Updates on the Development of the Aerosol Modeling Testbed

Jerome D. Fast[1], William I. Gustafson Jr. [1], Elaine G. Chapman[1], Jeremy Rishel[1], Douglas Baxter[1], Georg Grell[2], and Mary Barth[3]

[1]Pacific Northwest National Laboratory, Richland, Washington
[2]Cooperative Institute for Research in the Environmental Sciences / NOAA, Boulder, Colorado
[3]National Center for Atmospheric Research, Boulder, Colorado

1. Overview

The current paradigm in the scientific community of developing and testing new aerosol process modules is haphazard and slow. Aerosol modules are often tested for short simulation periods using limited data so that their overall performance over a wide range of meteorological conditions is not thoroughly evaluated. While several model inter-comparison studies have been performed that quantify the differences among aerosol modules, the range of answers provides little insight on how to best improve aerosol predictions. Understanding the true impact of an aerosol process module is also complicated by the fact that other processes such as emissions, meteorology, and chemistry are often treated differently.

To address this issue, we began the development of an Aerosol Modeling Testbed (AMT) a year ago with the objective of providing a new approach to test and evaluate new aerosol process modules. The AMT will consist of a more modular version of WRF-Chem [*Grell et al.,* 2005] and a suite of tools to evaluate the performance of aerosol process modules via comparison with a wide range of field measurements. Our approach is to systematically target specific aerosol process modules, while all other the processes are treated the same. The suite of evaluation tools will streamline the process of quantifying model performance and eliminate much of the redundant work performed among various scientists working on the same problem. Both the performance and computational expense will be quantified over time, analogous to meteorological forecast verifications made by the National Weather Service the past several decades.

The use of a testbed to foster collaborations and coordination of effort among the aerosol scientific community is the most important aspect of the AMT. While the initial development is being undertaken primarily by PNNL scientists, the long-term development and use of the AMT needs to be guided by users.

The AMT was introduced during the last WRF User's Workshop [*Fast et al.*, 2007] and the purpose here is to update the community on progress over the past year. Select tasks are described next in sections 2 - 4.

2. Modularity and Interoperability

Evaluating the performance and computational efficiency of new treatments for aerosol processes within a 3-D model requires the model to be sufficiently modular so that all other atmospheric processes are treated similarly. Since WRF-Chem is relatively new, its original form did not fully meet this criterion. This year, we have made two primary modifications to the code in addition to numerous minor modifications.

The first primary modification to WRF-Chem was to modularize how aerosol optical properties are handled. In version 2.2 of WRF-Chem, aerosol optical properties were computed within the Fast-J photolysis scheme and coupled only with the MOSAIC aerosol model [*Fast et al.,* 2006] as depicted in Fig. 1. The code was "buried" and it ws difficult for users to modify specific parameters and assumptions. We have created a more generic way of handling aerosol optical properties in WRF-Chem, via an "optical driver", that enables aerosol optical properties to be computed in a consistent manner for both the sectional (e.g. MOSAIC) and modal (e.g. MADE/SORGAM) representations of the aerosol size distribution. We also made it easy for the user to choose among three types of mixing rules (volume averaging, Maxwell-Garnett, shell-core) or add new treatments.

The second primary modification to WRF-Chem was to provide a means of fairly comparing the

MOSAIC and MADE/SORGAM models, the two aerosol models available to the community in version 2.2. The specific changes included adding anthropogenic emissions in the same way for both aerosol models, consistent on-line sea-salt and dust emissions, identical initial and lateral boundary conditions, use of the same trace gas chemistry for both aerosol models, and consistent treatments for aqueous chemistry and cloud-aerosol interactions. Previously, MADE/SORGAM was coupled only to the RADM2 and RACM photochemistry schemes and MOSAIC was coupled only to the CBM-Z photochemistry scheme. Now, both aerosol models can be run with CBM-Z so that differences in the aerosol predictions are not directly resulting from differences in gas-phase photochemical predictions. Similarly, we extended our treatments of aqueous chemistry and cloud-aerosol interactions [*Gustafson et al.*, 2007; *Chapman et al.*, 2008] to MADE / SORGAM so that differences between the two models do not result from different treatments of processes within clouds.

The new treatment of aerosol optical properties via the "optical driver" and some of the changes related to consistency between MOSAIC and MADE/SORGAM are now available in version 3 of WRF-chem.

