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Proposal Summary

The proposed activity here addresses the Health and Air Quality Application Area. The project anticipates improving the accuracy of the Decision Support Tools (DSTs) used by health and air quality managers to meet the health effect standards set by the Clean Air Act (CAA). The CAA is the comprehensive federal law that authorizes EPA to establish National Ambient Air Quality Standards (NAAQS) to protect public health and public welfare. The states are responsible to meet these standards through the use of the DST to develop and evaluate emissions control strategies under State Implementation Plan (SIP). SIPs are at the nexus of health effects and economics. Since the economic costs of such decisions can amount to billions of dollars nationally, the accuracy of the DST is critical to determining efficient, cost effective strategies for attaining NAAQS.

For this project, the target Decision Support Tool is the Weather Research and Forecasting (WRF) and the Community Multiscale Air Quality (CMAQ) modeling systems. CMAQ is an EPA-developed photochemical modeling system typical of the modeling systems now used by many regulatory agencies. The modeling system is also being used for operational air quality forecasting by NOAA. The objective of the proposed project is to utilize Earth observations and NASA science in the DST to improve key physical factors such as soil moisture and heat capacity, boundary layer development, and clouds that are critical in air quality photochemical simulations. A critical area in the DSS that will be targeted for improvement is in improving model location and timing of clouds. Clouds have a profound role in photolysis activity, boundary-layer development and deep vertical mixing of pollutants and precursors. Also, a new technique for near-realtime estimation of lightning generated NOx (LNOx) will be tested in the NASA Lightning <u>NO</u>-production <u>M</u>odel (LNOM). The technique introduces a methodology for directly estimating LNOx, on a flash-by-flash basis, from the observed cloud-top lightning optical energy detected from satellite lightning imagers. This will be a new capability made possible by geostationary observations of lightning events.

The satellite products include surface skin temperature, insolation, and albedo from Moderate Resolution Imaging Spectroradiometer (MODIS) on-board AQUA and TERRA satellites and Visible Infrared Imaging Radiometer Suite (VIIRS) instrument aboard Suomi National Polarorbiting Partnership (Suomi-NPP) satellite. In addition, we will be using Geostationary Operational Environmental Satellite (GOES) observations under NASA legacy science to complement polar orbiting observations obtained from VIIRS and MODIS. The project will take advantage of GOES-16 observations that offer a broad suite of observations relevant to this project at much higher temporal and spatial resolution. This will require retooling several NASA science products that are critical for our partner organizations. The applied partners in this project are EPA's Atmospheric Modeling Division (AMD) at the National Environmental Research Laboratory (NERL), the Lake Michigan Air Directors Consortium (LADCO), the California Air Resources Board (CARB), the Texas Commission on Environmental Quality (TCEQ), and the Georgia Environmental Protection Division (GAEPD). Note that this includes some of the largest most active state air pollution agencies in the country.

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1 Decision-making Activity

1.1 Description of Decision Making Framework:

The Nation's health related air-pollution control program is defined by the Clean Air Act that requires the attainment of National Ambient Air Quality Standards (NAAQS) that are set by the EPA. NAAQS are based on the pollutant's impact on human health and provide public health protection, including protecting the health of "sensitive" populations such as asthmatics, children, and the elderly. The standards are based on epidemiological and exposure studies which attempt to find minimum levels of pollutants which can be demonstrably connected to adverse health effects (morbidity or mortality). Air quality measurements are used to find those areas that are not attaining these health-based standards. Once an area is found to be in non-attainment for a particular pollutant, then a process is initiated in which the states' regulatory agencies must devise a plan for attaining the standards. This plan, called a State Implementation Plan (SIP), defines specific emission-reduction strategies for meeting the NAAQS and is the main vehicle for protecting human health and welfare.

The decisions made for the emissions reduction strategies under SIP are costly. Across the Nation, SIPs involve hundreds of billions of dollars in emission controls. For example, it is estimated that the cost of meeting the fine particle (PM2.5) NAAQS will amount to \$38 billion per year. Thus, it is imperative for the air quality managers to have confidence in the tools used to define emission control strategies. This is where NASA data, tools, and science can impact multi-billion dollar health decisions.

The Decision Support Tool (DST) used during the development of SIPs is an air quality modeling system comprising an atmospheric dynamics (meteorology) model coupled with an atmospheric chemistry (air quality) model. The retrospective modeling conducted in support of SIPs has to demonstrate that industry-specific emission reductions will result in future compliance with the NAAQS. Inaccurate characterization of the atmosphere by these models can bias the result and lead to development of ineffective emission control strategies. Since the cumulative costs of implementing these controls can amount to billions of dollars, reducing the sources of uncertainty and increasing the confidence in the model results is of outmost importance to the regulatory agencies.

The retrospective nature of the SIP process provides a greater window for the direct use of satellite. In modeling the SIP design period, satellite data can be assimilated throughout the modeling period. This allows using a combination of observations and model to dynamically fill the atmosphere on small space and time scales during the design period to better recreate a test atmosphere over which emissions-reduction scenarios can be assessed.

The DST most commonly used in SIP applications, and in particular by our partner organizations, employs the Weather Research and Forecasting (WRF) model to recreate the physical atmosphere and the Community Multiscale Air Quality (CMAQ) or the Comprehensive Air Quality Model with Extensions (CAMx) as the air quality model. Both the emission estimates of primary chemical constituents and atmospheric chemistry are highly impacted by physical factors such as temperature, moisture, winds, mixing heights, and clouds. In the present work we will concentrate on improving the performance of WRF model which is being used by both CMAQ and CAMx and is employed by our applied partners. Furthermore, the current project will provide a satellite-based estimate of lightning generated NOx (LNOx) that is a key component of natural NOx emissions and is of interest to our partner organizations.

1.2 Partners/End-users and Their Responsibilities:

We will be partnering with the EPA's Atmospheric Modeling Division (AMD) at the National Environmental Research Laboratory (NERL) in Research Triangle Park, NC, the Lake Michigan Air Directors Consortium (LADCO), California Air Resources Board (CARB), the Texas Commission on Environmental Quality (TCEQ), and the Georgia Department of Natural Resources (GA-EPD). As the original designer and developer of the WRF/CMAQ modeling system, NERL/AMD continues to update the system by including new science and innovations in the DST. UAH, being among the original developers of CMAQ, continues to have a close collaboration with EPA. This will ensure the dissemination of the tools and technology developed under this project to the broader user community and the realization of the health and societal benefits expected from this project. Our other partners from Midwestern States, California, Texas, and Georgia, represent some of the most influential and proactive states with respect to air quality and public health issues (**please see the letters in section 8**).

LADCO: LADCO is an organization established by the member States of Illinois, Indiana, Michigan, Wisconsin, Ohio, and Minnesota to provide the air quality modeling platform that is used by its member states to demonstrate NAAQS attainment. This is to ensure that the member states protect human health and the environment by attaining and maintaining health-based airquality standards. LADCO's interest in the proposed project stems from the results from recent field campaigns (e.g., LMOS-2017) and modeling studies that indicate the critical impact of land-surface temperature and lake temperature on the transport of precursors and the consequent chemical regime responsible for the elevated ozone levels.

CARB: CARB is a part of the California Environmental Protection Agency and reports directly to the Governor's Office in the Executive Branch of California State Government. CARB's mission is to promote and protect public health, welfare and ecological resources through the effective and efficient reduction of air pollutants while recognizing and considering the effects on the economy of the state. The project proposed here is of particular interest to CARB as it addresses some of the pressing issues CARB is facing in simulating boundary layer growth and transport over complex terrain in California.

