Annual Progress Report 2009-10

Improving an Air Quality Decision Support System through the Integration of Satellite Data with Ground-based, Modeled, and Emissions Data

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Abstract

The National Ambient Air Quality Standards (NAAQS) established by the Clean Air Act (CAA) amendments of 1990 were aimed at protecting human health and welfare, while the EPA Regional Haze Rule (RHR) of 1999 set targets to restore visibility to natural conditions by 2060 in national parks and wilderness areas. States and tribal associations are required to prepare Implementation Plans demonstrating attainment of the NAAQS and reasonable progress toward RHR targets. The air quality and emissions control assessments needed to support these plans can greatly benefit from satellite data, which have proven to be a valuable complement to surface observations, especially in locations where the latter are sparse, or where aloft processes affect ambient concentrations. The complex process of developing the Implementation Plans requires a synergistic integration of these data and the tools for their analysis into a "system of systems" that provides them in a framework designed to serve a diverse spectrum of end users. Thus this project aims to enhance the Visibility Information Exchange Web System (VIEWS) and its associated Technical Support System (TSS) by integrating NASA satellite data relevant to air quality and visibility assessments with surface observations, air quality model output, emissions information, and an advanced toolkit for interpretive analysis and visualization of the data.

The project objectives in support of this goal for VIEWS/TSS are to: (a) routinely capture, analyze, and process Earth Observations at a high temporal and spatial resolution to provide land use/land cover inputs to emissions and air quality modeling analyses; (b) acquire satellite data to improve activity data and emission rates for natural and anthropogenic area and point sources (individual and clustered) in remote and urban areas; (c) incorporate satellite data to improve boundary inputs and to evaluate regional-scale chemistry-transport models (CTMs); (d) develop and integrate advanced analysis tools for these data to better understand the relevant atmospheric processes and their representation in the CTMs, and (e) visualize and quantitatively analyze satellite data in combination with existing monitoring and emissions data, and modeling results within a unified data analysis and decision support platform.

Year 1 laid the groundwork for most of the data import and tool development for the VIEWS framework. In Year 2 of the project (1) the VIEWS/TSS satellite data image browser was further refined and automated for easy rendering of a large number of images in batch, including display on a clickable background map using Google Maps; (2) the VIEWS/TSS data storage and access capabilities were enhanced to accommodate the new data and toolkit integration; (3) substantial progress was made on dynamic import of data in VIEWS/TSS from NASA's Giovanni and EPA's Remote Sensing Information Gateway; (4) a regridding tool to project and map L2G and L3 OMI data on user-specified CMAQ domains and model resolution was developed and is being ported to the VIEWS/TSS Linux server; (5) the Atmospheric Model Evaluation Tool was enhanced to provide statistical comparisons of regridded satellite-, model- and surface-based data for selected air quality metrics, and has been ported to VIEWS/TSS; (6) CMAQ simulations of the Rocky Mountain Atmospheric Nitrogen and Sulfur (RoMANS) 2006 use-case study were completed; the output was integrated in the VIEWS database, and diagnostic model performance analyses for high ammonia deposition episodes were begun with the python-based Process Analysis tool, targeted next for VIEWS integration; (7) VPM, a visualization/animation tool for particulate matter size distributions has been developed and is nearly ready for beta testing; (8) a NASA satellite data training course for air quality applications was organized and offered at the annual Community Modeling and Analysis System conference in 2009, and (9) progress on these tasks was reported throughout the year at various meetings, including two conferences.

Contents

1 Introduction

The Clean Air Act (CAA) amendments of 1990 promulgated by the U.S. Environmental Protection Agency (EPA; EPA, 2001) led to the establishment of the National Ambient Air Quality standards (NAAQS), and provided the framework for managing air quality in the United States. Since the original CAA legislation of 1970, responsibilities have also been added to "prevent the significant deterioration" of national parks and other pristine areas and minimize human exposure to hazardous air pollutants, and to control emissions leading to acid deposition (NAS, 2004). In 1999 the Regional Haze Rule was added to the suite of EPA regulations (EPA, 1999) to improve visibility in pristine areas; it includes long-term targets to meet a national goal of restoring visibility to natural conditions by 2060 in 156 national parks and wilderness areas. These regulations require states and tribal associations to prepare State (and Tribal) Implementation Plans (SIPs/TIPs) demonstrating attainment of the NAAQS and reasonable progress toward visibility targets. There are many useful products and systems to help develop these plans; satellite data have proven to be a valuable complement to surface observations in the types of assessments required, especially in locations where the surface data are sparse, or where aloft processes affect ambient concentrations. However, the air quality and emissions control assessments entailed in air quality decision support require providing air quality managers and planning agencies more than just the raw materials, i.e., collections of data, products, and interesting images. What is needed in addition is a synergistic integration of data and analysis resources into a "system of systems" that presents the data and the tools for their analysis in a flexible framework that serves a diverse spectrum of end users from researchers and analysts to policy makers and air quality managers. The goal of this project, therefore, is to enhance an air quality decision support system (DSS) through such an integration of NASA satellite data products relevant to air quality and visibility assessments with surface-based observations, air quality model output, and advanced data analysis tools for comparing and interpreting the data.

The DSS selected for these enhancements is the WRAP Technical Support System (TSS), built upon the framework of the Visibility Information Exchange Web System (VIEWS), hosted by the Cooperative Institute for Research in the Atmosphere (CIRA). The system (hereafter VIEWS/TSS) integrates monitoring, modeling, and emissions data with decision support tools, standards interpretations, and procedural structure to guide planners through the analyses needed to develop effective and legally defensible emission reduction plans for compliance with air quality and visibility regulations. VIEWS/TSS has been designed with input from a diverse group of Federal Land Managers, states, tribes, and local agencies to add interpretive value to the products of several key data centers and support systems, and to optimize decision making.

This project is a joint effort by the University of North Carolina at Chapel Hill (UNC), CIRA, and the University of Maryland Baltimore County Joint Center for Earth Systems Technology (JCET); the UNC Institute for the Environment (IE) leads the overall project. The development of an advanced visualization tool for particulate matter (PM), an add-on task to the original scope in Year 2, is being done by IE in collaboration with visualization specialists at UNC's Renaissance Computing Institute (Renci). Guidance on end user needs for system enhancements has been provided by a project steering committee consisting of institutional representatives from the Western Regional Air Partnership (WRAP), the National Park Service (NPS), the Utah Division of Environmental Quality (UT-DEQ), the North Carolina Division of Air Quality (NC DAQ)and the EPA Office of Air Quality Planning and Standards (OAQPS).

1.1   Baseline System Performance

Although VIEWS/TSS included a solid suite of qualitative and quantitative databases and tools for state and regional air quality planning at the beginning of this project, it still needed to address some significant user needs by way of data and analysis tools:

1.1.1   Observational data

Surface measurements had been the staple of observational data in VIEWS/TSS for planning applications and control strategy development to address regional haze. However, they provide little insight into the source and spatial distribution of significant aerosol events, such as large fires and dust storms, which transport pollutants from distant sources and severely impair regional visibility. As it is impossible to infer the aerosol vertical profiles and compositional variability aloft solely from ground-based measurements; long-range transport and vertical mixing of pollutants cannot be adequately characterized during such events. This makes it difficult to properly attribute local vs. remote sources of pollution, and track pollutant precursors, both of which are important steps in effective control strategy development.

