changes in the WRF Registry and the 'real.F' program made the satellite data 'behave' like a new surface four-dimensional data assimilation field. The advantage of this approach was that two consecutive time periods of data are automatically read by the WRF IO system and are available for use in the needed subroutines where linear interpolation in time provides the needed values at the current model time. The disadvantage of this approach is that the code changes (especially in the WPS system) are significant.

For this project our team plans to use a simpler approach in which the needed data will be accomplished by dedicating a WRF io-stream (in the 'namelist.input' file) to import the needed data from NetCDF files created externally. In these NetCDF files variable names are chosen which correspond to pre-determined actual times. For example, corresponding to a file time of 12 UTC 1 September 2013, the variables 'TSKIN_OBS_E', 'TSKIN_OBS_M', and 'TSKIN_OBS_L' would correspond to the actual times of 1145, 1245, and 1345 UTC (most of the GOES data to be used will be the scan which starts at 45 minutes past the hour). The latter 3 times then allow time interpolation to create the needed data between 1200 and 1300 UTC before the next file read. In essence this approach has moved the complexity outside of WRF at the expense of repeating data (i.e., in reference to the latter example, the file time of 13 UTC 1 September 2013 would contain 'TSKIN_OBS_E', 'TSKIN_OBS_M', and 'TSKIN_OBS_L' corresponding to the actual times of 1245, 1345, and 1445 UTC so the first two times have been repeated). Most of the code changes in WRF will be confined to changes in the Pleim-Xiu scheme. The options will exist to use the default Pleim-Xiu NWS assimilation scheme or to use the satellite skin temperatures. Modifications to WRF will adhere to the current code structure. All modifications within WRF will be well documented in the code and will be included in the final report.

The insolation replacement in WRF will start as a stand-alone process to retrieve and regrid the insolation to the WRF grid. Modifications to the code within WRF will be provided to replace the model calculated insolation with the satellite-derived insolation. Options will be included to use either the model insolation or the satellite insolation. The same procedures to bring the skin temperature data into WRF described above will be used for the insolation data.

5.3 Hardware and Operating System Requirements

We expect to run all codes and scripts on a multi-core Linux cluster and supporting MPI (message Passing Interface) parallel processing directives. Model code will be compiled using Portland Group compiler for 64-bit architecture.

5.4 Verification and Validation

Functionality, interfacing, performance and design constraints for the modified WRF model will be verified mainly through the use of the test-bed program. Good Fortran coding practices (e.g., use of explicit type declarations) and Fortran compile-time checks will be employed to confirm that routine interfacing is working properly. Functionality, performance, and design constraints will be verified by applying the test-bed program to a case study. A simulation by modified code in which no satellite data is used will be compared to the baseline estimates to ensure that differences in atmospheric state variables are almost zero.

Code verification will primarily be carried out by controlled testing. There will be at least two programmers viewing code changes.

5.5 Audits of Data Quality

We will be performing Quality Assurance/Quality Control (QA/QC) procedures to ensure that all data and products used or generated by this project are of known and acceptable quality. QA/QC procedures will be performed in accordance with the Category III Quality Assurance Project Plan (QAPP). For this project category, data audits must be performed for at least 10% of the data sets and a report of QA findings must be given in the final report. A technical systems audit is not required.

All data generated from this project or used in the evaluation work will undergo a rigorous data quality check to remove the outliers. As explained in section 4.2, the determination of outliers for satellite-based LST is based on a threshold (1.5 times the standard deviation about mean value). At each stage of the project, the data (both generated and used in the evaluation) along with a metadata will be released to AQRP and TCEQ. In the final stage of the project, a metadata describing the data files, along with a document describing the data quality will be compiled. The document, metadata, and the data files will be delivered to AQRP and TCEQ as part of the final report.

The audit will take place as follows:
Satellite-based LST and insolation: A member of the team who is not involved in the generation or evaluation of satellite-based LST and insolation will review at least 10% of the data for quality assurance purposes.

WRF Model inputs: A member of the team who is not participating in the modeling exercise will review at least10% of the model input data and model output for quality assurance purposes.