TCEQ: Over the past decade the TCEQ has actively participated in many field campaigns and has been funding follow-on studies to advance the science and incorporate the results in Texas SIP activities. Currently, TCEQ (through AQRP) is funding a research project that uses satellite skin temperature to better specify physical parameters associated with land use classes. Therefore, the current proposal not only leverages the AQRP activity, it also has direct impact on TCEQ's decision making activity as it addresses a priority area for TCEQ.

GEPD: The GEPD was one of the initiators of the Southern Oxidant Study, a ten year study of the hydrocarbon rich southern atmosphere and one of the largest air quality research programs carried out in the country. Georgia's concerns are biogenic HC and natural NO emissions which are highly dependent on temperature and moisture. Photolysis fields due to the patterns of convective cloudiness that is part of the summertime climate and cloudiness associated with stationary fronts that have often been part of the SIP design periods in the Southeast are also of concern to Georgia (as well as Texas). In addition, these summertime convective activities also are responsible for a considerable burden of LNOx in the Southeast.

While the results from this project have transferability to the nationwide SIP activities and have a broader impact, certain parts of the project are more appealing to certain geographical locations.

However, since the results from this project tackle some of the more pressing modeling issues and has a broad implication, our partners from California to Ohio will benefit from the outcome.

1.3 Baseline Performance and Emissions Control Scenarios:

The SIP modeling process is based on a set of sensitivity simulations to test the impact of an industry-specific emissions control. Thus, the regulatory agencies strive to have the best model performance (closest possible to the real atmosphere) as their control simulation. The baseline performance for this proposal is the control simulations from our partner agencies. Therefore, our metric for success is to demonstrate that the use of NASA data and science will enable the end-user to out-perform their best model performance. This means demonstrating improvements over the control simulation (without satellite data), showing a reduction in uncertainties, and therefore increased confidence in DST and the decision making process.

2 Earth Observations

The satellite products include surface skin temperature, insolation, and albedo from Moderate Resolution Imaging Spectroradiometer (MODIS) on-board AQUA and TERRA satellites and Visible Infrared Imaging Radiometer Suite (VIIRS) instrument aboard Suomi National Polar-orbiting Partnership (Suomi-NPP) satellite. In addition, we will be using Geostationary Operational Environmental Satellite (GOES) observations under NASA legacy science to complement polar orbiting observations obtained from VIIRS and MODIS. The project will take advantage of GOES-16 observations that offer a broad suite of observations relevant to this project at much higher temporal and spatial resolution. This will require retooling several NASA science products that are critical for our partner organizations.

The data products and satellite assimilation techniques to be used and enhanced in this project have been largely developed with funding from NASA's Earth Science Division (ESD) over the past few decades. Some of the original geostationary work was funded in the mid 80s under a NASA research program related to the use of satellite data for understanding the initiation and evolution of moist convection. A second generation of assimilation and satellite products was developed in the early 90s under process related studies of surface energy budgets for use in regional and global climate models. In the late 90s, a NASA/NOAA U.S. Weather Research Project took these process and case study approaches into the operational forecasting arena. The assimilation techniques were incorporated into the MM5 modeling system and techniques for processing satellite data products were made efficient enough for use in operational environments. These activities took place under RTOP, USWRP, and GEWEX programs.

This long-term NASA support led to a successful collaboration with EPA through which UAH scientists used satellite derived products for assimilation of insolation and skin temperature data into the surface energy budget of the meteorological model and assimilation of photolysis fields into the photochemical model in the CMAQ. More recent NASA support resulted in the development of satellite-based photosynthetically active radiation (PAR) that has proven valuable for several state regulatory agencies in their SIP modeling activities.

3 Technical/Scientific/Management Approach

3.1 Relevance to the Priority Topic of Health and Air Quality Application Area

The main goal of this project to use Earth observing data to improve the decision support tool (DST) that is being used by the states' regulatory agencies to implement air quality standards, policy, and regulations for human welfare. The targeted DST is the Weather Research and Forecasting (WRF) and the Community Multiscale Air Quality (CMAQ) modeling systems. The project will improve the fidelity of WRF/CMAQ predictions through the utilization of satellite data and will provide the techniques, tools, and the data available for **routine** use by the air quality community. Our research group at UAH along with its NASA, USEPA, and State partners has been a leader in developing techniques that employ satellite data to improve the performance of regional-scale meteorological and chemical transport models, especially within the atmospheric boundary layer (McNider et al., 94, 95, 98, 2005, 2011; Pour-Biazar et al., 2007, 2010, 2011, 2012; Macharo et al., 2011; White et al., 2017). We are proposing here to implement these satellite data assimilation techniques within the framework of the WRF/CMAQ air quality modeling system and make them available to the air quality community, facilitating the utilization of NASA satellite data and science that has proven assenting in our previous research.

3.2 Application of the Erath Observations to the Decision Making Activity

Our objective is to demonstrate the use of NASA satellite data, science, and models for improved 1) cloud simulation, 2) characterization of surface energy budget, 3) boundary layer development, and 4) lightning-generated nitrogen oxides (NOx) emission estimates and to integrate them in the DST for the user community. This involves the use of IR surface temperature, and VIS derived insolation products from Visible Infrared Imaging Radiometer Suite (VIIRS) onboard the Suomi National Polar-Orbiting Partnership (Suomi NPP) satellite and the Moderate Resolution Imaging Spectroradiometer (MODIS) aboard TERRA and AQUA satellites. The project heavily relies on geostationary observations of clouds, surface temperature, insolation, cloud albedo, surface albedo, and lightning information from the Advanced Baseline Imager (ABI) and the Geostationary Lightning Mapper (GLM) aboard the new generation of Geostationary Operational Environmental Satellite-R series). The first in these series, GOES-16 as GOES-east, offers geostationary observations at much higher spatial and temporal resolution. The proposed activity here requires retooling our data processing software, as well as techniques used for data assimilation in DST, to work with the new satellite data.

In the following the rationale for each of these objectives along with the results from our previous research will be presented. We will also discuss the relevance of the proposed work to the issues that our partner organizations are facing. The results from this project will help our partners with respect to their regulatory decision making that impacts air quality and public health. In sections 3.3 and 3.4 the techniques for satellite data assimilation within WRF, satellite-based LNOx emissions estimates, and modeling efforts will be presented. The use of satellite skin temperature as a model performance metric also will be discussed. Section 3.5 presents an estimate of our current application readiness level (ARL) and our expectation at the end of the project. Anticipated challenges and risks will be discussed in section 3.6.

3.2.1 Role of the Physical Atmosphere in the Decision Making Activity

Atmospheric chemical composition is significantly affected by meteorology. In fact air quality often shows better correlation with physical parameters than with chemical measures such as anthropogenic emission variations or initial chemical conditions. For example in almost every geographic setting, ozone levels are strongly correlated with temperature (Sillman et al., 1995).

Clouds have profound impact on photolysis fields, which are first order drivers of photochemistry. Temperature greatly impacts evaporative anthropogenic emissions and biogenic emissions. Temperature also directly affects chemical reaction rate and thermal decomposition. Wind speed and wind direction have strong impact on source/receptor relationships and air quality background. Mixing heights inversely modulate concentrations of pollutants and precursors.

