QUALITY ASSURANCE PROJECT PLAN

AQRP Project 14-022

Use of satellite data to improve specifications of land surface parameters

PROJECT SUMMARY

QAPP Category Number: III
Project Type: Secondary Data Project and Research or Development (Modeling)
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
Audits of Data Quality: Cat III = 10% Required
Report of QA findings: Required in final report

Prepared for:
Texas Air Quality Research Program (AQRP)

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APPROVALS

This QAPP was approved electronically on February 9, 2015 by Vincent M. Torres, The University of Texas at Austin

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List of Acronyms

AQRP	Texas Air Quality Research Program
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
MPI	Message Passing Interface
MSFC	Marshall Space Flight Center
NASA	National Aeronautics and Space Administration
NOAA	National Oceanic and Atmospheric Administration
NO	Nitrogen monoxide
NO_2	Nitrogen dioxide
NO_x	Nitrogen Oxides (NO+NO2)
PAR	Photosynthetically Active Radiation
PI	Principal Investigator
PM	Particulate Matter
TCEQ	Texas Commission on Environmental Quality
GMU	George Mason University
WRF	Weather Research and Forecasting (WRF) model

1 PROJECT DESCRIPTION AND OBJECTIVES

1.1 Introduction

The land surface is a critical component in local, regional and global modeling. Heat, momentum and scalar fluxes at the surface control temperature, turbulent mixing, winds and dry deposition of chemical species. Because of the importance of the characteristics of the land surface there has been tremendous investment by the climate, weather forecasting and air quality communities. Much of this investment has gone into developing complex land surface models which include many intricate parameterizations that attempt to capture processes such as plant transpiration rates, leaf water interception, soil moisture and run-off and parameterizations which control thermal and water transfer through canopies and soils (Sellers 1997, Pitman 2003). Thus, these models require additional parameter specifications to close the model systems.

A second major area of investment has been the development of land-use classification data sets that attempt to define areas which are forested, croplands, urban areas etc. that can be used with the land surface models. The use of satellite data (with its observables such as greenness and albedo) have greatly improved the characterization of the surface into land use classes. However, land surface models such as WRF-NOAH don't use land use classifications directly, rather they use the physical parameters such as roughness, heat capacity, canopy thermal and water resistances, soil conductivity for water and heat etc. that are associated with the land use classes. Thus, in the models such as the WRF –NOAH land use schemes there are lookup tables that define these land-use associated parameters (Niu et al. 2011).

Difficulty in Specifying Land Use Parameters: Unfortunately, the specification of some of these physical parameters is difficult even in homogeneous land use classes (Rosero et al.2009). For example, the rate of temperature change in vegetation is controlled by plant transpiration and evaporation through water resistance parameters and by the canopy thermal resistance. Thermal resistance depends on the heat capacity of the canopy and the thermal conductivity through the canopy (Noilhan and Planton 1989). The water resistance depends on root zone moisture, the phenological state of the plant, leaf area, shaded leaf area etc. Field measurements using towers are usually conducted to try to establish these parameters. But, in effect, many of the parameters or processes have to be deduced as residuals in local canopy models which are tied to specific turbulence and radiative models (Yang and Friedl 2003, Pleim and Gilliam 2009). Thus, the parameters are often model heuristics as opposed to fundamental observables (Wegner and Gupta 2005) which is the reason a parameter such as canopy thermal resistance can vary by three orders of magnitude in different models (Pleim and Gilliam 2009). In inhomogeneous grid boxes which make up the real world the situation is even worse (McNider et al 2005). Here, dominant land-use classes are often used in models such as NOAH but they may not represent well the actual mix of urban, crop and forest land uses.

1.2 Purpose of Study

One of the challenges in understanding the Texas air quality has been the uncertainties in estimating the biogenic hydrocarbon emissions (Allen et al., AQRP State of the Science 2012 report). Biogenic volatile organic compounds (BVOCs) play a critical role in atmospheric chemistry, particularly in ozone and particulate matter (PM) formation. In southeast Texas, BVOCs (mostly as isoprene) are the dominant summertime source of reactive hydrocarbon

(Wiedinmyer et al., 2001). Despite significant efforts by the State of Texas in improving BVOC estimates, the errors in emissions inventories remain a concern. This is partly due to the diversity of the land use/land cover (LU/LC) over southeast Texas coupled with a complex weather pattern (Song et al., 2008), and partly due to the fact that isoprene is highly reactive and relating atmospheric observations of isoprene to the emissions source (vegetation) relies on many meteorological factors that control the emission, chemistry, and atmospheric transport.

