Chemical Data Assimilation: Integrating Atmospheric Chemistry Observations into Air Quality Modeling

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Goals

Our primary goal of assimilating atmospheric chemical observations into the Community Multi-scale Air Quality (CMAQ) Modeling System is **to generate better air quality analyses and forecasts.** The adjoint model associated with 4-Dimensional variational (4D-Var) data assimilation method model can provide a unique tool to study *receptor-based model sensitivities* to multiple model parameters. This will help **us understand the air quality model in its underlying physics, chemistry, as well as the numerical schemes implemented**. In addition, we can **mitigate the large emission uncertainties** caused by the outdated inventories through chemical data assimilation., i.e. *emission inversion***.**

Approaches

1. In data assimilation, background error covariance (B) not only determines the weighting between observations and a priori background model results, it also dictates the spread of the increment in space and between variables. We estimate the **CMAQ error statistics** through both the so-called NMC (National Meteorological Center) and Hollingsworth-Lönnberg methods.
2. A simple sequential data assimilation method, **Optimal Integration (OI) or 3D-Var**, is used to test the effects of assimilating in-situ and satellite observations on the air quality forecasts and re-analyses.
3. The **4D-Var** approach is investigated in its ability to provide re-analyses. It is also used to provide diagnosis to the air quality model , including its ability to generate receptor-based sensitivities. Emission inversion is going to be studied under the 4D-Var framework as well.

CMAQ Model Error Statistics

Hollingsworth-Lönnberg and NMC results are shown in Figs 1 and 2 respectively. The ozone horizontal error statistics from them agree reasonably well, in terms of error variances and correlation length.

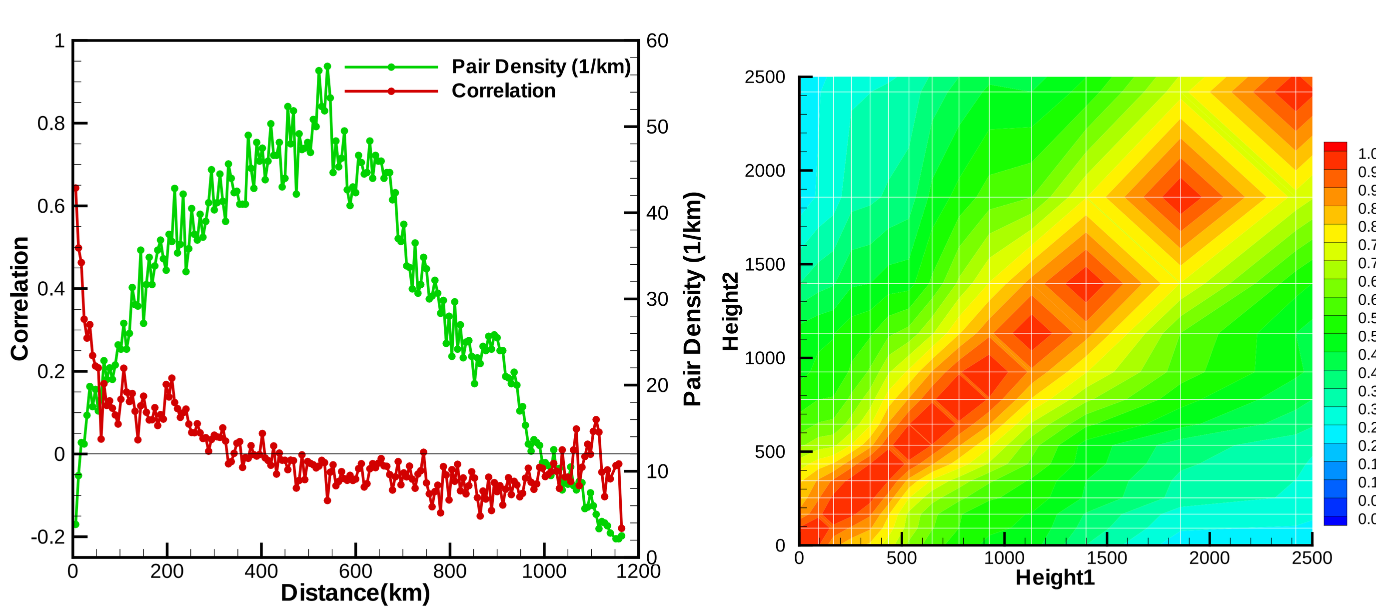

Figure 1 – Ozone error statistics results through Hollingsworth-Lönnberg approach. AIRNow observations are used to get horizontal error statistics (left). Ozonesonde observations are used in calculating vertial model error statistics (right). Unit of height: meter.

