Sensitivity Study on Generating Atmospheric Chemistry Reanalysis Field for the Contiguous Unites States Using Community Multi-scale Air Quality (CMAQ) Modeling System

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Three-dimensional multi-scale Air Quality (CMAQ) Modeling System has been used to generate ozone and particular matter (PM2.5) forecasts for the US. Similar to the meteorological reanalysis products, gridded data sets that best represent the atmospheric chemistry are needed for air quality, climate, epidemiology, and many other fields in their research and policy-related studies. To emulate the success of the National Centers for Environmental Prediction (NCEP) and the National Center for Atmospheric Research (NCAR) reanalysis products, efforts have been spent to generate atmospheric chemistry reanalysis field by assimilating the AIRNow surface network PM2.5 observations and MODIS (MOderate Resolution Imaging Spectroradiometer) aerosol optical depth (AOD) into the CMAQ model. In this work, sensitivity tests are carried out to study the impacts of observation insertion frequencies and schemes, different observation and background error covariance formulations on the atmospheric chemistry reanalysis products using a three-dimensional variational (3D-Var) data assimilation method. July 2011 is chosen as a test period to coincide with the Deriving Information on Surface conditions from Column and Vertically Resolved Observations Relevant to Air Quality (DISCOVER-AQ) field experiment. The field experiment observations as well as other un-assimilated observations will be used to evaluate the data assimilation performance. Effects of the data assimilation on aerosol components and their vertical distributions will be discussed. A data assimilation system using 3D-Var method to generate multi-year atmospheric chemistry reanalysis products will be proposed based on the sensitivity study results.

Data Assimilation for Space Weather: Specification of the Ionosphere-Thermosphere Environment

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Space weather has a dominant effect on many climate and weather patters across the globe. Therefore, it is important to understand and correctly specify the various space weather environments that influence Earth. Space weather refers to the variable conditions on the Sun and in the space environment that can influence the performance and reliability of spaceborne and groundbased technological systems, as well as endanger life or health. In this part of this talk we present an overview data assimilation for space weather problems, including heliophysics, radiation belts, magnetosphere, and ionosphere-thermosphere to name a few. In the second part we present our current efforts to correctly specify the ionosphere-thermosphere environment through the assimilation of direct and indirect data sources.

One of the most commonly used data assimilation technique for space weather is the ensemble Kalman filter (EnKF). The EnKF has been implemented to specify and predict radiation belts [1,2], Solar geomagnetic photosphere [3,4], Solar corona [5], and ionosphere-thermosphere-magnetosphere [6], among other problems. We will give an overview of the application of the EnKF to these and other problems, the challenges currently facing the predictability of extreme space weather events, and the future developments currently underway by a number of research groups to enhance the real time predictability of space weather environments.

In recent years, the accurate specification and prediction the global ionospheric-thermospheric environment has attracted much attention due to efforts in understanding the effect of the upper atmospheric environment on climate and weather patterns. In order to understand and accurately estimate the ionosphere-thermosphere environment, this talk presents the implementation of the local ensemble transform Kalman filter (LETKF) assimilation method to a global ionosphere-thermosphere model. In particular, the LETKF is utilized to estimate not only the model state, but also key model parameters that have a significant impact on the evolution of the total upper atmospheric density. The main parameters of interest are those who represent solar activity, such as $F_{10.7}$ and solar EUV spectrum parameters. A series of assimilation results are presented where the EnKF estimated a model bias correction through the parameters to obtain the correct model state. The assimilation experiments are shown for observational total density data from CHAMP and GRACE satellites, as well as indirect observation such as total electron content from a number of ground stations.