BVOC estimates depend on LU/LC, the amount of radiation reaching the canopy (Photosynthetically Active Radiation, PAR), and temperature. There have been many efforts in developing high resolution LU/LC data sets to better represent the diversity of vegetation over the State of Texas (Wiedinmyer et al., 2001; Byun et al., 2005). An on-going AQRP Project (Biazar and Cohan – AQRP – 14-022) is assessing the role of PAR and clouds on BVOC emissions. However, the treatment of temperature across different LU/LC classes presents a problem because of the uncertainties mentioned above.

The work proposed here is an attempt to improve surface temperature estimates by using geostationary satellite observations. Such temperature improvements should provide better temperature inputs into BVOC emission models and improve boundary layer and wind predictions. Under this activity we will perform a set of meteorological simulations using the Weather Research and Forecasting (WRF) Model. We will first diagnose a skin temperature from the Pleim-Xiu surface scheme in WRF and make a comparison to the skin temperature from GOES and MODIS (where available).

There are two principal objectives for this project:

(1) Use satellite observed skin temperature data as a verification product for WRF model LU/LC performance.

(2) Use satellite skin temperature to adjust LU/LC associated parameters such as soil moisture and heat capacity to improve model performance.

The final modeling period for this activity will be the Discovery AQ period September 2-September 29. However, some modeling early in the project where techniques are still be testing may include smaller time periods for efficiency. Figure 1shows the 12 km modeling domain of the project.

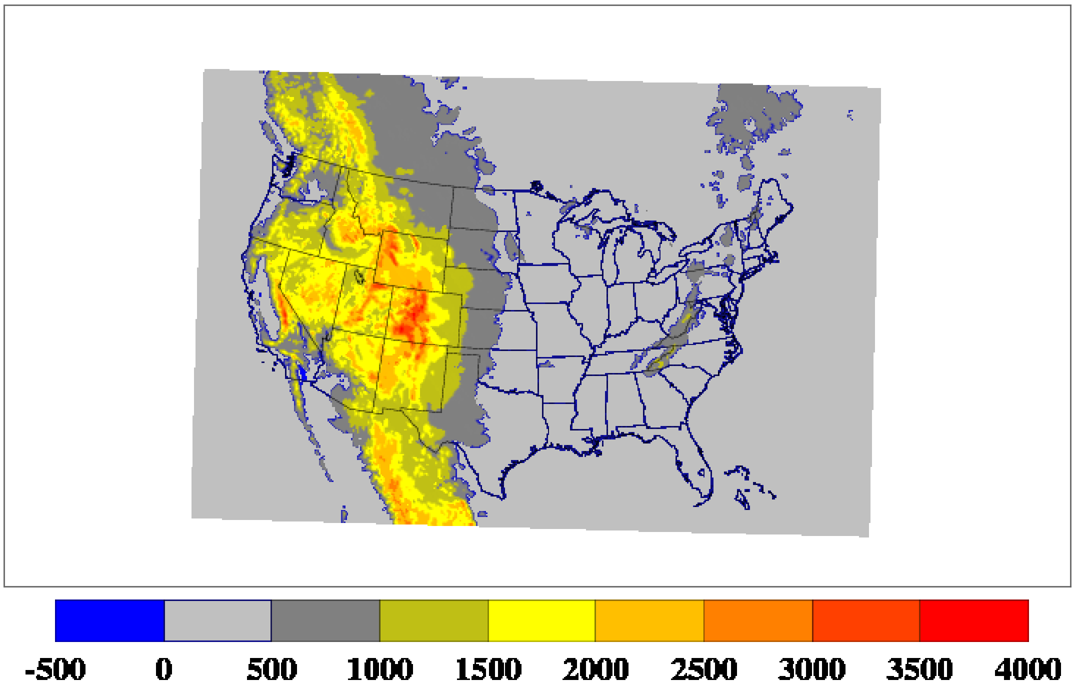

Figure 1 *Illustration of 12 km domain to be used in the project. As time permits a smaller 4 km grid will be used consistent with recomendations of TCEQ on the domain extent*

Consistent with the AQRP SOW the tasks and task deliverables under this proposal are:

Task -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.

