High Resolution Coupled RAQMS/WRF-Chem Ozone and Aerosol Simulations for GOES-R Research

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1. Introduction

The launch of the first in the series of Geostationary Operational Environmental Satellite-R (GOES-R) satellites is scheduled for FY2015. The instrumentation on these satellites will provide improved observations of a range of phenomena that can be used to improve weather prediction and the understanding of key processes affecting humankind.

Currently extensive efforts are underway to develop, demonstrate, recommend and set standards for a broad range of capabilities designed to make optimal use of the GOES-R data when it becomes available. One of these efforts, addressed herein, involves the generation of high temporal and spatial resolution Advanced Baseline Imager (ABI) proxy datasets to be used by a variety of GOES-R team members for algorithm development and demonstration activities.

In this research high resolution aerosol and ozone data sets have been created over the continental US to augment the current GOES-R Algorithm Working Group Weather Research and Forecast (WRF) model [(Skamarock et al. 2001, 2005)] ABI proxy data capabilities. These data sets have been generated with WRF-Chem [Grell et al., 2005] air quality simulations coupled to global chemical and aerosol analyses from the Real-time Air Quality Modeling System (RAQMS) [Pierce et al., 2007]. Both WRF-Chem and RAQMS include on-line aerosol modules from the Goddard Global Ozone Chemistry Aerosol Radiation and Transport (GOCART) model [Chin et al., 2002]. The addition of aerosol and ozone distributions into the WRF proxy data set allows generation of more realistic synthetic (proxy) radiances for all ABI bands, using the forward visible and

infrared radiance modeling capabilities from the Joint Center for Satellite Data Assimilation (JCSDA) Community Radiative Transfer Model (CRTM) [Han et al., 2006].

2. Models

WRF-Chem version 3.0.1 was used to produce the high temporal and spatial resolution simulation required for this effort. The final 30 hour high resolution simulation was obtained in several steps. First, a 36km resolution simulation, initialized at 00Z 20 August 2006, was integrated for 3 days. A second 12 km resolution simulation was initialized with the 36km forecast and integrated for an additional 24 hours. The final 30 hours of the simulation (00Z August 24 – 06Z August 25) were initialized with the 12km forecast and run at 4km resolution. Forty vertical layers with a top level of 50mb were used throughout the simulation.

Sub-grid scale processes were parameterized using the Thompson et al. mixed-phase cloud microphysics scheme, the Mellor-Yamada-Janjic planetary boundary layer scheme and the Goddard shortwave and Rapid Radiative Transfer Model long-wave radiation schemes. Surface heat and moisture fluxes were calculated using the Noah land surface model. The Grell-Devenyi ensemble scheme cumulus parameterization scheme was used for the 36km and 12km resolution simulations. No cumulus parameterization was used at 4km; therefore, all clouds were explicitly predicted by the microphysics scheme at this resolution.

The WRF-Chem simulation used the Kinetic Pre-Processor (KPP) [Sandu and Sander, 2006] capabilities of WRF-CHEM to couple GOCART aerosol predictions with the Regional Atmospheric Chemistry Mechanism (RACM) [Stockwell et al. 1997] chemical mechanism. The GOCART aerosol module predicts concentrations of seven aerosol species (SO4, hydrophobic OC, hydrophilic OC, hydrophobic BC, hydrophilic BC, and dust, sea-salt) which are the basis for the CRTM look-up tables for aerosol optical properties.

These simulations used high resolution (4km) continental US anthropogenic aerosol and ozone precursor emissions based upon the U.S. EPA's 1999 National Emissions Inventory (NEI-99, version 3) including March 2004 revisions, and biomass burning emissions produced from Wild Fire Automated Biomass Burning Algorithm (WF-ABBA) wildfire products.

The 36km WRF-Chem simulation was initialized at 00Z on 20 August 2006 using meteorological data from NCEP 1° Global Data Assimilation System analyses. Throughout the simulation the meteorological analyses were updated every 24 hours at 00Z (except at 00Z August 25) using NCEP 1° Global Data Assimilation system analyses. Chemical distributions were not updated throughout the entire simulation.