1.1.2   Emissions data

Currently available data in VIEWS/TSS include emissions from wild and prescribed fires that are important for visibility impairment. Trends in fire occurrence indicate that emissions from wild fires will continue to increase in strength and frequency in future years. Better information, especially by way of near real-time data on fire areas burned and fire counts, is needed to provide inputs to fire emissions models used in the current bottom-up inventories compiled for inputs to air quality models used in SIPs and TIPs. Similarly, dust emissions from far-away sources have a significant impact on air quality over the U.S., and are poorly characterized in most inventories. While wind-blown dust models have recently been developed to improve dust emission fluxes, they need to be evaluated against observations that adequately capture the origin and transport pathways of the dust plumes. Updated information on land use and land cover would help improve the characterization of both fire and dust emissions.

1.1.3   Model data

To improve the reliability of their predictions, air quality models must be thoroughly evaluated against observations. Absent the knowledge of how model results aloft compare with observations, most model evaluation studies, undertaken at considerable expense by air quality planners, are incomplete at present. Further, ground-based networks are resource-intensive, and thus lack extensive spatial and temporal coverage. Data from the periphery of these networks (especially over the oceans, and in the less populated regions in the Western U.S.) are often sparse, making it difficult to specify adequate model boundary inputs that capture the effects of emissions from offshore sources.

1.1.4   Analysis tools

VIEWS/TSS provides visualization of emissions data so that planners can get a qualitative sense of source locations, geographic distribution of pollutants, and the transport pathways for the emissions. However, analyses of primary emissions are in themselves insufficient for understanding the secondary production mechanisms in the atmosphere between the source and receptor sites. For example, three key atmospheric constituents responsible for regional haze, namely sulfate, nitrate and ammonia are governed by highly nonlinear, secondary chemical

reactions that cannot be understood solely by examining the primary emissions of precursors. A case in point is the problem of high nitrogen deposition in Rocky Mountain National Park (RMNP), which was identified as a critical need area at the start of this project by end users at the National Park Service. At issue is how much of the deposition during episodic periods is due to long-range transport of NO_x from the Southwest vs. local ammonia sources from the agricultural lands east of the Park; both of these produce volatile inorganic PM species that can contribute to the nitrogen loads in the sensitive ecosystems in RMNP. Current modeling of an intensive field campaign period in 2006 to study the issue showed severe underprediction of ammonia and particulate ammonium by the air quality model. Tools are needed for more in-depth analysis of the model algorithms and/or the model inputs.

Another seldom-examined aspect of the problem is the PM size distribution, which is a powerful diagnostic tool because it responds rapidly to atmospheric dynamics, chemistry and microphysics. Efficient visualization tools have not yet been developed to examine this response dynamically, i.e., with animation capability. Access to tools that can perform in-depth process-level analyses and more complete, dynamic visualizations of model results and observations, together and separately, is needed to understand the physical and chemical processes responsible for the measured pollutant levels, and to propose effective control measures.

1.2   Summary of Year 1 Accomplishments

The overall goal of this project is to improve the reliability and value of the air quality decision support system through the integration of Earth Science Research results, and to transfer the technology to the end-user community. The project objectives were finalized through discussions that began with the end user group representatives at the Design workshop that kicked off the project at CIRA in Year 1. The revised task list was communicated to NASA in our first quarterly project report and posted on the project wiki. These revised objectives are to:

a) routinely capture, analyze, and process Earth Observations at a high temporal and spatial resolution to provide land use/land cover inputs to emissions and air quality modeling analyses;

b) acquire satellite data to improve activity data and emission rates for natural and anthropogenic area and point sources (individual and clustered) in remote and urban areas;

c) incorporate satellite data to improve boundary inputs and to evaluate regional-scale chemistry-transport models (CTMs);

d) develop and integrate advanced analysis tools for these data to better understand the relevant atmospheric processes and their representation in the CTMs, and

e) visualize and quantitatively analyze satellite data in combination with existing monitoring and emissions data, and modeling results within a unified data analysis and decision support platform.

Our project tasks were also slightly modified to reflect these objectives to meet the end user needs in improving model inputs, interpreting model outputs, and assessing the source contributions to observed air quality metrics during routine operation of the surface-based networks, as well as during pollution episodes. The following is the revised list of project tasks that support the objectives:

- Task 1: Integrate satellite data into the VIEWS/TSS database
- Task 2: Enhance existing VIEWS/TSS tools for satellite data access
- Task 3: Incorporate current standards in web coverage/management services, and interoperability with other decision support systems used by the community
- Task 4: Investigate efficient ways to store/subset/serve modeled data for air quality analyses and evaluation against observational data
- Task 5: Explore and incorporate satellite data products in VIEWS/TSS to improve land use, land cover, emissions rates and activity data inputs to models
- Task 6: Incorporate tools in VIEWS/TSS for advanced analyses and intercomparisons of observational and modeled data
- Task 7: Demonstrate key applications of the enhanced VIEWS/TSS
- Task 8: Engage end users, transfer technology, and provide training
- Task 9: Develop an interactive animated visualization tool for PM size distributions derived from modeled and observed data (add-on task for completion in Year 2).

In Year 1, with the exception of future-year fire modeling, which was replaced with other tasks upon the recommendation of the end users during the initial Design Workshop, progress was made on all tasks originally proposed for the year. Task numbers are provided in parentheses, and additional or modified tasks are noted where appropriate:

- A Design Workshop was convened and the project scope was refined based on the end user feedback; tasks involving the future-year modeling of fires originally proposed were replaced with additional tasks on hind-cast modeling and analysis of relevance to end users, and investigating synergies with other data systems (Task 8)
- A project wiki was created for information exchange among team members and end users (Task 8)
- A number of satellite data products for air quality, meteorology and land use/land cover were acquired in collaboration with JCET for multiple years (2006-8) from the Ozone Monitoring Instrument(OMI) on board Aura, and the Moderate Resolution Imaging Spectrometer (MODIS) from both Terra and Aqua satellites, and loaded into VIEWS/TSS (Tasks 1 and 5).
- A prototype visualization tool for satellite data products was implemented in VIEWS, along with many other improved tools for browsing existing data (Task 2).
- Metadata were added for satellite data, and the capability for browsing data catalogs was improved (Task 3)
- Work began to explore synergies and interoperability with RSIG and CMAS within the VIEWS/TSS framework (added; Tasks 3 and 4)
- The groundwork was laid for modifying and porting AMET and pyPA to VIEWS/TSS (Task 6)
- Work began on data acquisition to model the RoMANS study as a use case for a demonstration of the analysis tools (replaces future-year fire modeling; Task 7)
- A NASA satellite data training pilot course for air quality analysis was organized and offered to project end users and team members (Task 8)

- Overviews of VIEWS/TSS capabilities were presented at two conferences, at the start and end of the performance period respectively (Task 8)

- In addition, a scope and budget were developed in collaboration with Renci and approved by NASA for the add-on task to visualize PM size distributions (Task 9) to be completed in Year 2.

2 Major Activities and Accomplishments of Year 2

2.1 Data and Tools Integration in VIEWS

2.1.1 Satellite Image Browser

The prototype "image browser" created in Year 1 for viewing satellite images was developed further in preparation for releasing a production-ready version on the VIEWS website. Efficient methods for automating the bulk production of web-formatted images from the source HDF data files were explored and tested. The Interactive Data Language (IDL) environment was found to be the most efficient means of reading and filtering the satellite data, and producing high-quality images for the web; IDL routines were therefore developed for batch processing of the data. This enables the satellite images to be produced as often as needed in bulk in an almost-fully-automated process. The resulting images are automatically named according to a specific convention to enable efficient, programmatic search and retrieval by the web tools. A specialized web page was developed to provide an intuitive user interface for selecting and viewing the images, and creating slideshows for animating a succession of images. After the next update of the VIEWS website (scheduled for March 2010), this tool will be available at: http://views.cira.colostate.edu/views/SatelliteData/Images.aspx.