These physical parameters also play a major role in the efficacy of control strategies. For example, if the physical model underestimates the mixing heights, the impact of emission reductions will be exaggerated. If temperatures are too hot in the model, it will increase thermal decomposition of organic nitrates, leading to steeper ozone-NOy curves and overstatement in NOx emission reduction strategies. Temperatures strongly impact biogenic emissions which can change the ratio of hydrocarbons to NOx, impacting efficiencies of hydrocarbon or NOx control strategies. Wind speed is the main factor diluting emissions of precursors. If models underestimate wind fields then sensitivity to emission reductions will be overstated.

Surface moisture impacts the partitioning of incoming solar energy between sensible and latent heat fluxes, directly impacting temperatures. Since the mixing heights are controlled both by land surface fluxes and synoptic or mesoscale subsidence, improvement in surface fluxes can also improve mixing height. Soil moisture also controls stomatal uptake of ozone which is one of the main losses of ozone in the boundary layer (Pleim et al. 2001). Thus, moisture may be one of the key factors in the viability of long-range transport of ozone impacting background levels.

One of the deficiencies of atmospheric models is their poor prediction of clouds. Clouds significantly impact photolysis fields and also alter the surface energy budget by reducing the incoming radiation. A modeling simulation that has photolysis rates too high will often show emission reductions to be more effective than in reality. In addition, clouds impact heterogeneous chemistry and aerosol recycling. Clouds also greatly impact biogenic hydrocarbon emissions (since the emissions are most sensitive to light).

Convective clouds generate lightning which in turn causes NO production (LNOx). LNOx is a significant source of NOx in the troposphere. With the ozone standards being reduced, the background ozone concentrations play an important role in devising SIP regulations. Thus, an accurate representation of this emission source in air quality models is crucial.

Use of satellite observations in the physical model can improve these key parameters. Satellite data have the potential to improve temperature predictions (Carlson 1986, Wetzel et al. 1984, Diak 1990, McNider et al. 1994, McNider et al. 2005). Satellites also provide the best observational platform for defining the formation and location of clouds. With geostationary observations of lightning, now available from GOES-16 Geostationary Lightning Mapper (GLM), it is possible to have satellite-based estimates of LNOx.

In the past, our research group has pioneered generating satellite data products and providing tools to assimilate satellite data in in meteorological and photochemical models to improve transboundary transport of air pollutants (Pour-Biazar et al., 2010, 2011), biogenic emission estimates (Zhang et al., 2017), cloud assimilation (White et al., 2017; Pour-Biazar et al., 2011, 2012), and photolysis rates and insolation specification (Pour-Biazar et al., 2007, 2011, 2012). While these techniques, the focus of previous NASA Applied Science (AS) projects, have improved the performance of models for SIP activity, there are still issues with the modeling system and data that need to be addressed. These issues include 1) the inadequate performance of

cloud assimilation in fine-scale simulations, and 2) disconnect between the model surface moisture, temperature, and fluxes and the attributes that were impacted by the cloud assimilation. We are proposing to address these issues and also provide a new technique for estimating LNOx based on satellite observations. These will be discussed further in the following.

The introduction of GOES-R series of geostationary satellites will provide geostationary observations at a much higher spatial and temporal scale. GOES-16 will replace GOES-13 as GOES-East, starting January 2018. Due to drastic differences in data stream, format, and resolution of the new data, many of the processing tools for our data products will cease to operate and need modifications. Many of our partner organizations (as indicated in their letter of support) rely on the availability of our satellite data products. This leads to a sense of urgency for retooling our processing software. Additionally, our assimilation techniques will be modified to take advantage of data with higher spatial and temporal resolution to address finer scale modeling issues.

3.2.2 Cloud Assimilation

Clouds play a critical role in the production and destruction of pollutants and the accurate prediction of clouds in space and time is essential for air quality modeling simulations. Clouds alter the photolysis rates (Pour-Biazar et al., 2007); affect the biogenic hydrocarbon emissions (Kesselmeier and Staudt 1999; Zhang et al., 2017); and impact the heterogeneous chemistry (Blando and Turpin (2000); Lim et al. 2010; Ervens et al. 2011). Clouds also modify the amount of vertical mixing; transport boundary layer air into the free troposphere, providing an important source of hydrogen oxide radicals (Tie 2003); alter the development of the boundary layer by suppressing the surface heat flux (Stull 1988); and in the case of precipitating clouds, present a significant removal mechanism for pollutants through wet deposition (Seaman 2000). Additionally, convective clouds, which generate lightning, provide a significant source of nitrogen oxides (NOx) into the free troposphere (Tie 2003). Pour-Biazar et al., 2007, showed that model errors in cloud simulation were responsible for large under- and over-predictions of ozone.

Previous Work: Despite many advances in microphysical and PBL parameterizations within weather forecasting models, creating clouds at the right time and location remains a challenge. This is especially the case when synoptic-scale forcing is weak (e.g. Stensrud and Fritsch 1994) such as often is the case during air pollution episodes. Because of the poor performance by the models, UAH has been pursuing data assimilation approaches to improve cloud simulation in the air quality models. Under a ROSES solicitation, UAH developed techniques to account for physical impact of clouds based on satellite observations, circumventing the problems associated with poorly predicted cloud fields. Model derived insolation, which plays major role in radiative fluxes and subsequent boundary layer evolution and is highly modulated by clouds, was replaced by satellite derived insolation (Gautier et al. 1980, Diak and Gautier 1983, and McNider et al. 1994).

However, since attenuation by cloud water can reduce photochemical rates beneath clouds and can accentuate production above clouds due to reflection (Madronich et al. 1987), further refinements were needed. Later, under another ROSES solicitation, satellite derived cloud transmittance and cloud top were used in place of model values in CMAQ (Pour-Biazar et al. 2007). Both of these direct replacements of the physical attributes of clouds made large differences in boundary layer characteristics and photochemistry in baseline tests (Pour-Biazar et al.

al. 2007). While these activities led to improvements in model performance, it produced a physical inconsistency in the model system. Insolation and photolysis fields did not agree with the model clouds. Thus, places where the photolysis was suppressed based on satellite observed clouds but the model was clear, the model did not have the appropriate mixing or venting. There was also no attempt at changing the liquid water content in the model to be consistent with observations. Thus, important chemical attributes such as moist chemistry for sulfur or organic aerosols were not handled properly.

To address this shortcoming, UAH pursued a separate activity that was initially funded under a NASA GEWEX project to improve the initialization of clouds for weather forecasting. While one might think that satellite estimates of liquid water would make the insertion of clouds relatively easy, this is not the case. Many research efforts have focused on assimilation of observations to improve model cloud fields (Chen et al. 2015; Spero et al. 2014; Jones et al. 2014, 2013, 1998; Zhang et al. 2013; van der Veen 2013; Otkin 2010; Yucel et al. 2003). However, the improvement in the model forecast, in time, has been limited. While these studies demonstrated limited improvements in model performance, they all concluded that the improvement was short lived.

The Need for Creating an Environment Conducive to Cloud Formation/Dissipation: Yucel et al. (2003) assimilated GOES visible and infrared data, but also found that enhancements to the forecast lasted a maximum of 3 hours. From this study, it was also concluded that the short term impact of cloud assimilation in NWP models is caused by the inconsistency between the model dynamic field and the thermodynamic field. The problem is that the production and sustainability of cloud water is dependent on the water vapor and temperature environment that provides the needed relative humidity. Therefore, the added cloud water in the model, where model has a dry environment, cannot be sustained. Conversely, when liquid water is removed from the model where observations show no clouds, the model will continue to produce new water. Direct insertion of liquid water can even deteriorate model performance. As an example, attempting to insert clouds (based on observation) at a position where the model is clear means that the cloud is likely being inserted where the model has subsidence as opposed to lifting. Inserting water where the model has subsidence will cause evaporation and further subsidence, exactly the opposite of supporting the observed clouds.