3. Testbed Case Development

The availability of field campaign measurements has always been an issue that hinders adequate model evaluation, since these measurements are usually located at multiple web and ftp sites or must be obtained directly from the principal investigator associated with each instrument. The time required to access and consolidate this disjointed mass of information is excessive and unfortunately limits the usefulness of field campaign data for the modeling community. The archival of field campaign measurements has improved somewhat in recent years, but the process is still far from perfect.

We have nearly completed assembling the MILAGRO [*Molina et al.*, 2008] field campaign data for our first testbed case. This has involved converting the disparate file formats into a consistent format that can be utilized by our evaluation tools. This has produced ~6 Gb dataset containing nearly 40,000 files of meteorological, chemical, and particulate measurements from ground and aircraft platforms. Satellite data and measurements from "research-grade" instrumentation that cannot be easily compared to model parameters remain to be converted.

4. Toolkit Software Development

We have developed a number of programs and scripts, as part of the "Analysis Toolkit", that extracts model output at aircraft and ground locations, creates plots, and generate statistics. By default, everything possible is extracted, although users can customize the scripts. The scripts are also relatively simple to operate, with the user needing to make only few changes, such as indicating the path where WRF output resides. The programs include "aircraft" and "lidar" simulators. The "aircraft" simulator extracts model output at aircraft locations and interpolates the model output in time. The "lidar" simulator is similar, except that vertical curtains of simulated lidar properties (e.g. backscatter, extinction) are extracted either along moving aircraft flight paths or at fixed ground sites.

"Quick-look" graphics are provided that are intended to provide the user an initial way to visualize the differences between observed and simulated quantities. Thousands of plots are generated automatically. Users can input the corresponding observation and model files into their preferred software for further analysis and publication purposes.

Statistics are also generated automatically from the corresponding observation and model files. Measures are computed include: mean, standard deviation, bias, root-mean-square error, correlation coefficient, index of agreement, percentiles, normalized mean bias factor, normalized mean absolute error factor, mean normalized bias, and mean normalized absolute error. Statistics for specific quantities can be generated for the overall field campaign or for selected aircraft flights and/or ground sites.

5. Other Developments

While much of the basic infrastructure of he AMT is complete, some work remains and the following is a list of tasks to be addressed over the next year:

- implement a generic and modular module for dry-deposition

- extend cloud-aerosol interactions to Thompson and Morrison microphysics schemes
- enable predicted aerosols and optical properties to be used by the CAM radiation scheme
- explore how to best handle framework for SOA so that multiple treatments can be tested
- explore alternative approach for chemistry "packages" in WRF-chem
- finish MILAGRO testbed case development
- develop a "cloudy" testbed case
- finish remaining items for the Analysis Toolkit ("satellite" and "radar" simulators, refine statistics, etc.)
- develop a web portal, obtain computational resources the operation of the AMT, and explore ways of handling large amount of output files for the dynamic archive
- let 3-6 "beta" users of the AMT test it's capabilities and provide feedback on its operation
- solicit funding to support the long-term operation of the AMT for the scientific community

The demonstration version of the AMT will likely be available in the next several months. Users interested of the AMT for their research should contact Jerome Fast (jerome.fast@pnl.gov). A journal article describing the AMT concept and presenting an example demonstrating its capabilities is being written.

6. Path Forward

We are continuing to 1) increase the modularity and interoperability of WRF-Chem to widen the variety of aerosol process modules that can be evaluated in the testbed, (2) expand the available testbed data to permit broader evaluations, and most importantly, 3) seeking user-feedback, both of the concept and of actual use of a beta-version of the AMT.

Acknowledgements: This research is supported by the PNNL Laboratory Directed Research and Development (LDRD) program through the Aerosol Climate Initiative. PNNL is operated for the U.S. Department of Energy under contract DE-AC06-76RLO1830.

References

Chapman, E.G., W.I. Gustafson Jr., R.C. Easter, J.C. Barnard, S.J. Ghan, M.S. Pekour, and J.D. Fast, 2008: Coupling aerosols-cloud-radiative processes in the WRF-chem model: Investigating the radiative impact of large point sources. Submitted to *Atmos. Chem. Phys.*

Fast, J.D., W.I. Gustafson, R.C. Easter, R.A. Zaveri, J.C. Barnard, E.G. Chapman, G.A. Grell, and S.E. Peckham, 2006: Evaluation of ozone, particulates, and aerosol direct radiative forcing in the vicinity of Houston using a fully-coupled meteorology-chemistry-aerosol model. *J. Geophys. Res.*, 111, doi:10.1029/2005 JD006721.