Deliverable – A report on the impact of specifying insolation on surface air temperatures and ground temperatures in the WRF model for a 12 km domain (see figure 1) for at least one week in September 2013 aspart of the Discovery AQ Period**. Delivery Date- March 1, 2015**

Task 2- Diagnosed Skin temperature in Pleim-Xiu Scheme: Under this task we will diagnose a true skin temperature from the Pleim-Xiu scheme using the approach in equation (4) above within the WRF framework.

Deliverable – Report describing the recovery of the skin temperature and tests of the recovery against FIFE data. The report will also include images of the recovered skin temperature in WRF for the Discovery AQ Period for the 12 km domain. **Delivery Date – April 1, 2015**

Task 3 – 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 will be provided for the DISCOVER-AQ and SEAC4RS 2013 intensive data collection periods. 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 compare three skin temperature products for the 12 km WRF domain. These will be the GOES standard LST product, a physical split window technique (Jedlovec 1987, Guillory et al. 1993) 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. Thus, we will compute anomalies and base the anomalies on the domain average LST for each satellite product. In the same way we can also compute anomalies in the WRF model so that the scatter plots and other spatial comparisons will be plotted versus the anomalies. Thus, any errors in satellite absolute values will be minimized. Also, for consistency we will use the same emissivity (correct for) in the model as used in the satellite skin temperature retrieval. 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. If so we may have to create our own cloud mask based on temporal changes in surface reflectance. This may impact being able to complete task 5 (see below). We don't expect a significant problem but we will be using a new skin temperature product from NOAA and this needs verification.

Deliverable – A report that includes images of the anomalies of satellite skin temperature products for the 12 km domain with parallel images of the land surface category. Similar images will be provided of the skin temperature from the WRF 12 km domain. It will also include differences between the satellite and WRF anomalies. Scatter plots of model versus satellite skin temperatures for the 12 km domain will be provided. **Delivery Date May 15, 2015**

Task 4 – Implement Pleim-Xiu assimilation technique using satellite skin temperature in WRF: The current Pleim-Xiu scheme uses NWS observations to adjust soil moisture. Under this task we will use the difference in skin temperatures in the model to adjust surface moisture as described in equation (2) above for the 12km domain in WRF for the Discovery AQ period. Comparison of model performance with and without the satellite assimilation will be provided both in terms of satellite skin temperatures and standard NWS observations.

Deliverable – A report describing the technique and implementation of Pleim-Xiu satellite assimilation in WRF. The report will include images of skin temperature for the control and assimilation case and difference images. Also, 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

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

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

Similar statistics will be provided for standard NWS observations. **Delivery Date – July 15, 2015**

Task 5 – Implement Three Stream MCN94/MCN05 Technique: Because of the short-time table on this project this is a tentative task and depends somewhat on the pace of progress on task 3 concerning cloud contamination. Under this task we will implement the three stream MCN94/MCN05 technique within the Pleim-Xiu scheme. We will determinedsurface moisture and surface thermal resistance. The results of this model experiment will be compared to the WRF Pleim-Xiu model and possibly a WRF NOAH control run for the Discovery AQ period if time is available for this task.

Deliverable – A report describing the implementation of the three Stream MCN94/MCN05 technique. The report will also include images of skin temperature with and without the technique. Scatter plots of (see examples figure 1 and 2) for theDiscovery AQ period against the satellite LST will be provided as well as bias and standard error statistics (see above). . We will also compare to standard NWS observations (see figure 3). The expectation is that scatter and bias will be reduced when compared to the satellite and NWS observations. Maps of surface moisture and surface thermal resistance will be provided. **Delivery Date August 15 , 2015**

Task 6 - Deliver temperatures/WRF model set up for use in biogenic models. We will provide WRF runs to other AQRP investigations and TCEQ to examine the impact on biogenic emissions from the above Discovery AQ period. **Delivery date September 15, 2015.**