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Operational Assimilation of Dust Optical Depth

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In desert regions mineral dust has a large effect on radiation and visibility and impacts on human health and safety and transport including aviation. Dust has been included in the operational Met Office global forecast model since July 2011 and the forecasts contribute to an international intercomparison (see http://www.metoffice.gov.uk/research/news/dust-forecasting and http://sds-was.aemet.es/forecast-products/dust-forecasts/compared-dust-forecasts). Originally there was dust uplift, transport and deposition [1] but no data assimilation. More recently a dust assimilation system was included, partly based on [2]. Trials have been performed assimilating Aerosol Optical Depth (AOD) retrievals from the SEVIRI instrument on Meteosat Second Generation (MSG) [3,4] and the MODIS instrument on the Aqua satellite [5,6]. The 4D-Var assimilation of MODIS AOD retrievals over land areas, where dust is expected to be the primary aerosol, became operational on 30 April 2013. (In some areas discrimination of dust and other aerosol types is problematic.) Overall the results show an improved fit to satellite AOD and to the sparse AERONET network [7] for short range forecasts. However by day five of the forecast the benefit has largely disappeared, this is expected given the relatively short residence time of dust in the atmosphere. The results [8] and future development options will be discussed.

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Variational Data Assimilation for Multiple Aerosol Species with WRF/Chem

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Aerosol data assimilation faces some fundamental difficulties that arise primarily in treating a large number of state variables. A sophisticated aerosol scheme often explicitly treats more than a dozen species, which involve not only mass concentrations but also number concentrations. The number of state variables is further multiplied for representing the wide range of aerosol size distributions, ranging from a few nanometers to around 100 µm in diameter. To circumvent these difficulties, a host of formulations are proposed and implemented in a three-dimensional variational data assimilation (3-DVAR) algorithm in a Weather Research and Forecasting (WRF) model coupled with Chemistry (WRF/Chem). The WRF/Chem model uses the MOSAIC (Model for Simulating Aerosol Interactions and Chemistry) aerosol scheme, which explicitly treats eight major species (elemental/black carbon, organic carbon, nitrate, sulfate, chloride, ammonium, sodium, and the sum of other inorganic, inert mineral and metal species) and represents size distributions using a sectional method with four size bins. To treat the large number of state variables associated with the MOSAIC scheme, this 3-DVAR algorithm first determines the analysis increments of the total mass concentrations of the eight species, defined as the sum of the mass concentrations across all size bins, and then distributes the analysis increments over four size bins according to the background error variances. The number concentrations for each size bin are adjusted based on the ratios between the mass and number concentrations of the background state. The system is evaluated using the analysis and prediction of PM2.5 in the Los Angeles basin, with assimilation of surface PM2.5, surface speciated concentrations, and aircraft profiles.

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Variational and Ensemble Aerosol Data Assimilation for Regional Air-Quality Forecasts Using WRF/Chem: an Overview

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In the past three years, aerosol data assimilation (DA) capability has been developed within NCEP GSI-3DVAR system at the NCAR MMM division. The system allows simultaneous assimilation of multiple aerosol observation types from both satellite platforms and ground-based networks to constrain 3D aerosol initial conditions for regional WRF/Chem model forecasts using the NASA GOCART aerosol module. 3DVAR control variables are 3D mass concentration of individual aerosol species (organic and black carbon, sulfate, sea salt, and dust) and the background error covariance (variance, horizontal and vertical correlation scales) for each species is obtained using the NMC method with no multivariate correlation considered.

The newly-developed system was firstly applied to a dust storm over East Asia by assimilating MODIS 0.55 μm total aerosol optical depth (AOD) retrieval products using the JCSDA's CRTM as the observation operator which led to substantial improvement for WRF/Chem air-quality forecasts when compared to independent aerosol data sources (Liu et al., 2011). Simultaneous assimilation of AOD and surface PM2.5 observations was then demonstrated over North American for a month-long period (Schwartz et al., 2012). The deficiency of assimilating MODIS AOD over western US desert area, where retrieval quality is problematic, was identified. Another noticeable thing is that the impact of assimilating surface PM2.5 is rapidly diminished with forecast range. This issue was also found when assimilating PM10 over China (Jiang et al., 2013). Process analysis for PM10 formation indicates that the rapidly-diminishing DA impact on aerosol forecasts, especially in early forecast hours, was caused by stronger vertical mixing created by surface aerosol DA.