2.1.2 Google Maps Visualization and Query Tool

The image browser capabilities have been intentionally limited to provide qualitative rather than quantitative information for quick exploration of the satellite data. To provide more comprehensive quantitative exploration of the data, a prototype for a more fully-featured visualization tool was developed to display satellite images on top of user-selected base maps via Google Maps. Google Maps can currently only display "overlays" (with associated opacity settings) if they are formatted in the Keyhole Markup Language (KML); therefore a process for producing KML files from the satellite data was needed. To accomplish this, a feature of KML was exploited whereby a reference to an external image file (in GIF, JPEG, or PNG format) can be embedded in a KML file such that the original image is rendered by Google Maps with additional settings (such as opacity). Thus the satellite image browser files can be leveraged for double duty in the Google Maps tool by simply creating KML "wrappers" for them. This new tool will allow a user to visualize the satellite data over a base map and click on a location in order to query the quantitative satellite data as well as any ground-based, modeled, or emissions data that are available for the selected location.

2.1.3 SQL Server 2008 Spatial Data Features

The latest version of Microsoft SQL Server introduced new capabilities for managing a wide range of geographical data, and these features have been leveraged to store a -selected subset of the satellite data in the VIEWS relational database for (a) enabling the query capabilities of the Google Maps tool, and (b) enhancing existing VIEWS tools to provide access to the data. As the

primary goal of this project is to enable the online comparison of ground-based, modeled, emissions, and satellite data through an integrated suite of tools, robust techniques for storing and cross-referencing the satellite data to these other datasets were developed by using the new capabilities of the SQL Server spatial database engine. Procedures for routinely extracting subsets from the raw HDF files and storing them in the relational database were developed, and the Transact-SQL queries for retrieving the data were designed and tested. The Google Maps tool was designed to use this infrastructure for performing *ad hoc* queries across all available datasets and presenting the results on the map (via pop-up "balloons"), and in other web components such as charts, graphs, and HTML tables. The beta version of this tool is currently in development and is planned for release on the VIEWS website i the second quarter of 2010.

2.1.4   Satellite Data Projection and Regridding Tool (regrid)

Satellite data are available with sufficient post-processing to enable visualization on a lat-long grid averaged over the specified days of data (1 day minimum), or as swath data (typically 10 km x 24 km pixel resolution), which include the time of overpass for each pixel. The spatial and temporal resolutions of the air quality model grid are typically not commensurate with those of the satellite data, making it difficult to quantify the differences between the two. To increase the usefulness of satellite data in air quality analyses which compare modeled and observational data, UNC has developed a Linux-based tool to project the satellite data from its native lat-long grid to that used by the Community Multiscale Air Quality model (CMAQ) described in Byun and Schere (2006) and Binkowski and Roselle (2003). The regrid tool uses the projection information and grid information specified by the user in a shell script to remap the satellite data on to the model grid using an area-weighting algorithm; this provides the user maximum flexibility in the grid specification.

In this period of performance, Co-I Dr. Prados provided PI Shankar and UNC developer Ran assistance on data retrieval, data formats and metadata interpretation, to download data from the Giovanni website and MIRADOR at GES DISC. The use of both HDF5 and HDF4 data formats in the data download were explored. Due to some instability with the geospatial data libraries used to read and process the HDF5 data, the tool currently processes HDF4 data from Giovanni. It is currently being used to regrid Level 2G (L2G) and Level 3 (L3) measurements from OMI. The data of interest for ozone analysis are tropospheric column (30% cloud screening) of NO_2, CO and HCHO, and for PM, the Aerosol (extinction) Optical Depth (AOD) at 388 nm, deemed to be the most reliable wavelength for OMI measurements of this quantity. Aerosol Absorption Optical Depth (AAOD) would also be very useful in the analysis of long-range transport of biomass combustion plumes.

The output data from the regrid tool are produced in both netCDF and ASCII formats for use in the Atmospheric Model Evaluation Tool (AMET) for comparison with CMAQ output. For the level of processing (L2G and L3) currently used in the satellite data, the regridded data are considered to be averages over the local daylight hours. The capability to grid swath data and match the overpass time with the CMAQ output time for a more fine-grained comparison is expected to be available around mid-March. The satellite metadata vary for each data product; to minimize effort, therefore, this tool will initially be enabled in VIEWS to batch process several data products currently served by VIEWS, and regrid the data to a pre-determined set of nested CMAQ grids (see Figure 1) used by a large class of end users. In addition, the ability for the user to specify the grid and projection information at run time through the web interface will be enabled. The tool will be available to the beta testers for a selected number of data products by

the beginning of the third year of performance. In addition, it will be enhanced to grid CALIPSO extinction profile data on user-specified grids.

2.1.5   CMAQ Post-processors for Aerosol and Tropospheric Trace-gas Products

To allow quantitative comparison of the air quality model output with the regridded satellite data UNC co-I Dr. Binkowski has developed two Linux-based post-processors of CMAQ output PM concentrations and gas phase mixing ratios to provide, respectively, the unitless Aerosol Optical Depth (AOD) and the tropospheric column abundance (molecules/cm^2) of any gas-phase species available in the model chemical mechanism.

The AOD calculator uses refractive indices provided as look-up tables as a function of spectral interval for the various aerosol types (e.g., water-soluble, insoluble, soot, and water) provided by the Optical Properties of Aerosols and Clouds (OPAC) software package of Hess et al. (1998). From these, the composite index of refraction for the aerosol is calculated as a function of aerosol volume concentration and chemical composition (e.g. sulfate, nitrate, black carbon, dust, and sea salt). Scattering, and absorption cross-sections for aerosols and gases and predicted aerosol size distribution parameters (number concentrations and mode mean diameters) from CMAQ are used in a highly optimized optics code based upon analytical expressions following Heintzenberg and Baker (1976), and Willeke and Brockmann (1977), to calculate the single scattering albedo, asymmetry factor and AOD. The tool was initially developed for a specific CMAQ chemical mechanism, but is being made more flexible to handle all operational mechanisms in CMAQ to get the aerosol species of interest from the model output. It will eventually be made available in the CMAS toolkit, m3tools, and also made available in VIEWS through the CIRA Linux server.

The vertintegral tool, currently available in the CMAS toolkit m3tools, uses a simple vertical integration of the gas-phase species through all the model layers and a unit conversion to provide the column amount in molecules/cm^2 to compare with the satellite data. The post-processing of CMAQ output in comparable units to the tropospheric column amount from the satellite has avoided the use of the averaging kernel to modify the satellite data. However, the inherent assumption in this calculation is that the model top is the location of the tropopause, and the uncertainty due discrepancies between the location of the model top in CMAQ, and that of the tropopause in the satellite retrievals needs to be examined.

2.1.6   Enhancement and Integration of AMET

AMET is a very useful analysis package for generating statistical analyses and plots of a variety of performance metrics, e.g., Normalized Mean Error (NME), Root Mean Square Error (RMSE), Mean Absolute Gross Error (MAGE), Mean Bias (MB), in comparing the atmospheric model output (both meteorological and air quality) against observational data. AMET version 2.0 is a significant redesign by developers at UNC relative to the previous version (v1.1) to incorporate satellite data as a data stream in addition to observations and air quality model outputs, and to greatly simplify the simultaneous comparison of these multiple data streams.