6 MODEL CALIBRATION: VALIDATION

6.1 Testing Strategy

In conjunction with AQRP and TCEQ a test period will be selected. Both a short (1 week) test period and longer period (1 to 2 months) will be identified. The short-term period allows for testing of model assimilation strategies without having to wait inordinately for model wall clock times. These selected test periods will be used as tasks 2-6 are carried out.

Under our previous project, the model evaluation period was the DISCOVER-AQ flight period (September 1-30, 2013). However, this period was selected in the AQRP RFP because of the aircraft data available - not because it was representative of extreme ozone events in the past. The synoptic situation for the month was especially active with multiple fronts producing excess cloudiness and higher winds in Texas and the Southeast (see Alrick et al. 2015). They showed that the DISCOVER-AQ Period was not as conducive to high levels of ozone as TEXAQS II. While last year's project showed that the satellite technique provided substantial improvement in land surface performance, the cloudiness reduced the number of times that the skin temperature data could be used. Examination of MODIS skin temperatures for the month of September 2013 shows virtually no thermal signal for Dallas (e.g., compared to Atlanta) indicating high winds may be reducing thermal gradients. Thus, the skin temperature technique may have even greater positive impact under other episodes where clear skies and light wind conditions most associated with high ozone events dominate. Therefore, for this project, in consultation with AQRP and TCEQ we will select another episode such as TEXAQS II 2006 or 2011.

We will be performing two types of model runs. The first are parameter selection runs where many different runs are made (usually using a short test period) to best determine parameters such as assimilation time scale or methods for using data. The second is where these are applied to assess model performance in a longer or independent test period.

6.2 Calibration: Parameter Selection

In the current investigation there is not a formal calibration. However, in carrying out tests of the technique for using skin temperatures to adjust soil moisture and heat capacity there is some adjustment of parameters such as the nudging time scale or the period of time that skin temperatures are used. We will provide sensitivity information on how these parameter selections change model performance according to metrics in Table 3. ***Figure 2*** provides an example. In this figure, bias (BIAS), root mean square error (RMSE), and differences between bias and RMSE (DBIAS and DRMSE) for each simulation as compared to control are presented. For example, for the simulation using satellite-derived albedo (marked as A) DBIAS and DRMSE are defined as:

DBIAS = |BIAS_A| - |BIAS_CNTRL|

DRMSE = |RMSE_A| - |RMSE_CNTRL|

The negative differences indicate a reduction of bias and RMSE compared to control. BIAS and RMSE are based on comparison with satellite-based observations. The labels indicate different sensitivity simulations: CNTRL for control simulation, I for the simulation with satellite insolation, I+SM for using satellite insolation and soil moisture nudging, I+A for using satellite based albedo and insolation, I+SM+HC+A for satellite insolation and albedo, soil moisture and heat capacity nudging. The times in seconds indicate the time scales for nudging. The last two bar charts indicate the period of time adjustment is applied. We will be selecting the configuration and parameters that yield the largest error reductions according to these metrics.

In the previous project the first 6 days of September 2013 were used in parameter selection. These were then applied to the entire month of September as an independent verification period. In the current project, the parameter selection will primarily take place during the September 2013 DISCOVER-AQ period. A second independent period probably July/August 2012 will be used as an independent test.