More recent development has focused on ensemble-based aerosol DA. Initial results using an EnKF did not show superior performance compared to 3DVAR (Schwartz et al., 2013), likely attributed to the inefficiency of EnKF when dealing with biased WRF/Chem forecasts. GSI-hybrid assimilation technique, however, exhibits some benefit. Efforts have also been made to directly assimilate MODIS visible radiances as an alternative to AOD assimilation, with encouraging initial results (Liu and Lin, 2013). These published and fresher results will be presented in the meeting.

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Global Aerosol Forecasting and Assimilation System at NCEP: Overview and Status

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Efforts to develop global prognostic aerosol capability at NOAA National Centers for Environmental Prediction (NCEP) have been underway, which in turn is part of NCEP's modeling efforts toward a unified modeling framework. In specific, NCEP is constructing NOAA Environmental Modeling System (NEMS) as its next-generation operational system and has collaborated with NASA Goddard Space Flight Center (GSFC) to develop NEMS GFS Aerosol Component (NGAC) system for predicting the distribution of atmospheric aerosols. NGAC Version 1.0 (NGAC V1) provides the first operational global dust forecasting capability at NOAA (http://www.ftp.ncep.noaa.gov/pub/data/nccf/com/ngac for real-time NGAC digital products and http://www.emc.ncep.noaa.gov/gmb/sarah/NGAC/html/realtime.ngac.html for the web-based graphics).

The rational for developing a global aerosol forecast and assimilation capability at NCEP includes: (1) to improve weather forecasts and climate predictions by taking into account of aerosols effects on radiation and clouds; (2) to better utilize satellite observations by incorporating aerosols as a key component, e.g., atmospheric correction; (3) to provide aerosol lateral and upper boundary conditions for regional aerosol/air quality models; and (4) to assess aerosol impacts on climate, human health, ecosystem, and visibility. The ultimate goal at NCEP is a full-blown Earth system with the inclusion of aerosol-radiation feedback and aerosol-cloud interaction. Due to resource constraints, the current operational configuration is to maintain a low-resolution system for aerosol prediction and a high-resolution system for medium range weather forecasting.

While development work remains, ground work has been laid for building a global aerosol forecasting/assimilation system within NGAC and Gridpoint Statistical Interpolation (GSI) at NCEP. This presentation will provide an overview of the NGAC global aerosol forecasting system, demonstrate the use of satellite-based biomass burning emissions for improving aerosol forecasts, and discuss the status on the development of GSI aerosol data assimilation.

Comparison of EnsKF and 4D Var chemical data assimilation with the BASCEO system

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The ensemble Kalman filter (EnsKF) using an observation perturbation approach has been applied to the stratospheric chemical transport model of BASCOE (Belgian Assimilation System for Chemical ObsErvations). BASCOE was developed originally with a 4D-Var and is providing near-real time analyses for the European project MACC-II. In this study we compare the results of 4D-Var with the EnsKF over a period of four months using MLS EOS-Aura ozone data. Each assimilation system uses the same observation error statistics and share the same spectral formulation of the prescribed error covariances (i.e. the model error covariance in EnsKF and the background error covariance in the 4D-Var). The model error variance and the observation error were also adjusted to yield a stable χ^2 over the whole integration time period. In their own respective setup, 4D Var and EnsKF are optimally tuned assimilation systems providing their best analysis [1]. The results shows the analyses of the EnsKF are more realistic and smoother than those of the 4D Var. Also the O-F of the EnsKF has systematically (all regions, all altitudes) smaller variances than the O-F of the 4D Var. Two aspects that can explain this discrepancy is discussed and explored through experimentation. One is the accumulation of information (or their lack of it) from one Var window to the next. Two is the effect of model error that is not accounted in 4D Var. The analysis shows that the continuous accumulation of information improves the performance of EnsKF but is limited in time by the presence of model error. Overall the absence of a strong constraint in the EnsKF, accounted by model error is responsible for the EnsKF performance over that of 4D Var.