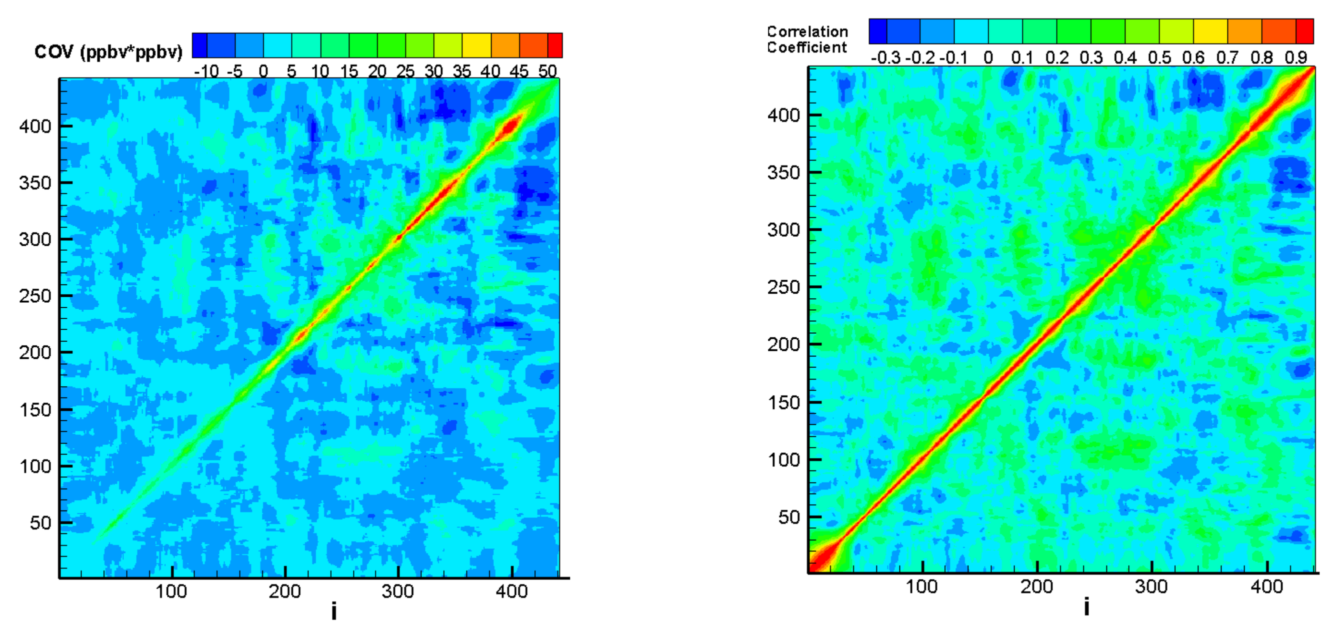

Figure 2. Horizontal error statistics (in east-west direction) results through NMC approach. Ozone error covariances are shown on the left and correlation coefficients are shown on the right. Numbers shown on both axes are in units of number of 12-km grid cells.

MODIS Aerosol Optical Depth Assimilation

We assimilated MODIS aerosol optical depth (AOD) using OI approach. At each time step, we solve an analysis problem

$$X^a = X^b + BH^T(HBH^T + O)^{-1}(Y - HX)$$

Where ***X*** and ***Y*** are the state and observation vectors, respectively. ***B*** and ***O*** are background and observation error covariance matrices. H is the observational operator. Superscripts *a* and *b* indicates analysis and background states. Observations far away (beyond background error correlation length scale) have no effect in the analysis. In the current study, the daily data injection takes place at 17Z.

