Assimilation of GOES-R ABI Aerosol Optical Depth (AOD) in a Regional Air Quality Model to Improve Surface PM2.5 Forecasts

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1. Objective

Ground level ozone and PM2.5 (particulate mass of aerosols smaller than 2.5 µm in median diameter, µg/m^3) concentrations are two of the leading indicators of air quality. National Weather Service (NWS) uses NOAA-EPA developed Community Multiscale Air Quality (CMAQ) model to provide air quality forecast guidance: the ozone forecast is operational, while the PM2.5 forecast runs in a developmental mode. Previous studies showed that the CMAQ model generally under-predicts PM2.5 concentrations in summer. Challenges for getting a better quantitative PM2.5 prediction come from imperfect meteorological inputs, inaccurate emissions and a lack of real time observations to specify the model initial conditions. Association between satellite derived Aerosol Optical Depth (AOD) and ground level PM2.5 makes it possible to improve PM2.5 prediction by assimilating AODs.

We developed an analysis-forecast-cycling data assimilation scheme based on a simple Cressman objective analysis in our previous research work to demonstrate the impact of satellite derived AOD values on surface PM2.5 predictions. Hourly GOES AOD retrievals and daily MODIS AOD retrievals, as proxy GOES-R ABI AOD data, were assimilated during two poor air quality episodes, one a sulfate haze case along the eastern U.S. and the other a biomass burning event in the western U.S. Evaluation studies showed that the assimilation of hourly GOES AODs largely improved surface PM2.5 predictions for the sulfate episode (reducing the False Alarm Ratio from 76.8% to 40.4% and increase the Critical Success Index from 2.6% to 21.5%, see Figure 1).

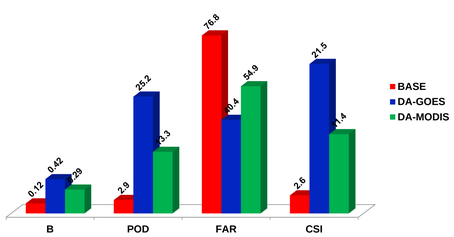

Figure 1. Categorical evaluation metrics for a sulfate haze episode.

To transition our research to operations and to be consistent with the development of the NWS aerosol assimilation system, we proposed to build a Grid-point Statistical Interpolation (GSI) assimilation system capable of assimilating operational AOD products in a regional air quality model. This work is expected to potentially improve NOAA's ability to use existing observations (operational GOES and MODIS AODs) to improve forecasts and prepare for the air quality observables from the next generation operational satellite sensors such as GOES-R Advanced Baseline Imager (ABI).

2. Accomplishments

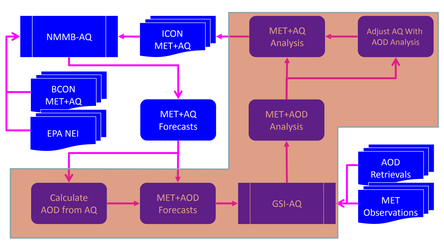

Figure 2. A diagram of the GSI system that is being built for assimilating satellite derived AOD products in a regional air quality modeling system. The shaded area represents the GSI software package.

NMMB-AQ: North American Mesoscale Modeling system on B-grid with Air Quality capability, NCEP's next generation Air Quality modeling system in plan. We'll take the current CMAQ model as a proxy for now
ICON: Initial Conditions
BCON: Boundary Conditions
MET: Meteorological fields
AQ: Air Quality concentrations
EPA: Environmental Protection Agency
NEI: National Emissions Inventory
AOD: Aerosol Optical Depth

2.1 Code development outside the GSI package

- ✓ **GOES AOD to BUFR format converter** – To satisfy NCEP's requirement for observation inputs
  - BUFR table for GOES AOD was setup
  - Encoder and decoder were developed
  - Data quality information based on retrieval screening criteria was introduced
  - Currently works for GOES-11, -12 and -13 satellites
  - Can be easily adaptable for other satellites
- ✓ **CMAQ IOAPI to NEMSIO format converter** – To satisfy NCEP's requirement for model I/O data
  - Combining data from multiple CMAQ IOAPI files into a single NEMSIO data file
  - Expanding domain size by one row and one column for scalar variables to match the wind vector domain size

2.2 Code development inside the GSI package

- ✓ **A branch was created in NCEP GSI subversion repository**
  - New code is developed in the working copy and committed to the branch
  - Working copy is kept current by merging changes from the GSI trunk frequently
- ✓ **GOES AOD read module**
  - A section of code to read GOES AOD BUFR data was developed
- ✓ **CMAQ first guess input module**
  - A collection of subroutines were coded to read CMAQ model first guess fields in NEMSIO format
  - A collection of subroutines were coded to convert CMAQ's C-grid variables at mass, U and V points on the expanded domain to analysis grid (A-grid)
- ✓ **CMAQ aerosol property module**
  - Defines aerosol data type to hold CMAQ aerosol related variables
  - Calculates aerosol size distribution parameters D_g and σ_g
  - Integrates Community Radiative Transfer Model (CRTM) for CMAQ aerosol package
  - Computes model AOD from the CMAQ aerosol fields with CRTM

2.3 Model AOD Background Error Statistics

The background error statistics play an essential role in a data assimilation system. In GSI, this is achieved by applying the recursive filters with a quasi-Gaussian self-adjoint smoother kernel. To construct the recursive filters, background error variance (or standard deviation) and length scale need to be specified for any analysis variable.