In AMETv1.1, the basic paradigm was to pair observations and model data before loading it into its underlying database. In this approach the user needed both the observation and the model datasets to load any dataset into the database, and it was very difficult to create the necessary database queries to compare two or more model datasets. The original database structure was tailored to comparisons with surface observations, and thus posed a series of challenges for

storing satellite data in that (a) there was no easy way of storing map scale projection information, (b) data locations were assumed to be points (useful for surface observations) but there was no way of storing area locations (e.g., satellite pixels), (c) the data tables were not structured to deal with the potentially much larger data demands of satellite datasets, and (d) the available variables (chemical species) were hard-coded into the database, necessitating modifications to the database to incorporate new species that might become available in newer datasets, for example, due to the use of a new chemical mechanism in the model.

AMETv2.0 addresses the above issues in several ways. First, it relaxes the requirement of having both an observation and a model dataset when loading data, instead loading a single dataset "mapped" to a generic grid. It should be noted that an AMET "grid" is a collection of points in time or space, called locations. For spatial grids, the projection information is stored along with information differentiating point grids (e.g. surface observations), area grids (e.g., surface model output or 2-D satellite data), and volumetric grids (e.g. 3-D model output and level-specific satellite data). This approach provides some significant advantages: (1) the data provider can take advantage of datasets that are already available in the AMET database. For example, model data can be loaded by interpolating to one of the generic grids without having to obtain and parse data from a new satellite dataset or observational network; (2) any dataset, independent of the data source, once loaded onto a specific generic grid, can be easily compared. This greatly simplifies the database queries needed for data analysis; (3) redundant data in the have been removed from the database, thus reducing its overall size; (4) the data table structure has been normalized to simplify the data queries and accommodate the much larger satellite datasets, and (5) the variables have been made a separate tabulated input so that the addition of a new chemical species does not require restructuring of the database tables. Additional metadata have been provided with the loaded data, and a quality metric has been added to provide a further means of subsetting the data.

In addition to these improvements in the database and loading components, AMETv2.0 includes a significantly redesigned analysis component. In AMETv1.1, a complicated R script typically performed all of the data access, statistics, reformatting, and plotting. While AMETv2.0 still performs the analyses in R, these have been significantly modularized into R libraries, which provide generic objects and functions for (a) accessing and storing the data, (b) transforming the data, (c) calculating a set of generic statistics, and (d) plotting the results. The advantage is that the R script can use these generic functions to greatly facilitate matching two or more datasets in the database and generating a statistical comparison plot. Thus the average user can much more easily understand, and potentially extend these scripts to perform more tailored analyses.

To facilitate the integration of AMET into VIEWS/TSS, an Ubuntu Linux server has been added to the CIRA network and connected to the VIEWS/TSS servers. Appropriate modifications to the CIRA firewall have been made to enable remote connections to the server, and the developers at CIRA and UNC have been collaborating to properly configure the server for AMET installation. A web-based interface is currently being developed for AMET and will be installed on the new server when complete; mechanisms for integrating this interface with existing web pages on VIEWS have been designed, which will use a series of forms for the user to select datasets and plot types of interest. The degree of integration that will be possible using this loosely-coupled approach, as well as methods for passing user selections to AMET from a VIEWS web page are being explored. A possible approach is for the VIEWS site to generate a

yaml configuration file and call the appropriate AMET script to run the analysis. The resulting plots and/or tables would then be written to disk and be displayed on the VIEWS web page.

2.2   *Model Evaluation Use Case for National Park Service End User*

2.2.1   Rocky Mountain Atmospheric Nitrogen and Sulfur (RoMANS) Study

To demonstrate the integration and use of the VIEWS/TSS enhancements being developed for this project, a case study was identified by end users at the National Park Service and agreed upon by steering committee members as a targeted application of satellite data for air quality assessment and performance evaluation of the CMAQ model. The Rocky Mountain Atmospheric Nitrogen and Sulfur Study (RoMANS) of 2006 described in Malm et al. (2009) was selected for this purpose as it provides intensive field observations to evaluate the model results and help assess nitrogen deposition in Rocky Mountain National Park (RMNP), which has exceeded a critical load in recent years. To enhance this analysis with satellite data and present the results on the VIEWS/TSS website, the RoMANS observational data were analyzed in conjunction with available satellite data to determine the best uses of the satellite data for providing additional insights; both OMI NO_2 and near-UV AOD data are being used along with MODIS Terra and Aqua AODs in the analyses. Next, specific configurations of both existing and planned VIEWS/TSS tools were designed to present useful visualizations and analyses of the results through interactive reports on the website. Efforts are ongoing to also compare CMAQ post-processed column data on NH_3 against Tropospheric Emissions Spectrometer measurements made on board the Aura satellite that could be available from the TES Science Team at NASA Jet Propulsion Laboratory toward the beginning of the next performance period (G. Osterman, private communication; see also Section 2.6).
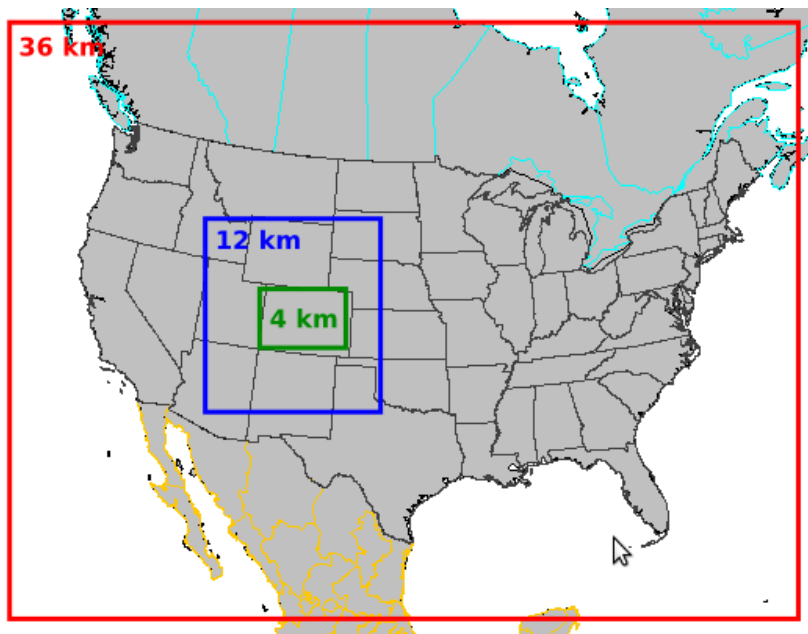

Figure 1. CMAQ and CAMx modeling domains at 36-, 12-, and 4-km resolutions that are used in simulating the RoMANS campaign period of spring and summer 2006.