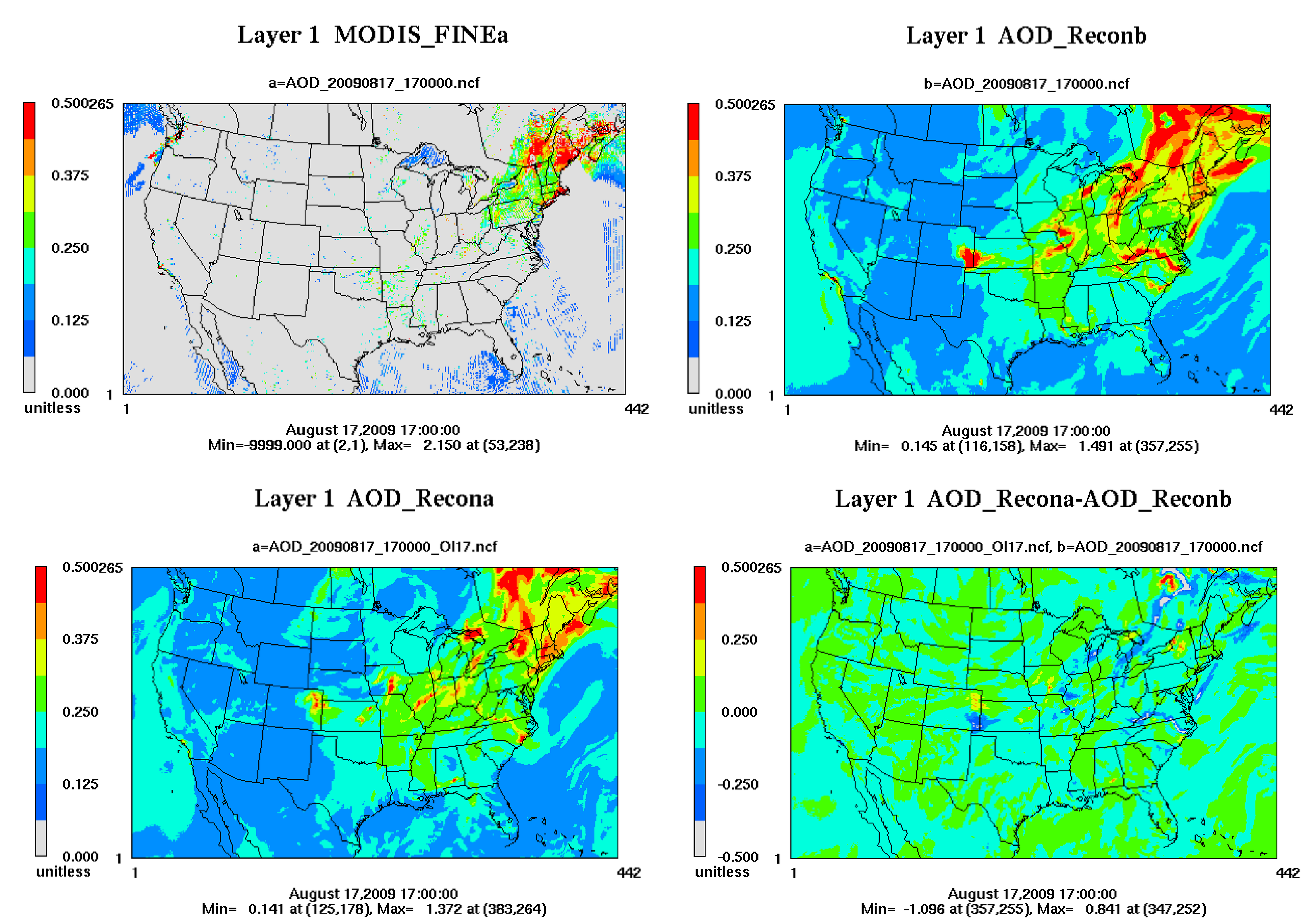

Figure 3. MODIS AOD (fine mode) and CMAQ reconstructed AOD. AOD_Recona and AOD_Reconb are calculated before and after assimilation. The differences (AOD_Recona - AOD_Reconb) are also shown.

Results (Fig. 3 and Table 1) show that assimilating MODIS AOD using OI method is able to improve AOD and PM2.5 predictions in selected regions, namely Upper Midwest (UM) and Northeast (NE) US. But, the improvement is not significant.

Table 1. Correlation between CMAQ PM2.5 predictions and AIRNow hourly observations in Upper Midwest and Northeast US before and after (OI) MODIS AOD assimilation.

R^2	8/15/09	8/16/09	8/17/09	8/18/09	8/19/09	8/20/09
UM	**0.420**	**0.138**	**0.355**	**0.154**	**0.234**	**0.021**
UM-OI	**0.399**	**0.178**	**0.311**	**0.180**	**0.270**	**0.041**
NE	**0.253**	**0.416**	**0.097**	**0.070**	**0.156**	**0.217**
NE-OI	**0.306**	**0.367**	**0.110**	**0.207**	**0.171**	**0.206**

CMAQ Adjoint and 4D-Var

CMAQ v4.5.1 adjoint model was originally developed at Virginia Tech University. We added the observational interface for 4D-Var applications. A receptor-based adjoint sensitivities are shown in Figs 4 and 5. Currently the adjoint of the newer CMAQ version is being developed, as a collaboration among several institutions.