Improving cloud forecasts, including non-precipitating clouds which are important for air quality, becomes even more challenging due to the reduction in the amount of available observations. Standard weather service observations are not dense enough to be used for cloud specification, and the NWS WSR-88D radar network is not designed to be sensitive enough to retrieve cloud droplet information. Therefore, satellites remain the only platform which provides sufficient temporal and spatial resolution to quantify cloud fields. The GOES-16 Advanced Baseline Imager (ABI) has a spatial resolution of .5-km over the visible channel at 0.64 µm and 2-km resolution over the infrared channels for timescales down to 15 minutes or less (continental U.S., every 5 minutes). Thus, cloud albedo can be retrieved from the visible channel while the infrared channel can be used to estimate the cloud top heights.

The satellite retrievals to be used in this project are described in White et al. (2017) and Haines et al. (2004) and are based on an implementation of the Gautier et al. (1980) method with improvements from Diak and Gautier (1983), Diak (2017), and subsequent refinements at UAH.

Refer to Pour-Biazar et al. (2007) and White et al. (2017) for further information about the retrieval method.

3.2.3 Improving Land Surface Parameters

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) has greatly improved the characterization of the surface into classes. However, land surface models such as WRF-NOAH do not 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 capacity 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 and the Role of Satellite Observations:

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 (Wagener 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 cells, 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.

To determine the heat capacity (or bulk thermal resistance) of a single entity such as a brick in a laboratory setting, one would measure the amount of energy added and measure the corresponding change in the brick's temperature. The ratio of heat added to temperature change defines the heat capacity and/or thermal resistance of the brick. Now, look out your window and try to think how you might define the heat capacity or thermal resistance of the landscape you see. It seems a difficult task, if not an impossible task, to imagine how you could *a priori*

amalgamate all the different features – trees, buildings, roads to arrive at a grid scale heat capacity. But the satellites can measure the aggregate thermal energy emitted from such landscape and measure the change of surface temperature caused by the change in input energy by the sun. Thus, in the same manner as in a laboratory setting, the heat capacity of the composite surface can be calculated.

3.2.4 Satellite-based Estimates of Lightning-generated NOx (LNOx)

Lightning constitutes a significant source of nitrogen oxides (NOx) in the middle and upper troposphere and plays an important role in tropospheric ozone production (Wang et al., 2015, 2013; Koshak et al., 2014b; Biazar et al., 1995). LNOx is emitted over a deep tropospheric column. However, due to large concentrated number of lightning flashes in the storms, LNOx has significant impact on the background tropospheric chemical composition and may impact episodic air pollution events. Wang et al. (2015) showed that a summertime lightning event resulted in 28 ppb mid-tropospheric ozone enhancement over Huntsville, Alabama. Under previous ROSES calls, NASA funded projects to facilitate incorporating LNOx emissions in CMAQ (Koshak et al., 2014b; Allen et al., 2012). However, the current implementation in CMAQ distributes LNOx according to model predicted convective activities which may not agree with observations. With the data that will become available from the Geostationary Lightning Mapper (GLM) onboard GOES-16, near-realtime estimates of LNOx is now a possibility. In this project we introduce a new technique for estimating LNOx based on observed lightning energetics provided by GLM, and we will be testing it within CMAQ.

3.2.5 Relevance to Partner Organizations' Decision-making Activities

Here we provide a short description of how these activities are of interest to the geographical setting of our partner organizations.

3.2.5.1 Lake Michigan Air Directors Consortium (LADCO)

Elevated ozone levels remain a concern for the Midwestern states. Similar to other regions in the eastern U.S., ozone episodes in this region are often under hot weather, clear or hazy skies, low wind speeds, high solar radiation, and winds with a southerly component that are associated with slowmoving high pressure systems. Previous field studies over this region have indicated that the transport of ozone precursors from urban centers to



Figure 1. LST retrievals for July 13, 2009 from MODIS onboard AQUA.

areas over Lake Michigan, allows ozone production and accumulation within the shallow boundary layer over the lake, and a return flow due to Lake Breeze bring the elevated ozone back onshore and over the population centers (Koerber et al. 1991, Dye et al, 1995; Lyons et al. 1995). However, it appears that the air quality models overestimate ozone concentrations over cooler bodies of water, e.g., over Lake Michigan and Chesapeake Bay (Cleary et al., 2015; Loughner et al., 2014). Combined with the inaccuracies in the timing and extent of the onshore flow during the day, that transports the high ozone and aged precursors back over land, levels of ozone at the shorelines cannot be simulated accurately. This may be partly due to the representation of the stable boundary layer in the model and/or due to errors in lake and land temperatures that define the strength of lake/land breezes.

One may suggest that ozone overestimation over water can be attributed to the model being too stable. Then, the shallow stable layer over water would be analogous to a smog chamber (Dye et al 1995) which allows ozone production with little surface loss and this process might be responsible for the over-prediction. However, we will also investigate the possibility that models with too much mixing might partly cause an over-prediction. Our preliminary results with respect to Lake Michigan simulations indicate that a combination of using MODIS lake temperatures and short-tailed stability function (England and McNider 1995) can improve temperature and wind statistics under stable conditions. Figure 1 shows LST retrievals from MODIS (AQUA) for July 13, 2009. Use of MODIS lake temperatures significantly improved WRF simulations for this period. These results together with other components of this project would be beneficial to LADCO in their SIP modeling activities.

3.2.5.2 California Air Resources Board (CARB)

The formation and transport of ozone and buildup of particulates in California is largely controlled by the complex terrain and mesoscale meteorology of the region. During the summer, marine stratus along the California coast is a common feature. This is due to the interaction between the North Pacific High (due to conservation of absolute vorticity) and the cool marine

boundary layer. Further inland, boundary layer heights are controlled by both surface forcing and the subsidence. In addition to the large scale subsidence, the mesoscale subsidence in the Central Valley (from daytime subsidence due to terrain and subsidence behind sea breeze fronts) also contributes to the descending air. Models often overestimate boundary layer heights over land, but overestimate marine stratus.

Along the coast photolysis rates driving photochemical production are often controlled by marine stratus (see figure 2). In the presence of marine stratus, temperatures which impact biogenic emissions, evaporative and thermal



Figure 2. MODIS visible image showing land use variations and marine stratus for July 26, 2017.

decomposition of nitrogen species and photochemical production is suppressed. Thus, ozone and fine particle levels will be low. However, inland where skies are clear, temperatures and photolysis levels can be quite high. Additionally the thermal difference between land, ocean, and elevated terrain drives mesoscale circulations which can both transport pollutants and precursors as well as produce stagnant zones where pollutants can accumulate.

California has large variations in land surface characteristics, both natural and manmade, which control surface temperatures and moisture fluxes which in turn impact boundary layer heights, mesoscale winds, biogenic emissions, and thermal decomposition. In fact it is the temperature difference between land and sea that determines the strength and timing of the inland penetration of the sea breeze through the Sacramento Delta area. This in turn affects ozone production in inland areas. Further inland, it is the smaller scale temperature variations that modify the flow. The assimilation of satellite skin temperature to recover moisture and heat capacity proposed here would be of particular interest in such a setting as it promises to improve model boundary layer development. Correcting model overestimates of marine stratus is also of interest to CARB.