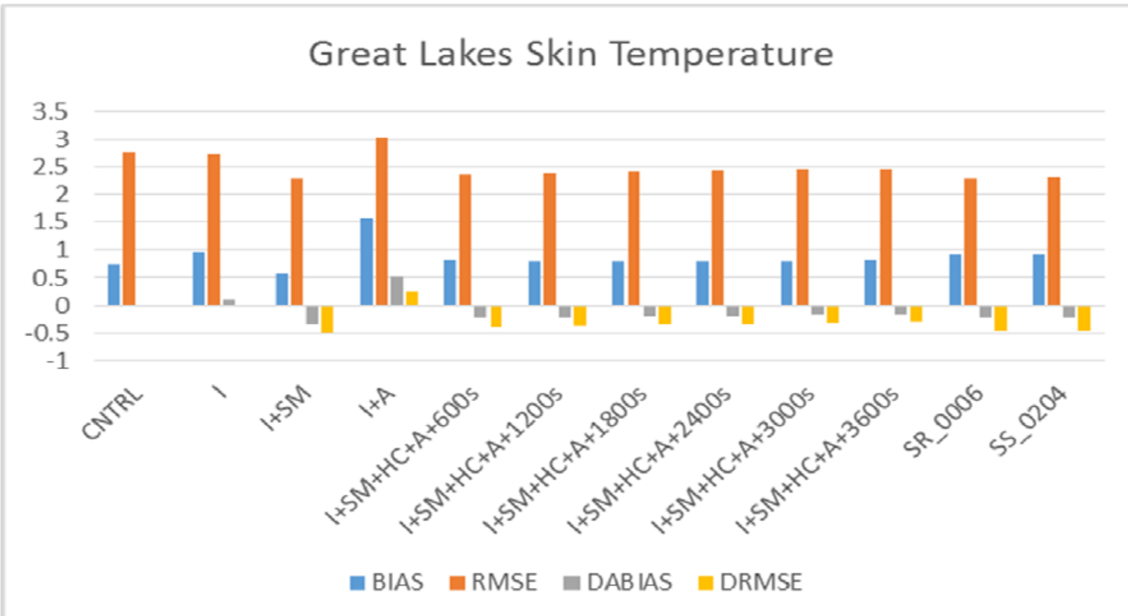


Figure 2. *Example of parameter sensitivity study for a Great Lakes Domain for the period September 1-6, 2013. The different runs on the x-axis correspond to differences in model configuration and nudging time scales.*

6.3 Checking Correctness of Outputs

Available air temperature and moisture measurements from National Weather Service (NWS) stations, as well as Continuous Ambient Monitoring Station (CAMS) operated by TCEQ will be used for model evaluation. Additionally, satellite skin temperature retrievals from Moderate Resolution Imaging Spectroradiometer (MODIS) and the Geostationary Operational Environmental Satellite (GOES) will be utilized for evaluating model skin temperature.

The evaluations will follow the recommendations made by weather and air quality community for these evaluations (Simon et al., 2012; Dennis et al., 2010). These evaluations will be based on standard statistical metrics such as error statistics and regression analysis with a focus on east/southeast Texas. A list of these performance metrics (adapted from Simon et al., 2012) is presented in Table 3. In this table, *M* stands for model value and *O* stands for observations.

In addition to these statistical metrics, the evaluation will also rely on model vs. observed scatter plots to quantify model deviations from observations and the improvements in correlation coefficient. Satellite-derived skin temperature and insolation will be the key observations used in these scatter plots. A separate evaluation of satellite products by comparing the retrievals to available surface observations will quantify uncertainties in satellite observations. In these evaluations, surface skin temperature observations from Atmospheric Radiation Measurement (ARM, https://www.arm.gov) facilities and surface insolation observations from U.S. Climate Reference Network (USCRN, https://www.ncdc.noaa.gov/crn), Surface Radiation Network (SURFRAD, http://www.esrl.noaa.gov/gmd/grad/surfrad), Soil Climate Analysis Network (SCAN, http://www.wcc.nrcs.usda.gov/scan), ARM, and Texas local broadband radiation monitoring stations will be used.

This project basically tries to correct fundamental parameters in the surface energy budget, such as surface moisture and heat capacity, by using observations. Thus, by modulating surface heat balance, indirectly corrects air temperature and moisture. While such correction will impact many aspects of boundary layer development and characteristics, our evaluation work will be focused on the impact of this technique on near surface air temperature and moisture.

Table 3. Definition of Performance Metrics (Adapted from Simon et al., 2012)