2 PROJECT ORGANIZATION AND RESPONSIBILITIES

2.1 Responsibilities of Project Participants

The University of Alabama-Huntsville (UAH) in collaboration with NOAA Air Resources Laboratory (ARL)/George Mason University will conduct this study under a grant from the Texas Air Quality Research Program (AQRP). UAH will be providing developing the techniques for diagnosing a skin temperature in the Pleim-Xiu scheme in WRF and using skin temperatures to hopefully improve model performance. NOAA ARL/George Mason University will be evaluating WRF performance both against satellite skin temperatures and standard National Weather Service Observations as well as any special observations made by TCEQ and NASA under the DISCOVERY AQ field program. /The key personnel working on this project and their specific responsibilities are listed below.

UAH has a worked in using satellite data to improve surface and boundaty layer performance for many years (e.g. McNider et al. 1994 and McNider et al 2005). UAH 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 will be provided for the TEXAQS 2005, TEXAQS 2006 and the DISCOVER-AQ and SEAC4RS intensive data collection periods. While satellite data can infer a land surface temperature (LST) it is not a clean observable. 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 compare three skin temperature products for the 12 km WRF domain. These will be the GOES standard LST product served by the NOAA, a physical split window technique (Jedlovec 1987, Guillory et al. 1993) and the MODIS operational LST product (see Wan and Dozier 1996 and updates). While we expect some differences in the absolute values of the different satellite LST we expect anomalies across land uses to be more invariant. Thus, we will compute anomalies and base the anomalies on the domain average LST for each satellite product. In the same way we can also compute anomalies in the WRF model so that the scatter plots and other spatial comparisons will be against the anomalies. Thus, any errors in satellite absolute values will be minimized. Also, for consistency we will use the same emissivity (correct for) in the model as used in the satellite skin temperature retrieval.

The NOAA Air Resources Laboratory and their contractor (George Mason University) have a long history of making physical atmospheric and air quality simulations. As part of this activity they have established tools and protocols for model evaluation

Richard McNider, PI, has a long history in mesoscale modeling and air quality. He served as an air pollution meteorologist with the State of Alabama. He was one of the five principals in the Southern Oxidant Study (SOS) and continued work in TEXAQS2000, TEXAQS2006 (nighttime transport and stationary fronts). He has also been a leader in the use of satellite data in mesoscale models and air quality models including developing techniques for using satellites to provide photolysis and surface energy budgets. He is currently a member of NASA's Applied Science Air Quality Team. Under the present proposal he will lead the implementation of the Pleim-Xiu and McN94/McN05 satellite retrievals of moisture and thermal resistance.

Pius Lee, Co-PI, has worked on both air quality models and weather forecasting models and currently leads NOAA's air quality forecasting system. He has recently been involved in the evaluation of model wind performance and his team was supported by the Texas AQRP. The paper by Ngan et al. 2013 was supported by this activity. He will take the lead on model wind evaluation and in running the BEIS experiments examining changes in biogenic emissions due to model temperatures.

Dr. Yu Ling Wu, Research Scientist at UAH, has significant experience in air quality transport and dispersion and in boundary layer chemical interactions. Dr. Wu will conduct the initial experiments with WRF testing the implementation of the skin temperature retrieval in the Pleim-Xiu scheme and in assimilating skin temperatures into the Pleim-Xiu scheme. She will pass the WRF code to NOAA/GMU for performance evaluation.

Table 1. Key project participants and their responsibilities.

Participant	Organization	Project Responsibility
Richard T. McNider	UAH	Develop implementation of skin temperature retrieval and assimilation. Advise on the overall direction of the project.
Pius Lee	NOAA	Oversee WRF model evaluation compared to satellite data and standard NWS observations and special DISCOVERY AQ data
Yu Ling Wu	UAH	Implement skin temperature retrieval and assimilation code into WRF

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. TCEQ staff will also receive remote training on the use of satellite-based skin temperature version of WRF.

Table 2. Summary of project schedule and milestones.