3.2.5.3 Texas Commission on Environmental Quality (TCEQ)

Texas has a varied physical atmosphere. In the east it is humid with substantial forest cover producing biogenic emissions. Fair weather cumulus and moist convection are a part of the air pollution climatology which must be dealt with in SIP modeling. Of particular note in Houston, the sea breeze is a critical part of the physical atmosphere. Late in the summer season, opposing synoptic flow can cause the sea breeze to develop late. Stagnant areas are produced as the opposing synoptic and sea breeze forcing battle. This leads to initial accumulation of precursors in the vicinity of the front with high photochemical potential that then moves northward across the metropolitan area. The temperatures and radiation impact biogenic emissions in the piney woods and mixed forest of SE Texas.

In northern Texas, stagnant conditions associated with stationary fronts are a challenge to the physical modeling, both in temperatures and photolysis fields. In fact, past extreme events and SIP design periods for Dallas have included stationary fronts. Overnight transport can bring elevated backgrounds into Dallas. In west Texas, terrain and low soil moisture can produce high temperatures and deep mixed layers. Convective clouds also pose a challenge to TCEQ SIP modeling efforts as they are the dominant feature along the stagnant fronts in northern Texas and also along the coast. Due to these diverse physical characteristics over Texas, TCEQ is interested in all components of the current proposal.

3.2.5.4 Georgia Environmental Protection Division (GEPD)

Georgia's physical atmosphere is not as diverse as California or Texas. However, it has unique aspects that make the physical modeling challenging. First, it has a high pollution potential due to its position relative to stagnating high pressure systems which have an axis along the Appalachians. This leads to low ventilation, and subtle land use changes from forests to urban surfaces can impact wind fields through surface temperature variations. As in east Texas, clouds can be a significant part of air pollution episodes.

However, it is probably winds that are the most challenging in SIP development. Large NOx sources around Atlanta can produce plumes of ozone in the rich hydrocarbon environment. Here temperature and radiation are important as they impact the biogenic emissions. Additionally, NOx from forest fires transported into the region can increase background levels of ozone.

3.3 Methodology for Improving the DST

3.3.1 Dynamical Adjustment of Clouds within WRF

The cloud assimilation technique is based on creating a dynamic environment that is conducive to creation/removal of grid resolved cloud through the use of GOES cloud information. The basic approach is to create positive vertical motion within the model to produce clouds and negative vertical motion to dissipate clouds based on observed cloud fields. The use of FDDA allows for the assimilation of horizontal components of the wind into the model in space and time. Therefore, the method provides a path to convert GOES cloud fields into vertical velocity estimates which are used to derive horizontal wind fields to be assimilated into the model through WRF FDDA.

The technique uses disagreement between the model and the GOES cloud fields to identify areas of under-prediction (model is clear and the satellite shows cloudiness) and over-prediction (model is cloudy and the satellite indicates clear sky). This is achieved by comparing satellite-derived cloud albedo with that of the model. A threshold cloud albedo is used to account for

uncertainties in both the satellite retrieval (i.e. impact of aerosols and water vapor) and the model derived cloud albedo. Then, a target vertical velocity necessary to produce or dissipate clouds within the model is estimated and nudged into the model through the use of a one-dimensional variational technique based on O'Brien (1970). The adjusted divergence field D_N^* needed to achieve the vertical motion prescribed at a certain height within a column based on an original "first-guess" field for each level *N* can be calculated as:

$$D_{N}^{*} = D_{N} + \frac{1}{\Delta h_{N}} \left[\frac{2N^{*}}{L^{*}(L^{*}+1)} \right] \left[\rho_{L} h_{L}^{*} - \rho_{L} h_{TL}^{*} \right]$$
(1)

Where D_N is the original divergence, Δh_N is the layer thickness, N^* is the current level index relative to the adjustment boundaries, L^* is the target level index relative to the adjustment boundaries, ρ_L is the density at the target level, $h_L^{\&}$ is the original sigma-h vertical velocity at the target level and $h_{TL}^{\&}$ is the target sigma-h vertical velocity. The adjusted divergence fields are then used to calculate the divergent component of the wind or the velocity potential. To determine the velocity potential from divergence, the Poisson equation shown in (2) is solved using a simultaneous over-relaxation (SOR) scheme.

$$MD_N = \nabla^2 \chi_N \tag{2}$$

Here, *M* is the sigma-h height scale, D_N is divergence and χ_N is the velocity potential at any level *N*. Once the velocity potential is known at each level, the new divergent component of the wind is added to the original rotational component of the wind field to fully construct a new horizontal wind field. Note that (2) will be applied everywhere within the model domain while the divergence adjustment is only applied to disagreement areas between the model and GOES. The result is a new divergent component of the wind at every grid point but it also acts to balance the mass throughout the model domain.

The inputs for the variational technique are estimated from a combination of satellite observation and model fields. For under-prediction case, a parcel of air should be lifted to saturation in order to produce a cloud comparable to GOES observation. For over-prediction case, the model has created a cloud in a grid location that GOES indicated is not cloudy. Thus, a downward displacement necessary to sufficiently warm the air parcels in order to evaporate the cloud will be estimated. In both cases, the displacement distance constitutes the target vertical velocity.

Applying this technique to a case study during summer of 2006 (TexAQS-II) improved model cloud performance, precipitation, insolation, and modestly improved surface statistics for wind speed, temperature, mixing ratio (White et al., 2017). The technique was also used in WRF simulations over the summer of 2013 (July-September, Discover-AQ field study) and resulted in similar improvements in WRF simulations. However, for 2013, the impact of these improvements on air quality simulations was also examined. Figure 4 shows the reduction in model insolation bias when compared to the U.S. Climate Reference Network (USCRN) surface observations. Cloud correction resulted in 10% reduction in biogenic emission estimates, which in turn improved ozone predictions and reduced ozone bias by 63%. As shown in Figure 5, cloud assimilation resulted in remarkable agreement with ozone observations over VISTAS region on certain days.

While model simulations with 36- and 12-km resolution might be adequate for the Clean Air Interstate Rule (CAIR), many of the SIP modeling activities requires model simulations with

finer grid spacing. In this project we will be testing the use of GOES-16 satellite observation, equipped with the Advanced Baseline Imager (ABI), which offers higher temporal and spatial resolution data. This new dataset is expected to improve the ability of the assimilation technique for higher resolution model simulations, which are expected to become the norm for both meteorological and air quality simulations.





3.3.2 LNOx Estimation from Recently Launched Satellite Lightning Imagers

A methodology has been introduced in Koshak et al. (2014a,b) and further expanded and refined in Koshak (2017) for directly estimating LNOx, on a flash-by-flash basis, from the observed cloud-top lightning optical energy detected from satellite lightning imagers. In basic terms, the total energy of a lightning flash is inferred from the observed cloud-top lightning optical emission, and then the total energy estimate is multiplied by a thermochemical yield for NOx [i.e., 1017 molecules/Joule as given in Chameides (1979)]. The methodology provides only a relative trend in LNOx since it is necessary to pick a calibration scaling factor (or " value") that sets the mean LNOx per flash in an arbitrary reference year to a widely accepted value (e. g., 250 moles/flash as given in the review by Schumann and Huntrieser, 2007). The methodology has already been tested and applied using data from the Tropical Rainfall Measuring Mission Lightning Imaging Sensor (TRMM/LIS) as discussed in Koshak (2017). The same basic methodology will be applied to data from the International Space Station LIS (ISS/LIS; Blakeslee and Koshak, 2016) and to the GOES-16 weather satellite Geostationary Lightning Mapper (GOES16/GLM; Goodman et al., 2013) when post launch validation testing of these sensors is completed. Therefore, independent relative trends of the LNOx on a flash-by-flash basis will be obtained by project collaborator Koshak. The results will be at exceptional spatial resolution (~ 5 km for ISS/LIS; ~10 km for GOES16/GLM), and temporal resolution (~2 ms for both sensors). In addition, GLM will of course provide 24/7 continuous monitoring which is a substantial improvement over the low-earth-orbiting observations offered by LIS.