Day zero chemical initial conditions and chemical lateral boundary conditions throughout the simulation were obtained from 6 hourly RAQMS two degree global analyses. The RAQMS analyses, produced in support of the 2006 INTEX-B field experiments, were constrained through chemical data assimilation of stratospheric ozone measurements from the Microwave Limb Sounder (MLS) and tropospheric carbon monoxide measurements from the Tropospheric Emission Spectrometer (TES) onboard the NASA Aura satellite, and aerosol optical depth (AOD) measurements from the Moderate Resolution Imaging Spectroradiometer (MODIS) onboard the NASA Aqua and Terra satellites.

The desired end product of the RAQMS/WRF-Chem model simulation was the final 24 hour, 4km horizontal resolution data. These data were saved at fifteen minute intervals for the period 06Z August 24 to 06Z August 25. Two 3-hour periods (06-09Z and 15-18Z August 24) were saved at 5 minute temporal resolution. The 4km resolution simulation was run at the Pittsburgh Supercomputing Center using 144 processors on a SGI Altix 4700.

The 4km resolution WRF-Chem model simulations are being used as input to the CRTM to construct physically realistic proxy ABI radiances consistent with the observed atmospheric state. ABI sensor specifications are included in the CRTM and appropriate satellite viewing geometry is used in the generation of radiances. The IR version of CRTM for ABI channel forward modeling has been available for some time. This project is also using a test version of CRTM which includes forward modeling capabilities for ABI visible channels (including aerosols).

3. Results

ABI visible and IR channel radiances are being produced for the 24 hour period of the 4km simulation. To test the quality of the proxy ABI radiances, comparisons with MODIS IR and visible radiances for 18:30Z August 24, 2006 MODIS Terra and Aqua overpasses have been completed using ABI channels and MODIS viewing geometry (Figures 1 and 2). Differences between MODIS and Proxy radiance distributions are quantified based on comparisons of observed and simulated radiance histograms (e. g, Figure 3).

As expected due to the increased complexity and relatively early nature of forward modeling of visible channels, agreement between the MODIS and Proxy IR channels (~3.9 to ~ 13.3 microns) is better than for visible channels (~ 0.47 to ~ 2.26 microns). The largest differences between observed and proxy radiances arise from timing and location of deep convective clouds, which result in high visible radiances (due to high reflectivity) and low IR radiances (due to cold cloud top temperatures) and errors in surface emissivity and reflectivity. For example, the increased frequency of high radiances in the proxy ABI 0.64 micron band (left panel of Fig. 3) and the increased frequency of low radiances in the proxy ABI 11.2 micron (IR) band (right panel of Fig. 3) relative to MODIS results from the WRF-Chem overestimation of convective activity over Arizona and off the coast of South Carolina.

Conversely, the increased frequency of low radiances in the proxy ABI 0.64 micron band

and the decreased frequency of high radiances in the proxy ABI 11.2 micron band relative to MODIS can be attributed to surface reflectivity and emissivity problems over of California and Utah.

4. Future Research

As discussed above proxy ABI radiances will be calculated for all ABI bands for the 24 hour period of 06Z August 24 to 06Z August 25, 2006. These dataset will be used by GOES-R team members for algorithm development and demonstration activities.

Validation of the simulated radiances will continue. In addition, a series of impact experiments will be run to assess the role of clouds and total and component aerosols on radiative balance. Input into the CRTM forward model can be controlled via the calling program. Radiances will be calculated where one or more fields are excluded from the forward modeling (e.g., clouds (total, ice, water, etc), total or component aerosols). Comparisons with the 'control' experiment will be used to evaluate the impact of these fields on top of the atmosphere (TOA) radiances.

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Fig. 1: Comparison of the 0.645 micron band MODIS Terra and Aqua L1 radiances (left panel) and 0.64 micron band ABI proxy radiances (right panel) using MODIS Terra and Aqua viewing geometry for 18:30Z on August 24th, 2006 (W/m²/sr/um)



Fig. 2: Comparison of the 11.03 micron band MODIS Terra and Aqua L1 radiances (left panel) and 11.2 micron band ABI proxy radiances (right panel) using MODIS Terra and Aqua viewing geometry for 18:30Z on August 24th, 2006 (W/m²/sr/um).



Fig. 3 Histograms of the MODIS (solid) 0.645 micron band and proxy ABI (dashed) 0.64 micron band (left panel) radiances, and MODIS 11.03 micron band and the proxy ABI 11.2 micron band (right panel) radiances.