One reason for choosing CMAQ for this study was its wide use in regulatory applications; another was to do a model-to-model cross-comparison, as previous simulations of the study

period by NPS with the CAMx model (Yarwood et al., 199X) showed significant underbiases in ammonia and particulate ammonium compared to observations. UNC augmented the emission dataset for this study by replacing the ones previously processed under a separate contract with WRAP to update key emissions sectors. NPS provided the meteorological data from the Fifth Generation NCAR/Penn State Mesoscale model for the study period; boundary conditions were generated by collaborator Yoshitomi at Harvard using the GEOS-Chem global chemistry model and mapped to the CMAQ modeled species by UNC. Co-I Dr. Arunachalam directed and quality-assured the CMAQ simulations at 36-, 12- and 4-km resolutions for the nested domains shown in Figure 1. The object was to examine CMAQ model performance compared to both CAMx results and the observations at the core RMNP site and the surrounding sites during spring and summer of 2006. The comparisons of time series plots at each site (not shown) for the spring found that while CMAQ performance was slightly better than that of CAMx for total ammonium, the trends in both models were severe under predictions at nearly all sites. Figure 2 shows results at the core field site (ROMO) and the 8 peripheral sites in RMNP for total ammonium on April 21 and 22, preceding a high ammonium deposition episode on April 23.
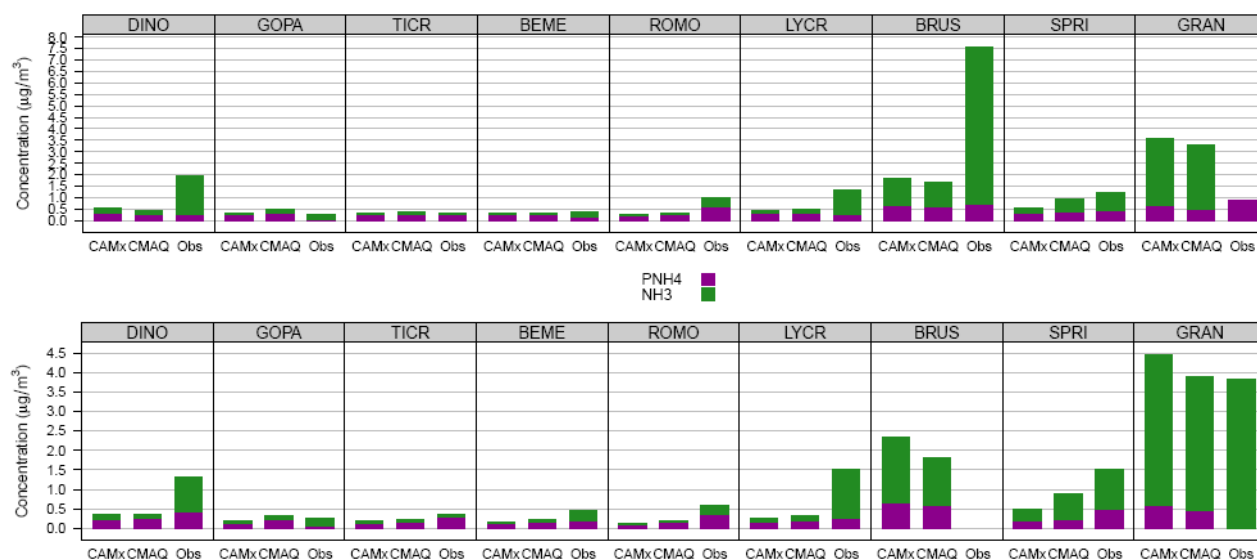

Figure 2. Comparison of CMAQ and CAMx performance for particulate ammonium (PNH$_4$) and gas-phase ammonia (NH$_3$) on April 21, 2006 (top panel) and April 22, 2006 (bottom panel) at the 9 intensive field measurement sites around RMNP during RoMANS. From left to right the site data are displayed in the order of west-to-east.

To diagnose the contributions of various processes (advection, diffusion, deposition) to the ammonium underprediction, UNC captured CMAQ output instrumented for processing through the python-based Process Analysis tool described in Section 2.2.2, for the 12-km domain, around the high ammonia deposition episode in April 2006. This case study will be further developed in the next year of the project, and serve as a practical demonstration of the enhanced capabilities of VIEWS/TSS. Figure 3 shows the tropospheric NO$_2$ column amounts (30% cloud screening) from OMI during on April 21 and 22, 2006 regridded to the CMAQ grid as described in Section 2.1.4, and those calculated by the vertintegral post-processor from CMAQ output, as described in Section 2.1.5.
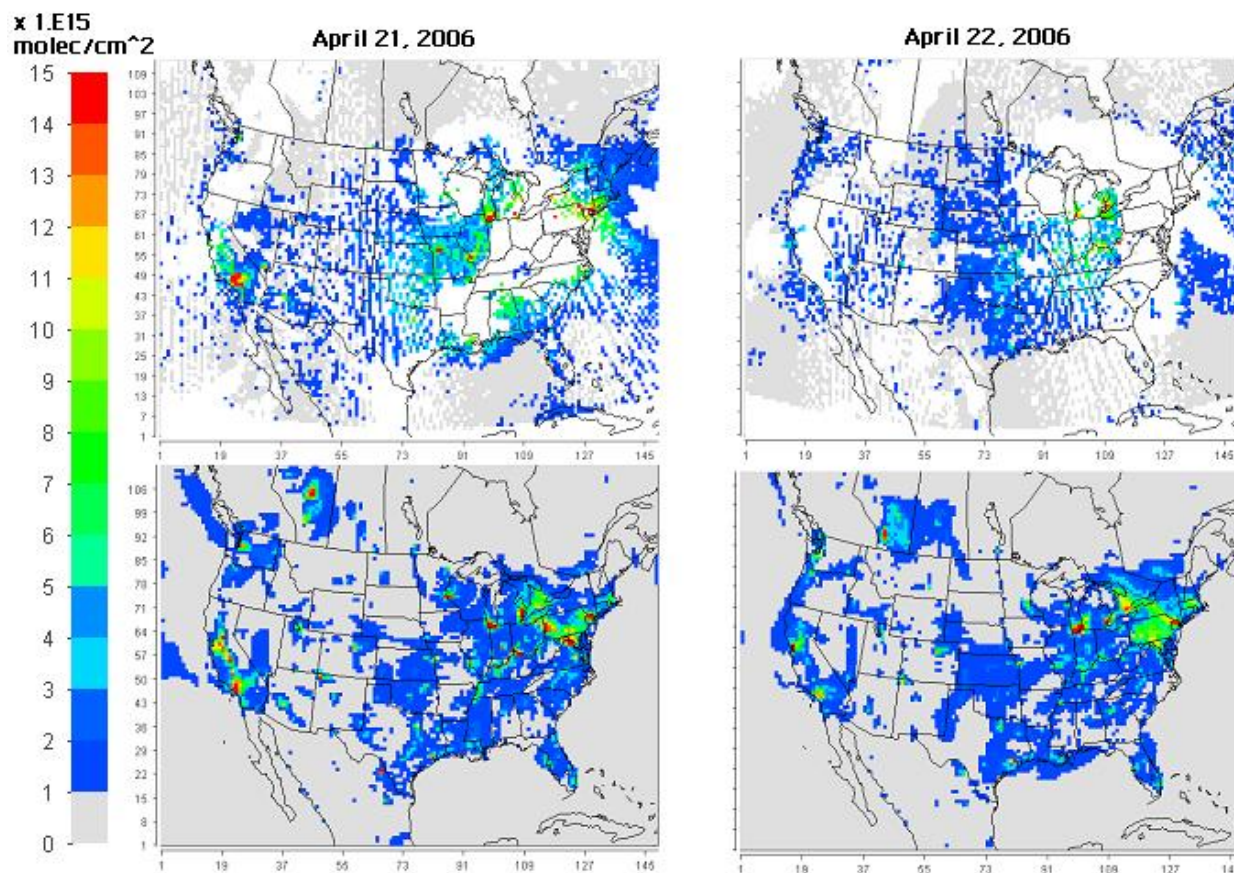
Figure 3. Tropospheric NO_2 column amounts (x 10^{15} molecules/cm^2) for April 21 and 22, 2006 using the regrid and vertintegral tools. Top panels: regridded from OMI L2G data to match the CMAQ grid; white areas indicate missing data; bottom panels: vertically integrated from CMAQ output. Column and row numbers for the CMAQ grid are shown on the axes.
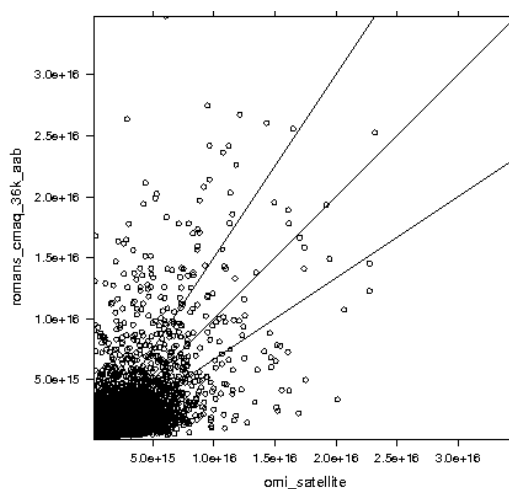