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Potential for Ensemble Assimilation of Stratospheric Ozone

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In the past decade, meteorological centers around the world have raised the lid of their numerical weather prediction models to include the stratosphere. However, comprehensive prognostic ozone fields are generally not included in these models even though ozone plays a strong role in the radiative budget of the stratosphere and influences the model forecasts. In addition, assimilating ozone observations can also have a strong impact on the temperature and wind fields analyses.

We will demonstrate the direct impact that the Ensemble Kalman Filter assimilation of ozone has on the wind analysis in the context of a perfect-model observation system simulation experiment (OSSE) [1]. The role of the multivariate background-error covariances and proper localization will be emphasized.

The assimilation process is also tested with times-lags between the analysis and the observations. Ozone data up to 48 hours posterior to the analysis time are being assimilated with an Ensemble Kalman Smoother. Again, promising results in terms of impact on the analysis errors of different model variables are obtained, at a computational cost similar to that of assimilating current observations [2]. This has implications for the improvement of current reanalysis systems and the production of ozone reanalyses.

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Assimilation of Fine Aerosols using an Ensemble Kalman Filter: Challenges for Predicting Atmospheric Chemistry and Meteorology

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Because of interactions between meteorology and chemistry future data assimilation systems will likely not only include meteorological but also chemical observations and state. Such systems hold a promise for improved prediction of both weather and chemical composition.

Prediction of atmospheric aerosols is the focus of this presentation. Aerosols not only impact radiation and cloud processes but are also a pivotal contributor to air quality and single most critical factor affecting human mortality due atmospheric pollution.

Current skill of prediction of aerosol composition and concentrations is poor compared to the skill of weather forecasts as demonstrated by evaluation statistics and large discrepancies between results from different global and regional chemical models. Such state of the art originates mainly from

- weaknesses of chemical parameterizations;
- strong sensitivity of the system to uncertain and burdened with large errors emission source estimates;
- limited availability of observations of vertical profiles and aerosol composition and shortcomings of satellite retrieval for assimilation and verification;
- deficiencies in forecasting boundary layer meteorology.

In the presentation, we examine the impact of assimilating MODIS AOD and in-situ measurements on the prediction of fine aerosol concentrations over North America in the summer of 2012. We use an on-line meteorology-chemistry model WRF-Chem and a hybrid data assimilation system which includes the Gridpoint Statistical Intepolation (GSI) and an Ensemble Kalman Filter. Similar to our earlier publications ([1], [2]), we note large initial benefit of data assimilation and relatively quick deterioration of forecast verification scores with time. Simultaneous assimilation of meteorology and chemistry allows us to elucidate both positive and negative effects of regression relationships derived by the Kalman filter. We further seek to improve forecasts by increasing model error using stochastic parameterizations of selected model parameters. We present a comprehensive evaluation of the results, identify deficiencies of the system and outline future work.

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Assimilation of CO2 from ACOS GOSAT and AIRS into the GEOS5 constituent assimilation system

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We present the results of assimilating CO2 retrievals from Atmospheric CO2 Observations from Space (ACOS) of the Greenhouse gases Observing Satellite (GOSAT) combined with retrievals from the Atmospheric Infrared Sounder (AIRS). These two instruments are sensitive to CO2 in significantly different levels of the atmosphere, with lower tropospheric information from ACOS GOSAT and mid-tropospheric information from AIRS. These observations are assimilated into the GEOS5 constituent assimilation system and we show how the combined measurements can be used to improve estimates of tropospheric CO2 profiles through comparisons with aircraft and ground based in---situ measurements. We also describe the extraction of systematic errors in the data, and the development of a bias correction scheme for the assimilation system.