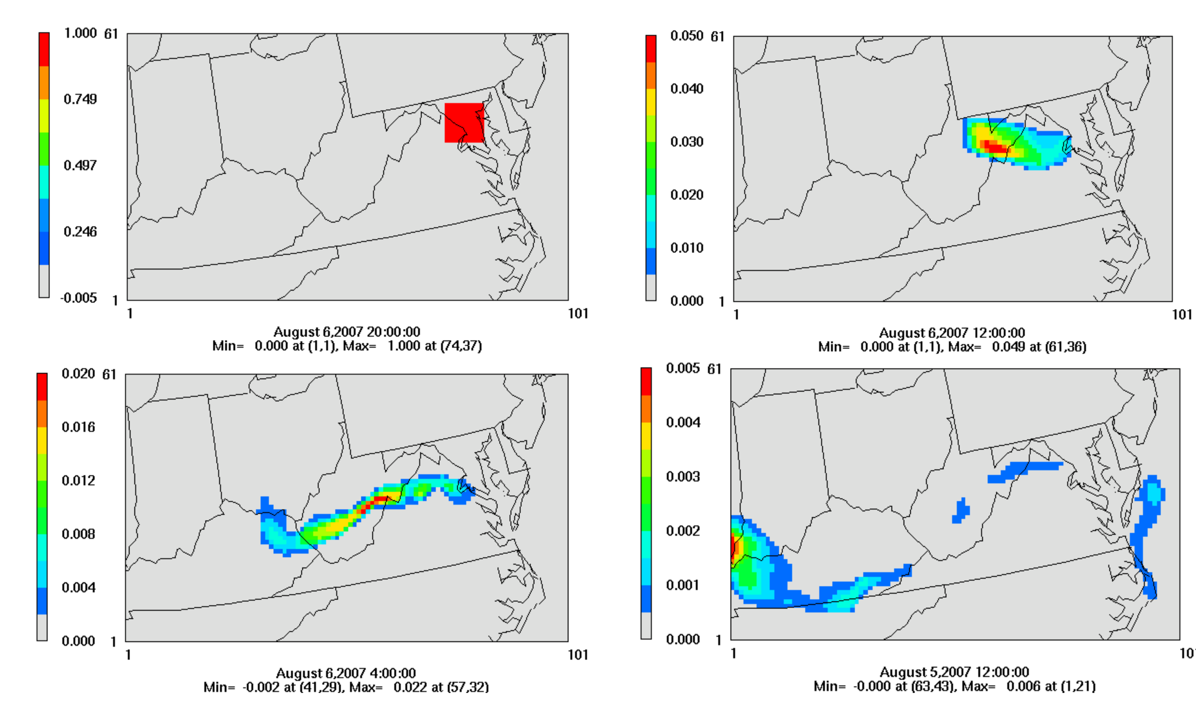

Figure 4. Adjoint sensitivities of "target" to surface ozone at earlier hours. Target is defined as the sum of ozone concentrations in a selected region covering Washington DC area, extending from layer 1 to 4, at the final time (20Z, 08/06/2007).

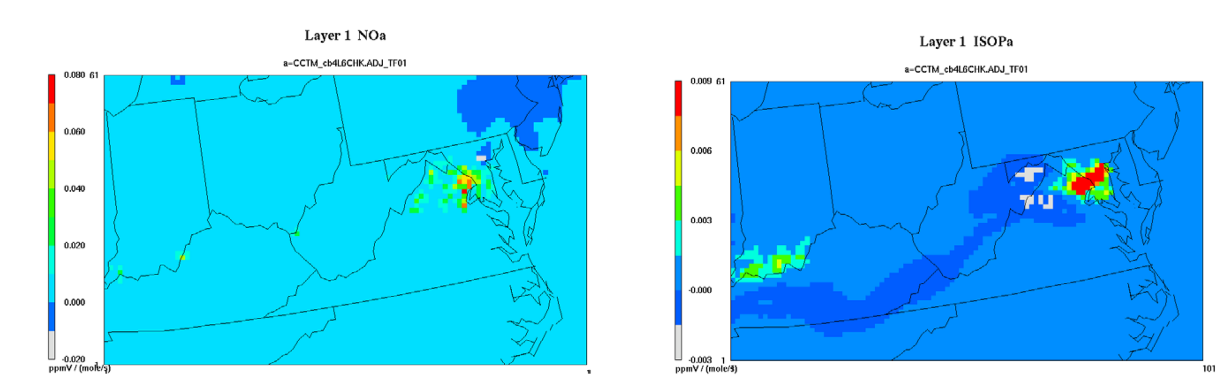

Figure 5. Adjoint sensitivities of "target" to NO and isoprene emissions in a 32-hour simulation. Target is defined as the sum of ozone concentrations in a region covering Washington DC area, extending from layer 1 to 4, at the final time (20Z, 08/06/2007).

Future Directions and Collaborators

1. Assimilate MODIS AOD and AIRNow PM2.5 predictions to generate PM2.5 re-analysis and forecast products using OI method (in collaboration with US EPA)
2. Improve operational air quality forecasting capabilities using GSI 3D-Var method (with NOAA/NESDIS, NOAA/NWS, NASA, NRL, and University of Wisconsin, Madison)
3. Develop adjoint model and its interface for assimilation capabilities, to be released with the next CMAQ release (with US EPA, Univ. of Iowa, Virginia Tech, U. of Colorado, and others)
4. Evaluate and/or reduce emission uncertainties using data assimilation approach.