Figure 4. AMET statistical comparisons of the CMAQ and OMI NO_2 values shown in Figure 3; off-diagonal lines indicate ±33% bias; diagonal indicates 1-1 agreement.

Figure 4 shows the scatter plot from AMETv2.0 comparing the CMAQ NO_2 column against regridded OMI values for the same two days s in Figure 3 at all the grid points for which both sets of data were available. Although the spatial patterns of satellite and modeled data compare reasonably well in the tile plots for each day shown in Figure 3, the scatter plot clearly shows the overbias in the model at the upper end of the range, and underprediction at the low end. A full diagnostic evaluation of all the contributing factors to these biases is ongoing.

2.2.2   python-based Process Analysis Tool (pyPA) Application

Towards providing air quality end users a powerful analysis tool to help diagnose model performance and reconcile differences in comparison with satellite- and ground-based data, UNC has been testing the pyPA post-processor for analyzing CMAQ output for the RoMANS study at 12-km resolution. Process Analysis post-processing has traditionally been a researcher's tool, but recent developments help make diagnostic analysis available to policy makers and others not familiar with algorithm details in the model. Specifically, UNC has worked on improving the user-friendliness of the post-processing utilities, focusing on the Python-based Process Analysis (pyPA) and Python Environment for Reaction Mathematics (PERM) packages.

Although the primary feature of pyPA is the extraction and aggregation of complex 4 dimensional air parcels from air quality model output, its typical usage can be automated to reduce the technical knowledge necessary to operate it. First, dynamic windowing of standard model inputs and outputs have been added to simplify the process of running pyPA. In addition, subsetting of the domain for the process analysis output uses both netCDF, and the simpler ASCII format to generate binary data masks (1 = yes, 0 = no) to further simplify the process of selecting which grid cells will be used in the post-processing.

The primary function of PERM is to provide the mathematical analysis and plotting of process analysis data. Typically, PERM operates on data that have been extracted and merged by pyPA, but it is sometimes more useful to look at the unmerged data from the model to better understand the spatial variability of the data. Thus PERM I/O has been simplified to read CMAQ outputs directly. In addition, PERM has been extended to recognize all currently available CMAQ chemical mechanisms. pyPA developer Henderson directed the testing of the PERM tool in stand-alone mode to generate output for Integrated Process Rates (IPR) from the CMAQ RoMANS simulation results for NH_3 ands NH_4, and is currently helping examine these process rates to diagnose the underbias cited in Section 2.2.1. In ongoing communications about these analyses, and in an *ad hoc* training teleconference conducted by Henderson, the end users at NPS expressed strong interest in diagnosing CAMx model performance with pyPA using the results that they have generated from that model with the same set of inputs as in CMAQ. As pyPA is already set up to process the CAMx binary outputs, this analysis would allow a rigorous inter-model comparison of the process formulations responsible for the underbiases seen in total ammonium in each model.

In a parallel effort CIRA and UNC are also collaborating on the VIEWS web implementation of pyPA, which will use the same loosely coupled paradigm as in the VIEWS implementation of the other analysis tools.

2.3   *Visualize PM (VPM) Tool Development for PM Size Distributions*

In the first year of performance, PI Shankar and co-I Zubrow, in collaboration with Renci's institutional co-PI Steve Chall submitted a Statement of Work (SOW) to NASA to develop an

advanced, interactive visualization and animation tool for PM size distributions from modeled and observed data. This was approved by NASA as an addendum to the existing grant in the second year. The purpose of this task is to facilitate advanced diagnostic investigations of model performance and comparison with the detailed PM composition and size distribution data from field campaigns, aircraft campaigns and satellite platforms; of note are surface-based data collected during RoMANS in 2006, and the 2009 CalNex aircraft campaign in California, as both involved active participation from end users at NPS and WRAP. The VPM development is scheduled for completion within Year 2, and will be beta tested beginning in Year 3.

Renci Co-I Dr. Borland, the lead developer of VPM, has made considerable progress toward fulfilling the major goals of the VPM effort as described in the SOW. He has used the Visualization ToolKit (VTK) to provide all graphics and visualization functionality in its primary C++ binding. The Input Output Applications Programming Interface (I/O-API) library, incorporated into a VTK reader subclass, performs all functions for opening and extracting CMAQ output data. In integrating it into the VPM environment, Dr. Borland has incidentally performed some useful QA on the I/O-API libraries for different platforms, improving their usefulness for the CMAQ user community. The VSNdist5 subroutine initially developed in CMAQ has been fully integrated into VPM to generate the modeled size distribution plots. PI Shankar is providing guidance on an ongoing basis on QA of CMAQ output and on the expected size distribution characteristics; the ability to visualize observed distributions is currently under development.

Interactive selection of the map location for visualization has been prototyped and is currently being integrated into the production code. Custom-generated maps for widely used model domains are available (see Figure 5); a more general solution to generate the background map from the input metadata is being explored. Color coding of the map to display concentrations of user-selected variables is robustly supported in current versions; the simulation time and vertical level are selectable and animatable. The ability to select a streamline from input meteorological data is a capability in VTK that was demonstrated during the prototype development, and will be integrated into VPM in the near future. Visualization and animation of the PM size distributions along these streamlines is under development.

The VPM interface has been redesigned as a single VTK class with two presentation modes. The VPM application was developed to run on a Linux machine because the models are run on a Linux server and the model output, due to its size, would likely be analyzed on that same server. An advantage of this development platform is that the VPM could be installed and used by a researcher independent of VIEWS. Thus one mode of VPM operation is as a standalone application with a graphical user interface based on the Qt open-source C++ toolkit. The Linux platform, however, raises some challenges for integrating the VPM into VIEWS, as VIEWS runs on a Windows server. To address this issue, UNC Co-Is Ross, Zubrow, and Borland are designing and implementing a web interface to the VPM.