Deliverable	Deliverable Due Date
1. Satellite derived insolation Report	March 1, 2015
2. Diagnosed Skin temperature in Pleim-Xiu Scheme Report	April 1, 2015
3. Satellite Skin Temperature Report	May 15, 2015
4. Pleim-Xiu satellite skin temperature assimilation technique in WRF Report	July 15, 2015
5. Implement Three Stream MCN94/MCN05 Technique Report (this is tentative deliverable based on progress)	August 15, 2015

3 FUNCTIONAL REQUIREMENTS

3.1 Required Functions

The functional requirements of the new satellite-based skin temperature improvement in land-use technique and the responsible institution:

- Retrieve solar derived insolation for the Discovery AQ period from UAH archives and assimilate into WRF (UAH);
- Develop retrieval of skin temperature in Pleim-Xiu scheme and for FIFE data and Discovery AQ period (UAH);
- Carry out model evaluation using GOES and NWS observations for Discovery AQ – (NOAA/GMU)
- Develop adjustment of surface moisture using satellite skin temperature in Pleim-Xiu scheme (UAH);
- Evaluate the impact adjustment of moisture from skin temperature on model performance using satellite and surface observations during Texas Discover-AQ campaign (NOAA/GMU)
- Implement the Three Stream MCN94/MCN05 Technique into Pleim-Xiu. Because of the short-time table on this project this is a tentative task and depends somewhat on the pace of progress on task 3 and 4
- Evaluate the impact of the Three Stream MCN94/MCN05 on model performance using satellite and surface observations during Texas Discover-AQ campaign (NOAA/GMU)

3.2 Functionality, Interfacing, Performance, and Constraints

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.

The regridding and subsetting of the skin temperature data will be carried out as a stands-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.

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 SYSTEM DESIGN

4.1 System Overview

The skin temperature retrieval system will be constructed as a stand-alone system that will interact with the observational system through external files containing data and instructions. Currently, UAH collaborates with the Infrared (IR) group at the National Aeronautics and Space Administration (NASA) at Marshall Space Flight Center (MSFC) to generate and archive several GOES derived products. The retrieval system, GOES Product Generation System (GPGS), provides routine near real-time retrievals of skin temperature and surface insolation to be used in the meteorological (Haines et al., 2003). However, under this activity, we also plan to use a NOAA operational skin temperature product which is available through NOAA NCDC CLASS system. Our only concern with the new product is how good the cloud mask is that ensures that surface skin temperature retrievals are not contaminated by clouds. If we find potential issues we may use other cloud detection algorithms. The first phase of evaluations will cover September 2013. For these evaluations NOAA skin temperature product will be compared to the NASA split window skin temperature product. More information on the system constructs is provided in Section 3.2.

4.2 Component Description

Detailed information on the component description is provided in Section 3.2. Specific details about satellite skin temperatures and modifications to WRF will be provided in the final report.

4.3 Rationale for Selected Software/Hardware Tools

The software and hardware selected for this project are consistent with the current WRF programming code, compilers and platforms used to develop, build and run these models, respectively. This will ensure compatibility with TCEQ's current computer system.

5 IMPLEMENTATION

5.1 Software System Development

We expect to develop the skin temperature retrieval system as a stand-alone process accessing the NOAA web site. The process will retrieve the skin temperature data 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 report on April 15, 2015. 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 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 predetermined 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.

5.2 Verification and Validation

Functionality, interfacing, performance and design constraints for the new satellite insolation and skin temperature 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 WRF code in which no satellite data is used will be compared to the baseline WRF estimates to ensure consistent responses.

The initial evaluation for satellite-based skin temperature comparison will be made for the Discovery AQ period. UAH will make the first comparison of the model versus satellite skin temperature. Then NOAA/GMU [George Mason University]will make a comparison with standard NWS data and with special Discovery AQ data(See below for a discussion of Discovery AQ data to be used). This will be considered the control case, Next the satellite skin temperature assimilation technique will be carried out in WRF. UAH and NOAA/GMU will the carry out an evalution of the impact of the assimilation against both skin temperature and independent NWS observations and Discovery AQ special observations. Example, NWS data will be two-meter temperature and relative humidity. Discovery AQ data will include flight track temperature. The evaluations will be based on standard statistical metrics such as error statistics and regression analysis with a focus on east/southeast Texas. 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

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

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

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.