Fast, J.D., W.I. Gustafon Jr., E.G. Chapman, D. Baxter, G. Grell, and M. Barth, 2007: The Aerosol Modeling Testbed: Coordinating the development of aerosol treatments using WRF-chem. 8th Annual WRF User's Workshop, 11-15 June, Boulder, CO.

Grell, G.A., S.E. Peckham, R. Schmitz, S.A. McKeen, G. Frost, W.C. Skamarock, and B. Eder, 2005: Fully coupled "online" chemistry within the WRF model. *Atmos. Environ.*, 39, 6957-6975.

Gustafson Jr., W.I., E.G. Chapman, S.J. Ghan, and J.D. Fast, 2007: Impact on modeled cloud characteristics due to simplified treatment of uniform cloud condensation nuclei during NEAQS 2004. *Geophys. Res. Lett.,* 34, L19809.

Molina, L.T., S. Madronich, J.S. Gaffney, and H.B. Singh, 2008: Overview of the MILAGRO/ INTEX-B Campaign. *IGACtivities Newsletter*, 38, 2-15.

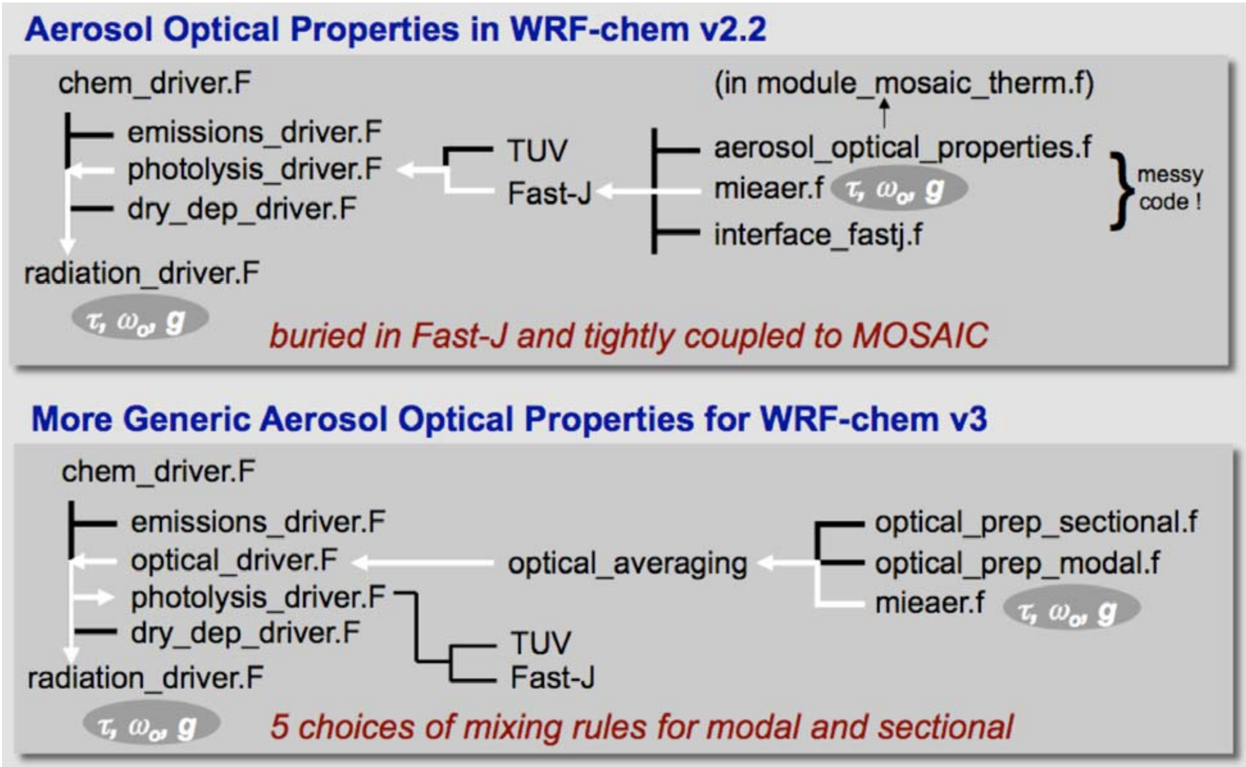

Fig. 1 Schematic diagram of the flow chart of the code related to aerosol optical properties in versions 2.2 (top) and 3 of WRF-Chem.