Abbreviation	Term	Definition[a]
MB	Mean bias	$\frac{1}{N}\sum(M_i - O_i)$
ME	Mean error	$\frac{1}{N}\sum\lvert M_i - O_i\rvert$
RMSE	Root mean squared error	$\sqrt{\frac{\sum(M_i - O_i)^2}{N}}$
FB	Fractional bias	$100\% \times \frac{2}{N}\sum\frac{(M_i - O_i)}{(M_i + O_i)}$
FE	Fractional error	$100\% \times \frac{2}{N}\sum\frac{\lvert M_i - O_i\rvert}{(M_i + O_i)}$
NMB	Normalized mean bias	$100\% \times \frac{\sum(M_i - O_i)}{\sum O_i}$
NME	Normalized mean error	$100\% \times \frac{\sum\lvert M_i - O_i\rvert}{\sum O_i}$
MNB	Mean normalized bias	$100\% \times \frac{1}{N}\sum\left(\frac{M_i - O_i}{O_i}\right)$
MNE	Mean normalized error	$100\% \times \frac{1}{N}\sum\left\lvert\frac{M_i - O_i}{O_i}\right\rvert$
UPA	Unpaired peak accuracy	$100\% \times \frac{(M_{peak} - O_{peak})}{O_{peak}}$
I of A	Index of agreement	$1 - \frac{\sum(M_i - O_i)^2}{\sum(\lvert M_i - \overline{O}\rvert + \lvert O_i - \overline{O}\rvert)^2}$
r^2	Coefficient of determination	$\left(\frac{\sum_1^N((M_i - \overline{M}) \times (O_i - \overline{O}))}{\sqrt{\sum_1^N(M_i - \overline{M})^2 \sum_1^N(O_i - \overline{O})^2}}\right)^2$

As an example, bias and standard error statistics for the runs will be provided. That is the bias is defined as difference of the means

$$Bias = 1/N \sum (T1\,(i,j) - T2(i,j))$$

and mean standard error is

$$RMSE = sqrt\,\left(\frac{1}{n}\right) sqrt\,\left(\left(\sum\left(\left(T1\,(i,j) - T2(i,j)\right) ** 2\right)\right)\right)$$

where T1 and T2 are two variables to be compared and the sums are over all i,j grids.

The primary initial model comparisons will be made against satellite observed skin temperatures and NWS observed surface data.

In addition to the overall statistics, the spatial and temporal variability of error statistics will be examined using visual graphical imagery (and subsetting of statistics if visual inspection warrants) to determine geographical variations in performance.

Final parameter selection will be based on sensitivity studies that show the best model performance. Since this project seeks to improve surface and near surface air temperatures, the parameter selection will be based on a configuration that yields a better agreement with observed temperatures as described in section 6.2.

6.4 Determining Conformance to Requirements

The Principal Investigator (PI) and his team will review all testing configurations, applications, and results from the simulations. Results of all tests will be documented and submitted to AQRP and TCEQ as one of the deliverables in this project.

6.5 Verification

The initial evaluation for satellite-based skin temperature comparison will be made for the Discover-AQ period. UAH will make the first comparison of the model versus satellite skin temperature as described in previous sections above.

A second model test period will be selected based on information from AQRP and TCEQ. This will likely be during July/August 2012 based on information at this time. This second period will provide for an independent check beyond the DISCOVER-AQ period using the same metrics for evaluation.

6.6 Evaluation

The final model results will be evaluated against available surface observations using the metrics in Table 3 (as described in section 6.3). The final model validation on whether the technique and modifications proposed here will be used for regulatory actions is the decision of the TCEQ. However, publication of results from this project in a peer-reviewed article, as planned, provides one component of potential acceptance.

7 DOCUMENTATION, MAINTENANCE, AND USER SUPPORT

7.1 Release and Delivery Management

The testing described in Section 6. above will encompass "alpha" testing of the new satellite-based skin temperature model. Once the system is verified to be working correctly, the revised WRF model code and the satellite data will be transferred to TCEQ for installation on their computer system. Toward the end of the project we foresee that TCEQ can commence "beta" testing using one of their current ozone modeling applications in which the NOAA skin temperature or Marshall Spaceflight Center (MSFC) split window data are available (after 2010). Any problems or issues will be reported back to the project team, who will promptly address them and provide a revised version to TCEQ for further testing if warranted. It should be noted, however, that this will be the first attempt at the implementation of such a system. TCEQ's feedback together with the lessons learned during the evaluation of the system will be used to compile a list of recommendations for improving the system for operational use.

7.2 Version Control, Documentation, Archival

The satellite-based retrieval system is a new attempt and the final satisfactory outcome will be offered as version 1. All codes and modifications will use standard FORTRAN. Additional code checks will be applied to ensure that standard FORTRAN techniques are used throughout all model routines. The core model and all Probing Tools (if applicable) will be run in a systematic series of tests to ensure that all systems are working correctly. The new system and the modifications to WRF will be documented and communicated to AQRP and TCEQ.
All the source codes (including WRF and the skin temperature and insolation files) and documentations from this project will be compressed into a single Linux "tar" archive file and will be backed up at UAH and shared with AQRP and TCEQ.