Under this proposal, we will be providing the data and as another standard product from our retrieval system (GPGS). The data will be made available through the Global Hydrology Resource Center (GHRC) which is one of NASA's Earth Science Data Centers.

3.3.3 Surface Assimilation Techniques for Simple Land Use Models:

The development of complex land surface models mentioned above (section 3.2.3) was consistent with the need in the climate modeling community for surface models that could be run for years without being touched by data. Thus, they needed vegetative surface interaction, water balance models, etc. However, Diak 1990, McNider et al 1994, Anderson et al. 1997 and others argued that for short-term weather forecasting and for retrospective air quality simulations (McNider et al. 1998, Pleim and Xiu 2003) simpler models that could be constrained by observations might be preferred. The simple models avoid setting many uncertain parameters as in the complex models. This is the path to be pursued here with observational constraints provided by satellite skin temperature data. We will employ two techniques – 1) the Pleim-Xiu assimilation scheme (P-X) modified to use satellite skin temperature rather than NWS observed 2m temperatures and 2) an updated form of the combined McNider et al 1994 (here after McN94) and McNider et al 2005 (here after McN05) incorporated into the Pleim-Xiu framework in WRF.

Pleim-Xiu technique: Pleim and Xiu (2003) uses observed NWS surface temperatures to nudge moisture. The P-X approach adjusts surface layer moisture using the difference between model temperatures and relative humidity and analyses of observed temperatures and relative humidity. The Pleim-Xiu approach has been widely used and in recent California inter-comparisons, AND has performed better than the NOAH complex land surface scheme (Fovell 2013). Because NWS observations are coarse, we propose to replace the observed temperatures with satellite skin temperatures, and replace model 2-m temperature with derived diagnostic skin temperature from the Pleim-Xiu scheme.

McN94/McN05 technique: Basically, the McN94/McN05 retrieval of moisture and surface resistance performs a laboratory type experiment in the real world. Carlson 1986 proposed that the two most uncertain parameters in the surface energy budget in terms of their impact and specification are the surface moisture and thermal resistance. We use the morning rise in satellite skin temperature to recover moisture and the evening decline to recover the thermal resistance. Mathematically,

$$E_{s} = C_{b} \left[\left(\frac{dT_{G}}{dt} \right)_{m} - \left(\alpha \frac{dT_{R}}{dt} \right)_{s} \right]_{Morning} + E_{m} \qquad \text{and} \qquad C_{bs} = C_{bm} \left[\left(\frac{dT_{G}}{dt} \right)_{m} / \left(\alpha \frac{dT_{R}}{dt} \right)_{s} \right]_{Evening}$$

where E_s is the satellite derived evaporative flux as an adjustment to the original model evaporative flux, E_m , $(dT_G/dt)_m$ and $(dT_R/dt)_m$ are the ground temperature tendency in the model and satellite radiating skin temperature, respectively. Following Mackaro et al 2011 $\alpha = (dT_G/dt)/(dT_R/dt)$ is the internal fractional relationship in the model between the ground and skin temperatures (this is to avoid mixing the use of model ground temperatures and skin temperatures). The surface moisture is analytically recovered from the surface similarity relations. Here C_{bs} represents the satellite adjusted surface bulk heat capacity or thermal resistance to the model default C_{bm} . Note that the use of tendencies avoids issues with errors in absolute temperatures. Due to space limitations here we cannot provide the complete equations. We have successfully implemented the McN94/05 technique within the Pleim-Xiu scheme in WRF and have carried out successful initial tests against flux tower observations.

Land Surface Model Performance from Previous Studies: In a case study over TexAQS2000 period, which was an extraordinary hot and dry period and the model was not able to reproduce maximum temperatures, the application of the McN94 was able to dry the surface and produce

much warmer temperatures and deeper boundary layer heights. While the moisture recovery alone over corrected and produced daytime temperatures that were too hot and humidity values that were too low, the addition of thermal resistance recovery (McNider et al. 2011) resulted in remarkable improvements in model moisture and temperature fields. However, we also noticed that in the surface energy budget formulation, there was no distinction between ground temperature and skin radiative temperature. This correction is described in Mackaro et al. (2011).

More recently, the technique was implemented in WRF for Pleim-Xiu scheme and was tested in simulations for summers of 2013 and 2012. The assimilation improved model performance compared to NWS observations and the bias was reduced. The assimilation also improved model comparison to profiler wind data with substantial improvement in the low level jet at night. This is of particular interest to our partner organizations as it impacts long range transport and has implications for meeting EPA Clean Air Interstate Rule (CAIR).

3.4 The Integration of Earth observations into the decision-making activity

A major component of the current activity facilitates the retooling of software and updating the archiving system so that the satellite products continue to be available for our partner organizations as well as the broader user community. We will also make the tools and model codes available through EPA and CMAS websites. Throughout this process we will be working closely with the partner organizations to solicit their input and accommodate their needs. To facilitate the routine use of Earth observations, we adhere to the air quality modeling system that our partner organizations are currently using. This will ensure the successful integration of the techniques in our partners' decision making process. The following describes the models and the data to be used.

3.4.1 Modeling Activities

We will be using the latest version of WRF/CMAQ (WRF-3.9/CMAQ-5.2). Under a previous NASA Applied Science funded project, UAH has partly developed a technique for assimilating GOES skin temperature and cloud observations in the WRF. These techniques have proven to improve WRF performance. Our baseline simulations will take advantage of these advancements. We will be measuring the incremental improvements made by our assimilation techniques (discussed previously in this proposal) to the meteorological modeling as well as air quality model performance by carrying out several sensitivity studies.

UAH will be collaborating with our NASA collaborators on the implementation and testing of LNOx emissions estimates. A module will be added to CMAQ for ingesting the new LNOx emission estimates and distributing it vertically according to the profiles described previously. Since our activities impact both NOx and BVOC emissions, we will be testing the impact of cloud assimilation and LNOx separately in different simulations to quantify and document the incremental improvements from each activity. We will conduct WRF/CMAQ simulations for the summers of 2013 and 2016. The 2013 period will be used for preliminary evaluations as it coincides with Discover-AQ field campaign. Summer of 2016 has been suggested by our partner organization as a period of interest. We also will be using the techniques developed under previous NASA Applied Science funding that are relevant to the current activity.

3.5 Estimate of the ARL of the Application

Both cloud assimilation and skin temperature assimilation techniques have been developed and partially tested in the DST. Following NASA guidelines for Application Readiness Level (ARL) these activities are at ARL level 3. Because these components of application have been tested

and validated independently in WRF which is used in our partners' decision making process and have produced promising results. With respect to the LNOx estimates, since more work is needed before it can be tested and validated independently, it is still at ARL 2. We will be following ARL guidelines to follow the progress of this project and anticipate reaching ARL 7 (while having the potential of reaching ARL 9) by the end of this project. The added-value of the results from this project to our partners' decision making process is significant and the project has the potential of reaching ARL 9. However, the sustained use of these techniques within the partner organizations may take longer and may happen beyond the life of this project.