The conceptual design of the web interface is nearly complete, and allows for a loosely-coupled interaction between VIEWS (on the Windows server) and the VPM (on the Linux server). It calls for implementation of a web page in VIEWS that uses an iframe to host the VPM web interface. This web page is being designed to provide a consistent appearance with the other pages within VIEWS. Through the VIEWS page, the user would select various datasets and then select a plot type from a hierarchy of choices: (a) modeled, (b) observed, or (c) both types of distributions, at user-selected non-contiguous locations, or along the air parcel trajectory

(streamline). Once these selections are submitted, the commands would be transmitted through the VPM web interface to the VPM application on the Linux server. The resulting plots generated on the Linux server would be sent via the web interface back to the VIEWS web page. The user will then be able to interactively create additional plots, e.g., by changing the model layer, animating the plot through time steps, or selecting a different map location for the size distributions. A capability has been added to compare the size distributions from multiple locations on a single plot as shown in Figure 5.
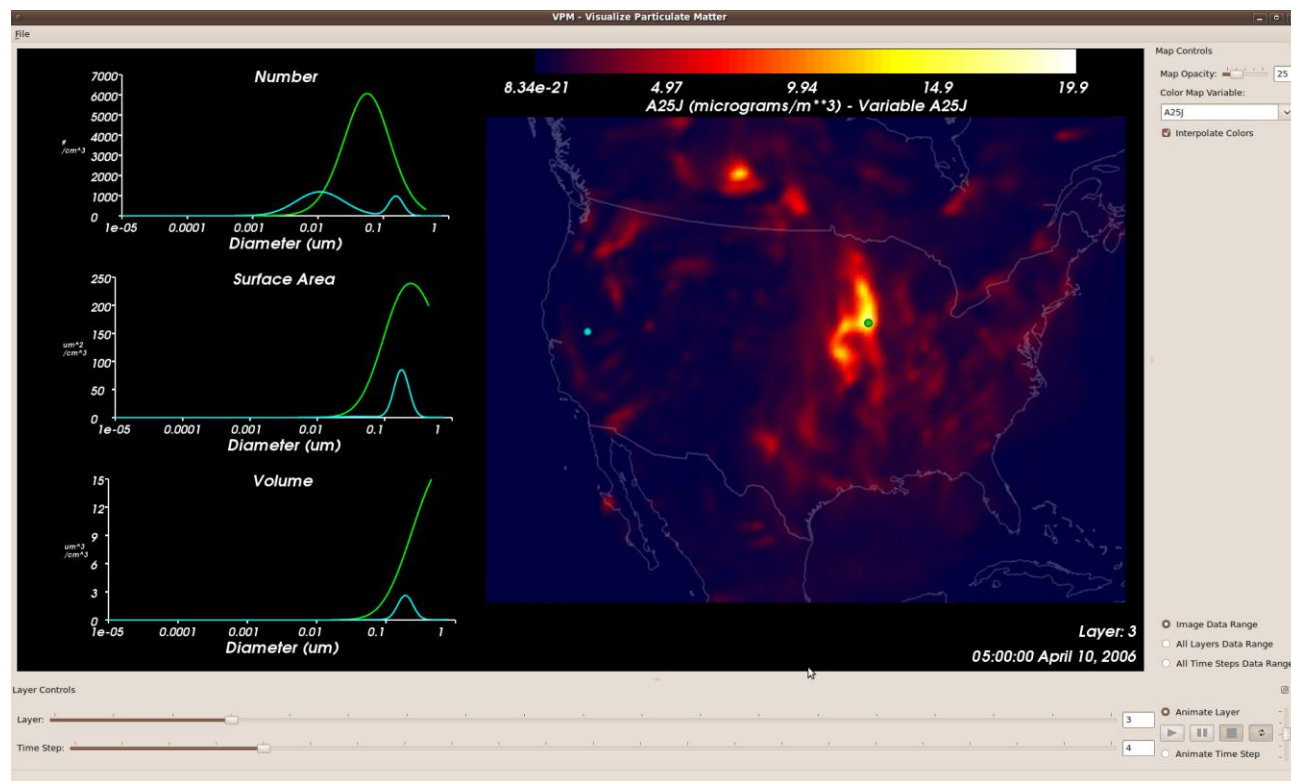

Figure 5. Screenshot of VPM output showing a color map of species A25J, unspeciated fine PM (fugitive dust) from CMAQ on a day during the RoMANS spring campaign, and the size distributions of total PM number, surface area and volume concentrations (left panel) at selected locations. Plot color corresponds to location marker color on the map; the green line represents aged (polluted) aerosol, and the blue line, a strongly bimodal aerosol population with a significant mode of newer (smaller) particles. Scroll bars at the bottom control the plot display through vertical layers, and time steps.

Co-I Borland has implemented a Java wrapper to the VPM application, allowing the application to be directly called from Java. Investigator Ross has designed a Java server that will control the interactions between the web interface and the VPM. This will allow multiple VIEWS users to call the VPM application via the VIEWS web page. He has also implemented a test web interface to demonstrate the possibility of displaying images generated from the VPM application and having the user dynamically interact with that image (e.g., using a slider to animate the image). This test application has not yet been ported to the Linux server at CIRA and will require additional development to more fully exploit the VPM functionality. Investigator Zubrow has begun porting the web interface and the VPM application onto CIRA's Linux server.

2.4   Interoperability and Synergistic Developments with Other Systems

2.4.1   Use of Web Services from Giovanni and RSIG

The design of the VIEWS/TSS system architecture already supports multiple levels of interoperability with systems within the WRAP domain of air quality decision-making activities. These include the WRAP Emissions Data Management System (EDMS) and the Fire Emissions Tracking System (FETS), as well as the Regional Modeling Center (RMC). New systems being connected to VIEWS include EPA's Air Quality System, Air Quest, AirNow, DataFed, Giovanni, Remote Sensing Information Gateway (RSIG), and NASA DAACS.

In the past year, in collaboration with Co-I and Giovanni developer Dr. Prados, and RSIG PI, Dr. Szykman, Co-PI McClure investigated the capabilities and web services offered by Giovanni and RSIG for accessing satellite data to determine their suitability for use by VIEWS/TSS tools. The Giovanni team has indicated that they are interested in this approach and in working with the VIEWS/TSS team to help facilitate access to GES DISC satellite imagery and data files. Both Giovanni and RSIG offer a certain subset of their capabilities as OGC-compliant web services, and the communication protocols used by each (such as WMS, WCS, WFS and OPeNDAP) are inherently compatible with the VIEWS/TSS infrastructure. While particular subsets of the satellite data will be stored locally in VIEWS/TSS for analysis and performance reasons, other subsets will be accessed remotely via dynamic interaction with these remote systems. A substantial amount of additional work is required to fully enable this interaction; however significant progress was made in designing the programmatic methods to request and receive data from these systems, and to incorporate the results into VIEWS.

2.4.2   Public Repository for CMAQ Output

While some CMAQ output, particularly subsetted (surface-layer) data are currently stored in the VIEWS database, multi-year, and/or complete model outputs, such as those needed for comparing with satellite data, would entail access of CMAQ output from a larger, more permanent repository. The Community Modeling and Analysis System (CMAS) Center, hosted by UNC, used a recent work assignment (WA) under a current EPA contract, to provide public access to archived CMAQ output and metadata from EPA's model evaluation runs. Toward addressing Tasks 3 and 4 of the project, Co-I Zubrow worked with CMAS Center and the Data Intensive Cyber Environments (DICE) group at UNC to develop an approach for storing and serving CMAQ output data and metadata to the user community. DICE, which recently relocated to the UNC School of Information and Library Sciences with research space at Renci, is an award-winning research group that brings expertise in developing digital data technologies, including open source software that enables data sharing in collaborative research, publication of data in digital libraries, and preservation of data in persistent archives for use by future generations. DICE has developed for this purpose the "i" Rules Oriented Data System (iRODS), which offers great flexibility and ease of use via searchable metadata catalogs for accessing and serving data residing on distributed computing platforms, and serves the data needs of a world-wide scientific user base. iRODS also has the capability to do hierarchical searches of duplicate datasets from nearest to most remote data location, providing remote users the fastest possible access to the data. As a proof of concept, UNC loaded a full year of model data into the iRODS repository and developed a web interface for easily query the available data and metadata. In addition to the public web-interface, there are a series of command line interfaces that could be leveraged to develop interoperable calls between the VIEWS server and the iRODS repository.