7.3 Archiving Data and Software

Data produced by the WRF model systems will be stored on a UAH Linux Cluster disk system that uses RAID technology to automatically distribute any archived data on different disks in the RAID disk cluster so that the likely hood of one disk failure destroying all the data is minimized. The final run (but not all intermediate runs) data will be stored on the system till the end of the project. At the end of the project we will off-load the data from the system to two removable disks. UAH will retain the data for a period of five years; all metadata, data, and documentation will be provided to AQRP for its archive as well as to the TCEQ.

WRF source code and related tools will be compiled into a single Linux compressed tar file and archived as described in previous sections. Source codes (in addition to the automatic system backups) are archived manually each week at UAH.

7.4 Audits of Data Quality and Model Inputs

Most all of the input data for the WRF simulations such as the large scale weather analyses, land use variables such as roughness have wide use and have had their own data audits. Thus, we will not audit or quality-assure such data unless we see a specific problem as we compare model output to observations. Under this project we will be using two data sets which do not have such wide use. These are the satellite skin temperature data and satellite derived insolation data. The following discusses quality control and data audits.

Skin Temperature: All the satellite skin temperature data generated from this project or used in the evaluation work will undergo a rigorous data quality check to remove erroneous data. We are mostly concerned about cloud contamination of the surface skin temperature data. We will implement stringent tests to check and remove cloud contamination using both absolute values and independent visible data. For example any visible brightening or time tendencies in the cloud GOES albedo product will be used to flag skin temperature retrievals. There is still the concern that sub-visible detected clouds can contaminate the skin temperature. The final report of the prior year's project provides an extensive discussion of cloud screening. This can be mostly a problem in the afternoon when small cumulus may go undetected.

Satellite derived insolation: The satellite-derived insolation we will use is a product produced by UAH and MSFC. This has several quality control steps as part of the retrieval process. Biazar and Cohan under another AQRP project have evaluated the insolation product against pyranometer data. Under this activity we will carry out a similar comparison of the satellite derived insolation product with available surface pyranometer data for the Discover-AQ period.

Model Inputs and Configuration: We are fortunate under this project to have three different modelers who will be carrying out the model runs. Thus, as part of our QA activity we will have the three modelers examine the model set up. If TCEQ is agreeable we will also send the model run files to them to ensure that the model set up is consistent with their WRF protocols except where we depart in the specific aspects related to the surface system.

At each stage of the project, the data (both generated and used in the evaluation) along with a metadata will be released to AQRP and TCEQ upon request. In the final stage of the project, a metadata describing the data files, along with a document describing the data quality will be compiled. The document, metadata, and the data files will be delivered to AQRP and TCEQ as part of the final report.

7.5 Maintenance and User Support

The core model and all Probing Tools (if applicable) will be run in a systematic series of tests to ensure that all systems are working correctly. The new system and the modifications to WRF will be documented and communicated to AQRP and TCEQ.

All the source codes (including WRF and the skin temperature and insolation files) and documentations from this project will be compressed into a single Linux "tar" archive file and will be backed up at UAH and shared with AQRP and TCEQ.

The Weather Research and Forecast model WRF model is a well-known community model http://www2.mmm.ucar.edu/wrf/users. WRF allows researchers to generate atmospheric simulations based on real data (observations, analyses) or idealized conditions. WRF offers operational forecasting a flexible and computationally-efficient platform, while providing advances in physics, numerical algorithms, and data assimilation contributed by developers in the broader research community. WRF is currently employed within EPA, NOAA and several states for producing the physical atmosphere for conducting air quality simulations. WRF has a large worldwide community of registered users (over 25,000 in over 130 countries), and workshops and tutorials are held each year at the National Center for Atmospheric Research (NCAR).

The WRF code modifications will conform to WRF code structure and will be thoroughly documented. The project team will archive all the source codes, scripts, and documentations for modified WRF with the satellite skin temperature options using Linux "tar" command. A backup will be kept at UAH and AQRP/TCEQ will be provided with a copy.