Discovery AQ data to be used. While the Discovery AQ program contains many air chemistry and aerosol data our interests are in the physical measurements listed in the table below. NOAA ARL will take the lead on obtaining observed data for model evaluation.

P3 Aircraft in situ temperature	Provides temperature at flight level so that temperature profiles are available during air

	spirals
P3 Aircraft in situ Dewpoint/Humidity	Provides temperature at flight level so that dewpoint profiles are available during air spirals
P3 Surface IR Temperature	This is one of the most useful products for the project since it will provide an independent measure of the surface skin temperature
University of Houston Sondes	We will also use temperature and dew point information when available from these special balloon borne instruments.
Planetary Boundary Heights	This is not listed as a specific observable but if instrument investigators produce a mixed layer height from aerosol or ozone profiles we will compare these to model PBL heights

5.3 Release and Delivery Management

The testing described in Section 5.2 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.

5.4 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.

5.5 Archiving Data and Software

Data produced by the WRF model systems will be stored on a UAH Linux Cluster disk system (called MATRIX) 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 keep one for three years and the other will be sent to TCEQ.

WRF source code and related tools will be compiled into a single Linux compressed tar file and archived as described in Section 5.4. Source codes (in addition to the autaomatic MATRIX backups) are archived manually each week.

5.6 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 and that is 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 audit 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. This can be the most problem in the afternoon when small cumulus may go undetected. We may follow McNider et al. 1994 and only use morning skin temperatures in the Pleim-Xiu assimilation. Second, anomalous temperature tendencies will be examined. As an example should morning skin temperatures decrease over time then these will be flagged for possible contamination. Such flags will be used to exclude such data in model comparisons or in the data used in assimilation.

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 are evaluating and auditing 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 prynaometer data for the Discovery 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 auditthe 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. 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.

A minimum of 10% of the data, model scripts and model results will be audited by a staff member who did not perform the analyses. The results of these audits will be included in the final report.

6 VALIDATION, VERIFICATION, AND TESTING

6.1 Testing Strategy

The testing strategy is presented in Section 5.2.

6.2 Checking Correctness of Outputs

The approach to checking correctness of outputs is described in Section 5.2.

6.3 Determining Conformance to Requirements

The Principal Investigator (PI) and his team will review all testing configurations, applications, and results from the stand-alone skin temperature retrieval system and the modified WRF model for the Discovery AQ 2013. Results of all tests will be documented and submitted to AQRP and TCEQ as one of the deliverables in this project.

TCEQ modeling staff will also play a role in this quality assurance step through their "beta" testing of the revised WRF model. TCEQ staff will report back to the project team on any problems, unexpected results, or confirmation of appropriate outcomes from the use of the skin temperature assimilation.

7 DOCUMENTATION, MAINTENANCE, AND USER SUPPORT

7.1 Project Documentation Requirements

The project documentation requirements are listed in Section 2, Table 2. The required documentation includes this QAPP and the documentation listed in Table 2.

7.2 Maintenance and User Support

Code maintenance is detailed in Section 5.4. 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, numerics, 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.

TCEQ staff may contact the project team directly for user support. Contact information is listed below:

- Dick McNider, mcnider@nsstc.uah.edu,256/961-7756
- Yuling Wu, **wuy@nsstc.uah.edu**, 256/961-7942
- Kevin Doty, kevin.Doty@nsstc.uah.edu, 256 961-7904.

7.3 Methods and Maintenance Facilities

The methods and facilities used to maintain, store, secure, and document code versions and related items are described in Sections 5.4, 5.5, and 7.2.

8 REPORTING

8.1 Project Deliverables

8.1.1 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

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.

Due Dates:

Report	Period Covered	Due Date
Quarterly Report #1	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

8.1.3 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

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 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

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. The final run (but not all intermediate runs) data will be stored on the system till the end of the project. As the project goes forward and at the end

of the project we will off load the data from the system to two removable disks. UAH will keep one for three years and the other will be sent to TCEQ.

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. **Due Date: Tuesday, August 18, 2015**

8.1.6 Final Report

A 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**

8.1.7 AQRP Workshop

A representative from the project will present the findings of this project at the AQRP Workshop in June 2015.

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