Further extensions of this system could include adding additional data servers to host new model datasets or archive copies of the current datasets, further investigations of iRODS capabilities for querying the metadata of the loaded datasets, and creating new functions for subsetting and transforming the data on the iRODS server before downloading to the VIEWS server.

2.5   *Training on Satellite Data Use for End Users*

In conjunction with the CMAS conference in October, and under funding from the NASA Applied Sciences Program, a three-day training course tailored to the air quality community on the use of satellite data was offered, and attended by 12 participants. The course was led by Co-I Dr. Prados and Mr. Kleidman from NASA GSFC, and covered many of the web-based tools and technology currently available for querying and downloading from NASA data archives, and additional modules tailored to this community of students. The goals of the training activity were to 1) provide air quality modelers and other professionals the background needed on relevant NASA data products to facilitate their use in air quality applications; 2) provide an introduction to satellite data visualization and analysis tools, and 3) introduce key concepts for enabling comparisons between NASA satellite data and CMAQ model output. A large fraction of the course time was spent on hands-on activities with guided instructions on the use of web-based tools and other software for visualization and analysis of satellite imagery. The final hands-on activity on Day 3 involved CMAQ model output and satellite data comparisons. One of the unique aspects of the course was the development of a teaching module by PI Shankar on CMAQ trace gas and aerosol species relevant to satellite data comparisons and details on how to generate model output to better enable direct comparisons to satellite data. This teaching module leveraged the data sets generated in ongoing studies by UNC over North America and the Middle East, which were post-processed with the tools described in Section 2.1.6, to compare with the regridded data from OMI for selected episodes. It also included a discussion of some of the opportunities and challenges when comparing CMAQ model output to satellite data.

All course attendees were provided with computers by UNC staff. The computers were preloaded with the power point presentations, as well as instructions, software, satellite datasets, and model output for the hands-on activities. Prior to the training a list of URLs of remote sensing online tools and datasets were also added to the CMAS website by UNC staff.

Based on the course evaluation provided by the students, the material was well-received, with most of the students reporting that they had better knowledge of satellite data use as a result of the training. Compared to the CMAS pilot training in the spring of 2009, the overall prior knowledge of satellite products was higher for the attendees in this more tailored and lengthier training course. The course surveys indicate a high degree of satisfaction with the workshop, with half of the attendees giving the training an overall rating of 4 out 5. Areas that received particularly high ratings were the ability of the instructors to answer questions and the overall content and relevance of the curriculum. The students found the pace to be fast despite the longer schedule compared to the pilot training (2.5 days instead of 2), and the virtual computing environment in which the hands-on exercises were attempted proved to be a serious limitation in the execution speed of web commands. These issues will be addressed before the next training course, slated for the end of October 2010.

2.6 Conference Attendance

PI Shankar and Co-I Zubrow attended the Earth Science Information Partnership (ESIP) Federation meeting in Santa Barbara, CA in July 2009. This was a follow-up to the GEOSS Architecture Implementation Pilot – Phase 2 (AIP-2) workshop in Boulder, CO in September 2008 on use cases for data sharing, and implementation of metadata and web service standards in the Air Quality societal benefit area. Shankar and Zubrow participated in the Air Quality Working Group break-out session to provide inputs to the model evaluation process; Shankar presented the status of the VIEWS/TSS data services in the session on Air Quality. The conference also provided an opportunity to discuss the project goals with the Program Officer and some of the end users who attended the conference, and to meet developers of other decision support systems, as well as members of other Working Groups.

In October 2009 PI Shankar attended and presented a paper on the RoMANS campaign simulation results from CMAQ at the 8th Annual CMAS Conference (Shankar et al., 2009). She subsequently made contact with Greg Osterman, a TES Science Team member at NASA's Jet Propulsion Laboratory and will coordinate with him to obtain TES NH_3 data, as an additional model evaluation dataset; this will be valuable as gas-phase ammonia measurements are often unavailable in the surface monitoring networks. She also interacted with other users of satellite data to find out about their needs for processing tools, and their experience with the satellite data, especially the use of swath data in comparisons against time-dependent model output.

Pi Shankar presented the status of the project at the All-Investigator meeting in November 2009 in Washington DC. She and Co-I Dr. Arunachalam also participated in discussions on the requirements for an Applied Sciences Team to advance the mission of the NASA Applied Sciences Program through the use of Earth Observations in air quality assessments.

PI Shankar also attended the ESIP Federation winter meeting in Washington D.C. in January 2010, and participated in the discussion sessions on the Air Quality societal benefit area, and on formulating plans for GEOSS AIP-3.

3 Summary

In the period of performance covered thus far in Year 2, significant progress was made on almost all tasks originally proposed for Year 2, including the add-on visualization task (Task 9).

- The prototype image browser in VIEWS for satellite images was prepared using as a production-level tool in VIEWS (Task 2)
- A project Google Maps visualization and query tool was developed in VIEWS to allow clickable query of any of the diverse VIEWS data streams on a background map (Task 2)
- New features in the SQL spatial data server were leveraged for easier access and cross-referencing of the diverse datasets in the VIEWS database (Task 4)
- OMI Level 2G and Level 3 data for tropospheric NO_2 column and Aerosol Optical Depth were regridded with a newly developed projection and regridding tool for test periods in 2005, 2006 and 2007 to match two North American CMAQ modeling grids and a Europe/Middle East modeling grid at two different horizontal resolutions (Task 6).
- Post-processors were developed to calculate trace gas tropospheric column amounts and Aerosol (extinction) Optical Depth from CMAQ output to facilitate quantitative comparisons with satellite data (Task 6).

- Synergies and interoperability with RSIG and Giovanni are being explored within the VIEWS/TSS framework (Tasks 3 and 4)

- The public repository of CMAQ data, iRODS was put into operation with a year of model output and associated searchable metadata, and data subsetting capabilities (Task 4)

- The AMET analysis tool was significantly improved to create Version 2.0, which facilitates loading multiple modeled and observation (including satellite) datasets and performing statistical comparisons among them (Tasks 4 and 6)

- Work to provide a loosely-coupled implementation of AMETv2.0 in VIEWS was begun (Task 6)

- The CMAQ simulations of the RoMANS study period were completed to provide a use case demonstration of the analysis tools and the complementary evaluation data from satellite platforms (Task 7)

- Output from CMAQ for the RoMANS study period was archived in the VIEWS database for access by end users (Task 7)

- The pyPA analysis of CMAQ performance for the RoMANS study period was begun to provide insights to the NPS on the cause(s) of the ammonia underpredictions (Tasks 7 and 8)

- A NASA-sponsored-satellite data training course for air quality analysts was organized and offered to the community through the CMAS training program (Task 8)

- Overviews of VIEWS/TSS capabilities were presented at two conferences and the all-investigator meeting (Task 8)

- Significant progress was made on developing a new visualization/animation tool for interactively visualizing PM size distributions (modeled and observed) (Task 9)

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