8 REPORTING

8.1 Project Deliverables

AQRP requires certain reports to be submitted on a timely basis and at regular intervals. A description of the specific reports to be submitted and their due dates are outlined below.

UAH will be responsible for submitting the reports for this project. UAH also will submit the Financial Status Reports (FSRs). The lead PI (Dr. McNider) will submit the reports, unless that responsibility is otherwise delegated with the approval of the Project Manager. All reports 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. Report templates and accessibility guidelines found on the AQRP website at http://aqrp.ceer.utexas.edu/ will be followed.

8.1.1 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: Wednesday, August 31, 2016

8.1.2 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 TCEQ.

Quarterly Report Due Dates:

Report	Period Covered	Due Date
Quarterly Report #1	June, July, August 2016	Wednesday, August 31, 2016
Quarterly Report #2	September, October, November 2016	Wednesday, November 30, 2016
Quarterly Report #3	Dec. 2016, January & February 2017	Tuesday, February 28, 2017
Quarterly Report #4	March, April, May 2017	Friday, May 31, 2017
Quarterly Report #5	June, July, August 2017	Thursday, August 31, 2017

Quarterly Report #6	September, October, November 2017	Thursday, November 30, 2017

8.1.3 Monthly Technical Reports

Technical Reports will be submitted monthly to the Project Manager and TCEQ Liaison as a Word doc using the AQRP FY16-17 MTR Template found on the AQRP website.

MTR Due Dates:

Report	Period Covered	Due Date
Aug2016 MTR	Project Start - August 31, 2016	Thursday, September 8, 2016
Sep2016 MTR	September 1 - 30, 2016	Monday, October 10, 2016
Oct2016 MTR	October 1 - 31, 2016	Tuesday, November 8, 2016
Nov2016 MTR	November 1 - 30 2016	Thursday, December 8, 2016
Dec2016 MTR	December 1 - 31, 2016	Monday, January 9, 2017
Jan2017 MTR	January 1 - 31, 2017	Wednesday, February 8, 2017
Feb2017 MTR	February 1 - 28, 2017	Wednesday, March 8, 2017
Mar2017 MTR	March 1 - 31, 2017	Monday, April 10, 2017
Apr2017 MTR	April 1 - 28, 2017	Monday, May 8, 2017
May2017 MTR	May 1 - 31, 2017	Thursday, June 8, 2017
Jun2017 MTR	June 1 - 30, 2017	Monday, July 10, 2017
Jul2017 MTR	July 1 - 31, 2017	Tuesday, August 8, 2017

8.1.4 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 FY16-17 FSR Template found on the AQRP website.

FSR Due Dates:

Report	Period Covered	Due Date
Aug2016 FSR	Project Start - August 31	Thursday, September 15, 2016
Sep2016 FSR	September 1 - 30, 2016	Monday, October 17, 2016
Oct2016 FSR	October 1 - 31, 2016	Tuesday, November 15, 2016
Nov2016 FSR	November 1 - 30 2016	Thursday, December 15, 2016
Dec2016 FSR	December 1 - 31, 2016	Tuesday, January 17, 2017
Jan2017 FSR	January 1 - 31, 2017	Wednesday, February 15, 2017
Feb2017 FSR	February 1 - 28, 2017	Wednesday, March 15, 2017
Mar2017 FSR	March 1 - 31, 2017	Monday, April 17, 2017
Apr2017 FSR	April 1 - 28, 2017	Monday, May 15, 2017
May2017 FSR	May 1 - 31, 2017	Thursday, June 15, 2017
Jun2017 FSR	June 1 - 30, 2017	Monday, July 17, 2017
Jul2017 FSR	July 1 - 31, 2017	Tuesday, August 15, 2017
Aug2017 FSR	August 1 - 31, 2017	Friday, September 15, 2017

Report	Period Covered	Due Date
FINAL FSR	Final FSR	Monday, October 16, 2017

8.1.5 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: Tuesday, August 1, 2017

8.1.6 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: Thursday, August 31, 2017

8.1.7 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 (September 29, 2017). 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. **UAH will retain the data for a period of five years. Also, all metadata, data, and documentation will be provided to AQRP and TCEQ.**

8.1.8 AQRP Workshop

A representative from the project will present at the AQRP Workshop in the first half of August 2017.

8.1.9 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.

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