Upper-Tropospheric and Lower-Stratospheric Ozone from Assimilation of EOS-Aura Data into GEOS-5

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Accurate knowledge of the abundance, structure and variability of ozone fields in the Upper Troposphere – Lower Stratosphere layer (UTLS) is critical to our understanding of Stratosphere – Troposphere Exchange processes, radiative forcing and the tropospheric ozone budget. Data assimilation provides a unique opportunity to generate a representation of global ozone fields by combining satellite observations with general circulation model output in a manner that is consistent with atmospheric dynamics. In this paper we present validation results of an eight year long assimilation of data from the Ozone Monitoring Instrument (OMI) and the Microwave Limb Sounder (MLS), both on the EOS-Aura satellite, into the GEOS-5 Data Assimilation System (GEOS-DAS) developed at NASA's Global Modeling and Assimilation Office (GMAO) in collaboration with NCEP. This version of GEOS-DAS uses state-dependent background error variances for ozone, which help resolve sharp tracer gradients in regions of high dynamical variability. In particular, we will show that small-scale laminar structures in the UTLS ozone are well resolved in this product despite a relatively low vertical resolution of the input data. We will demonstrate that sharp ozone gradients in the vicinity of the tropopause are correctly represented in this assimilation allowing studies of cross-tropopause ozone transport.

Accounting for Representativeness Errors in the Inversion of Atmospheric Constituent Emissions: Application to the Retrieval of Regional Carbon Monoxide Fluxes

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A four-dimensional variational data assimilation system (4D-Var) is developed to retrieve carbon monoxide (CO) fluxes at regional scale, using an air quality network. The air quality stations that monitor CO are proximity stations located close to industrial, urban or traffic sources. The mismatch between the coarsely discretized Eulerian transport model and the observations, inferred to be mainly due to representativeness errors in this context, lead to a bias (average simulated concentrations minus observed concentrations) of the order of magnitude of the concentrations. 4D-Var leads to a mild reduction of the bias because it does not adequately handle the representativeness issue. For this reason, a simple statistical subgrid model is introduced and is coupled to 4D-Var [1]. In addition to CO fluxes, the optimization seeks to jointly retrieve *influence coefficients*, which quantify each station's representativeness. The method leads to a much better representation of the CO concentration variability, with a significant improvement of statistical indicators. The resulting increase in the total inventory estimate is close to the one obtained from remote sensing data assimilation. This methodology and experiments suggest that information useful at coarse scales can be better extracted from atmospheric constituent observations strongly impacted by representativeness errors.

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Ensemble-based Assimilation of Aerosol Observations in GEOS-5

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The MERRA Aerosol Reanalysis (MERRAero) is the aerosol reanalysis produced at NASA's Global Modeling Assimilation Office (GMAO). This reanalysis is based on a version of the GEOS-5 model radiatively coupled to GOCART aerosols and includes assimilation of bias corrected Aerosol Optical Depth (AOD) from the MODIS sensor on both Terra and Aqua satellites.

The AOD analysis in GEOS-5 is performed by means of *analysis splitting.* First, a 2D analysis of AOD is performed using error covariances derived from innovation data. The 3D analysis increments of aerosol mass concentration are computed using an ensemble formulation for the background error covariance. In MERRAero, as well as in the GEOS-5 near real-time system, this calculation is performed using the Local Displacement Ensemble (LDE) methodology under the assumption that ensemble perturbations are meant to represent misplacements of the aerosol plumes. These ensemble perturbations are generated with full model resolution, without the need for multiple model runs.

Currently, the GEOS-5 meteorological data assimilation system is transitioning to a hybrid Ensemble-Variational formulation. In line with these advances, we are updating the aerosol component of our assimilation system to an Ensemble Kalman Filter (EnKF) type of scheme. Since aerosols are an integral part of the GEOS-5 forecast model, aerosol ensemble members are routinely produced by the meteorological assimilation.

In this talk we will explore several strategies for generating aerosol ensemble members by a combination of perturbed transport afforded by the meteorological EnKF and careful perturbation of emissions, chemical production and removal processes. Before a full aerosol EnKF is implemented, we will examine the impact of replacing the current LDE perturbations with the new ensemble members in the existing *analysis-splitting* scheme. We will discuss the impact of this new ensemble formulation on AOD forecast skill, as well as on aerosol vertical structure as validated by independent ground-based, airborne and space-borne LIDAR observations.