In this study, the "NMC" method was followed: the error statistics are estimated with the differences of 24- and 48-hour forecasts valid at the same time. Three months' CMAQ model forecasts running from July 1 – September 30, 2010 were downloaded and model AOD fields were computed with a standalone version of CRTM AQ package.

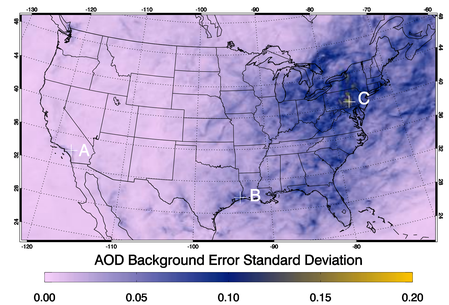

Figure 3. The AOD background error standard deviation shows significant spatial variation.

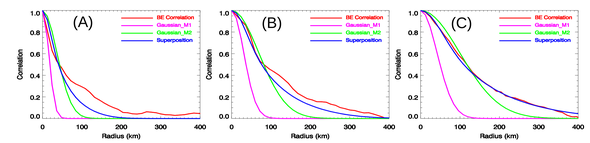

Figure 4. Different ways to estimate the correlation length scales were tested.

BE Correlation: At each grid point, correlations with all surrounding grid points were calculated and binned according to the distance. The AOD correlations at the three hot spots show remarkable "fat-tailed" distributions.

Gaussian_M1: Commonly used for estimating length scales for meteorological variables. The formula $L = (8\mathbf{V}_\tau / \mathbf{V}_{\nabla^2\tau})^{1/4}$ is used to find the length scale of the variable, where $\mathbf{V}_\tau$ is the variance of the variable and $\mathbf{V}_{\nabla^2\tau}$ is the variance of its second derivative. **This method results in serious under-estimation for AOD.**

Gaussian_M2: An effective length scale is determined such a way that the resulting Gaussian distribution and BE correlation reach a value of 0.5 at the same distance. **This method results in better fit** with slightly over-estimation within short distance and under-estimation in longer distance.

Superposition: Superposition of three equally weighted Gaussian distributions with 0.5, 1.0 and 2.0 times the effective length scale estimated as in Gaussian_M2. The "fat-tailed" distributions can be achieved.

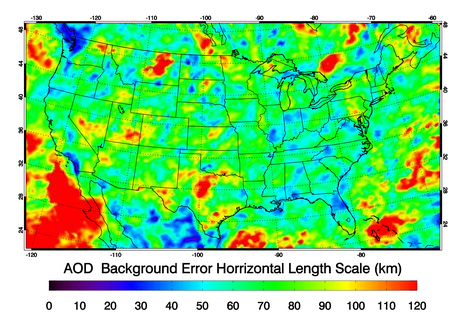

Figure 5. The effective length scales (estimated with Gaussian_M2 method) show significant spatial variation, indicating that the background errors covariance may not be treated homogeneously.

3. Accomplishments anticipated at end of FY12

- Complete GSI code development
  - Conduct GOES AOD observation error (OE) statistics
  - Re-conduct CMAQ model AOD background error (BE) statistics upon the fully functional CRTM (with hygroscopic effects) release.
  - Integrate CMAQ AOD BE and GOES AOD OE covariance matrices into GSI system through cost function construction
  - Integrate the whole GSI system as needed
- Conduct data assimilation experiments with GSI and analyze the results
  - With GOES AOD retrievals
  - With GOES-R proxy data

4. Initial feedback from potential user

This project is to develop and deliver to NCEP a GSI system capable of assimilating GOES AOD for CMAQ model to improve the surface PM2.5 forecasts. As a potential user, NCEP has been supporting this project by providing computing resources, the CMAQ model with necessary input data sets, as well as guidance and regulations of software development for its operational use. Through a coordinated community effort, NCEP has taken this project as one part of its plan to develop an aerosol assimilation system, which can use satellite and *in situ* observations in a regional or a global air quality model.

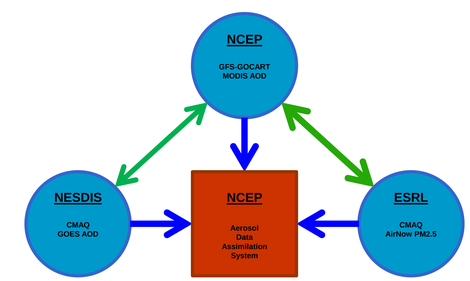

Figure 6. A coordinated community to develop an aerosol data assimilation system.

5. Future work

Due to budget shortfall, NWS/NCEP has decided to stop work on GSI aerosol assimilation activities. This change requires NESDIS/STAR to separate the 3D-var code development from NCEP's GSI framework and make it a "stand-alone assimilation system". Discussions with EPA are underway for use of this system in its applications.

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