3.6 Challenges and Risks Impacting Project Success

Our work for transitioning from GOES-13 to GOES-16 is based on the projected timetable suggested by NOAA for decommissioning GOES -13 and replacing it with GOES-16. NASA SPoRT center is currently in the process of transitioning to GOES-16. We anticipate that by the starting date for this project GOES-16 data will be available. Since we will be relying on SPoRT to produce the operational products, any interruption in their operation may adversely affect this project. However, since we are colocated with SPoRT (at the NSSTC), and share resources, we will be able to coordinate our efforts quickly to overcome such interruptions. Another issue for this project would be a change of priority with some of our partner organizations. Since our goal is to have the results of this project integrated in the DST, we will be working closely with our partners to make necessary modifications to fit their needs.

4 Performance Measures

We will be using NASA guidelines and Application Readiness Level (ARL) to track the progress of this project. Project performance will be measured by closely following the schedule and adhering to the timetable and milestones. Standard tools and measures established by EPA and the end-user community will be used to evaluate the added-value of this project to the DST. Model performance will be evaluated against a base case in which the best practice in the use of DST in its current state will be employed. For the base case we adhere to the guidelines of the partner organizations for their SIP development. In addition to standard statistical metrics, the evaluation will use the Atmospheric Modeling Evaluation Tool (AMET) (Gilliam et al., 2005) developed by U.S. EPA. This tool is being used extensively by EPA and our partner organizations to document the overall quality of meteorological and air quality modeling simulations which are being used for emission control strategy development. Data for meteorological model evaluation is obtained from Meteorological Assimilation Data Ingestion System (MADIS), provided by National Oceanic and Atmospheric Administration (NOAA).

For evaluating performance of the meteorological model, EPA recommends statistical metrics and benchmarks suggested by Emery et al., (2001). A major component of this work targets improvements in model cloud simulations, surface fluxes and the boundary layer development, and LNOx estimates. Since EPA does not provide any guidance on how to assess the adequacy of these fields, we consider it prudent to suggest "interim" performance benchmarks for these variables. Through a comprehensive literature review, the benchmarks will be reviewed, and if necessary revised during the course of this project.

Additionally, working closely with our partner organizations, we will be convening regular conference calls and meetings to convey the progress of the project and to solicit their input about the priorities of the project. We will work with our partner organizations, so they can perform their own independent evaluation of the impact of assimilation techniques. This will also ensures the successful integration of our techniques in the DST.

4.1 Satellite Skin Temperatures as a Model Performance Metric

While National Weather Service and other observations of air temperature have been used to examine the performance of meteorological models in air quality settings, the spacing of these thermometers and their sitting criteria means they cannot capture the variation in temperatures across all the different land uses. Almost all modern land surface models used in climate or weather forecast or air quality settings have a grid average radiating temperature or skin temperature. The NOAH land surface model (Niu et al. 2011) has a diagnosed skin temperature as one of its fundamental outputs. Satellites have long used atmospheric window thermal IR temperatures to provide estimates of surface radiating temperatures. Unlike standard thermometer based temperatures the skin temperatures observed by satellites (approximately 2km in GOES-16 and 1 km in MODIS) provide a rich base for model inter-comparison. We will be using satellite skin temperatures as an additional observational set for model performance evaluation.

5 Anticipated Results/Improvements

The end result of this project will be the incorporation of an option to use NASA satellite data and science in the NERL/AMD supported and distributed WRF/CMAQ modeling system. Also, a web site with all the relevant documentations, tools, and links to the required satellite data will be provided and maintained through the NASA data center (GHRC) to be accessed by government and private users. Based on expected positive benchmarking, the contributions from the proposed project should improve model characterization of the physical atmosphere by improving model surface properties, boundary layer development, cloud radiative impacts, and the representation of the chemical atmosphere by improving lightning generated NOx emission estimates and ozone and aerosol distribution.

We anticipate improving surface O_3 and total $PM_{2.5}$ mass prediction through improvements in meteorological simulations and satellite-based LNOx estimates. The expected improvements in model performance are based on results from our previous research funded by the NASA ESD and briefly mentioned earlier. The generation and archiving near-real-time satellite-based products as explained in this proposal will benefit the larger air quality community beyond our partner organizations.

The benefit to the Nation's air-quality management system is the use of improved models to assess the efficiency and efficacy of control strategies for meeting the NAAQS. In a modeling environment where tens of billions of dollars in industrial and mobile source controls depend on the outcome of these SIP activities, reducing errors in the specification of the physical atmosphere that bias or change the impact of emission reductions would be invaluable.

Not only can the satellite data improve the robustness of the control strategy testing, but improved model performance will give confidence to regulators and to the industries being regulated that the models can be trusted. The SIP process is one in which a consensus must be developed on how costly control measures will be implemented. If regulated industries are not convinced that models are performing satisfactorily, then they may be reluctant to accept the results. This in turn could mean SIPs would not be approved by State regulatory commissions, or if approved over the objections of industry, then costly and antagonistic litigation could result. When NASA set up its new Application Program to improve decision-making systems, CMAQ was one of the examples in the Air Quality focus area that might be improved by NASA science and data. We believe that the present proposal is exactly in keeping with this paradigm.

6 Transition and Sustainability Plan

We will be working closely with our partner organizations to solicit their input about the priorities of the project and have them engaged in the progress of the project. In the third year of the project, we will begin transition activities. The transition and distribution are made up of two parts. The first is the code additions and changes within the WRF/CMAQ modeling system. The second is the dissemination and processing of satellite data. Scripts and software tools developed during this project will be part of the official WRF/CMAQ release that is distributed by U.S. EPA through Community Modeling and Analysis System (CMAS) center. Additionally, the tools will be tested at multiple locations including LADCO, California ARB, Georgia EPD and TCEQ. This will ensure a smooth integration within the end-user existing system. According to the needs of the end-users, a training meeting will be held towards the end of the project to provide additional support to the users.

Model Code and Scripts: A key aspect of the present project is to transfer the needed modifications to the DST (WRF/CMAQ system) supported by NERL/AMD. This will be carried out by transferring UAH's code changes to EPA. While UAH will be directly interacting with scientists at EPA, CMAS center will provide the needed support to EPA for implementing and testing the code. Initial tests will include replicating past satellite assimilation cases such as the 2013 Texas DiscoverAQ field study. Additional benchmarking can be carried out for other episodes or special periods of interest to EPA and our partners. These episodes include the periods of interest to our partner organizations (currently, summer of 2016). UAH and the NASA Short-term Prediction Research and Transition Center (SPoRT) will work closely with CMAS and EPA in the code transfer and testing process. If the benchmarks are successful, NERL/AMD, working with OAQPS through CMAS, will be the focus for disseminating the codes in their supported versions of WRF/CMAQ. This will be accomplished through their normal processes including workshops and including the EPA model clearinghouse. In addition to a User's Manual, we will also provide a document that describes the rationale, scientific basis, and benefits of the enhancements in this project. The PI is a member of CMAS steering committee and will oversee the transition activity.

Satellite Data: While implementing the code changes is straightforward, the real heart of work is the ingestion of the satellite data. Currently NASA-SPoRT center generates near-realtime products that will be used in this project. A major task in this project is the adaptation of retrieval software for GOES-16. Currently, UAH is archiving these products. These products, along with documentation and tools are provided to the user community through a web interface. Under the present project, we will be upgrading the web interface and will be providing skin temperature along with other derived products. The most cost efficient mechanism for disseminating the satellite data for use in WRF/CMAQ and other models is to provide the tools, document, and the links to the raw satellite data through the Global Hydrology Resource Center (GHRC) a NASA data center. At the end of this project we will work with GHRC toward such transition. The distribution of the data would also take advantage of the existing GHRC structure. This arrangement would parallel EPA relationships for land-use data sets with U.S. Geological Survey or meteorological data sets with NOAA-National Centers for Environmental Prediction. In these cases, the data sets are critical to EPA's modeling mission but because taking full responsibility for maintaining such a system lies outside EPA's main mission and expertise, EPA relies on the other agencies.

7 Project Management and Schedule

Dr. Arastoo Pour Biazar, University of Alabama in Huntsville (UAH, PI) will be responsible for coordination of all aspects of this research. He also will be responsible for modeling efforts. Dr. Pour-Biazar has been a member of EPA's Models3 development team and has been involved in air pollution and atmospheric modeling studies from plume- to global-scale, and will oversee the implementation, benchmarking, and transition activities in this project. Dr. Pour-Biazar is the PI of an ongoing project that has made the satellite-based photosynthetically active radiation (PAR) data available for the air quality community. He is also a member of CMAS steering committee and served as co-PI on NASA's Air Quality Applied Science Team (AQAST). Dr. Pour-Biazar will be assisted by the following Co-Is for implementing different components of the current project.

Dr. Richard McNider (Distinguished Professor, UAH, Co_PI) is well known in the air pollution community for his numerous scientific contributions over the years, among others, in mesoscale model development, atmospheric dispersion, boundary layer predictability, and satellite assimilation. Dr. McNider, will be serving as a science-PI and will be directing the activity with respect to the surface energy budget and will oversee the implementation of this technique within the DSS. He will be participating in the modeling effort and also in the interpretation of the results. He will be assisted by Dr. Maudood Khan (Co-I) and a post-doc for WRF and Air quality simulations. Additionally, Drs. Shuang Zhao (Co-I, economist) and Susan Alexander (collaborator, nursing) will perform societal impact analysis to quantify the added-value of this project.

Drs. Christopher Hain (NASA, Co-I), Bradley T. Zavodsky (NASA, collaborator), and William Koshak (NASA, collaborator) are also accomplished NASA scientist in the area of remote sensing. Dr. Hain will lead the efforts at SPoRT (the NASA Short-term Prediction Research and Transition) for near-real-time satellite surface temperature retrievals. Dr. Zavodsky will lead efforts for generation of GOES-16 ABI products. Dr. Koshak (NASA, collaborator) will be responsible for satellite-based LNOx. They will be assisted by UAH personnel.

7.1 Schedule

The following presents a timeline for individual tasks as described in the text.



8 Budget Justification: Narrative and Details

The attached budget, requesting \$870,753, provides the cost of the three years effort by UAH and partners. The majority of the budget is for personnel to carry out the data retrieval, analysis, and model runs. Dr. Arastoo Pour Biazar will devote approximately 1.5 months per year to this project and will serve as the Principal Investigator. He will oversee the project direction and will be responsible for coordination and communications with EPA and end-users to ensure a successful transition of the techniques to the user community. He will also have a major role in performing model simulations and evaluation.

Dr. Richard McNider will be responsible for surface energy budget activity and the implementation of the satellite assimilation technique within Pleim-Xiu scheme in WRF. Dr. Maudood Khan will be responsible for WRF and CMAQ simulations. Dr. Shuang Zhao will assist in performing impact analysis.

Drs. Christopher Hain (NASA, Co-I), Bradley T. Zavodsky (NASA, collaborator), and William Koshak (NASA, collaborator), an accomplished NASA scientist in the area of remote sensing, will lead the efforts at SPoRT (the NASA Short-term Prediction Research and Transition) for near-real-time satellite retrievals. Dr. Koshak will provide satellite-based lightning NOx estimates. A UAH research associate and a student will be assisting them in adapting the retrieval software for GOES-16.

The team will be assisted by research associates and graduate students who will be helping the PI, CO-Is, and NASA collaborators to fulfill their responsibilities. During the third year of this project, UAH will work with EPA and partner organizations on transition activities. UAH will be upgrading the satellite data distribution web-interface and will work with the NASA SPoRT center and GHRC for near-real-time production and distribution of derived products.

UAH computing facility will be used for model runs and storage. Since this project requires visualization, analysis and archiving of a large volume of satellite data, in addition to UAH computing facility we will purchase additional storage and PCs, dedicated to the needs of this project. These will complement the existing UAH facility. The additional data storage is needed to store the new satellite products from GOES-16 (due to higher spatial and temporal resolution of observations). Additional computing and storage purchased for this project will be dedicated to the scientific needs of this project. Dell PowerEdge will be used for reprocessing the historical data and also for the upgrade to the web-site. The PCs will be used for producing images for graphical display on the web-site, data ingest, and monitoring data flow between NASA and UAH machines.

Funds have also been allocated for publications and travel to meetings with EPA, partner organizations, and other professional meetings.

9 Facilities and Equipment

Under the present project UAH and NASA (NSSTC) would operate and maintain the satellite processing system. The NASA Short-term Prediction Research and Transition (SPoRT) center, co-located at NSSTC, currently operates the Geostationary Operational Environmental Satellite (GOES) Product Generation System (GPGS). GPGS is a set of computer programs designed to generate meteorological data products in real-time or case-study mode using measurements from the GOES-East Imager and Sounder instruments. GPGS has been operating since 1998 and has been generating Imager and Sounder products since 2000. Products generated from the Imager and/or Sounder instruments are skin temperature, total precipitable water, cloud top pressure, cloud albedo, surface albedo, and surface insolation. Intermediate products used to create the primary products are cloud mask and 20-day clear-sky composite images in the visible and infrared spectral regions.

UAH facilities comprise total of 37 GIS & RS computers with powerful state of the art GIS and image processing software. The workstations are equipped with industry standard ESRI ArcGIS 10.5 with Spatial, 3D, and Geostatistical Extensions as well as ENVI 5.4+Zoom and ENVI 5.0, and IDL 8.6 software packages. For CPU intensive applications/models, we operate a high performance Linux cluster with 1224 processor cores and 9 TB of memory. Network based storage is available for high volume data, as is a high speed network link (Internet 2) for collaboration with other educational institutions and government agencies. We are a Tier2 level provider for LDM data feeds.

Through our collaboration and colocation with NASA SPoRT center we will have access to realtime GOES-16 data. NASA's Marshall Space Flight Center GOES-R series GOES Rebroadcast (GRB) receiving system consists of a 6.5 meter diameter antenna with motorized pointing, a dual-channel L-band feed, Low noise amplifiers and demodulator. A data acquisition computer is directly connected to the demodulator unit; a data processing computer is used to derive Level 2 products from the ABI instrument. The current system receives data from GOES-East. The system receives data from the ABI, GLM, SUVI, MAG, SEISS and EXIF instruments. Data is disseminated via the Ethernet within NASA and to our partners in near-real time. A second receiving station is in process of being installed and will be used to acquire data from the GOES-S satellite once it launches.

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