The Aerosol Modeling Testbed: Coordinating the Development of Aerosol Treatments using WRF-chem

Jerome D. Fast[1], William I. Gustafson Jr. [1], Elaine G. Chapman[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 direct (scattering and absorption of radiation) and indirect (cloud-aerosol interactions) effects of aerosols predicted by climate models still contain large uncertainties. To address this issue, the goal of a new project which began this year is to develop an *Aerosol Modeling Testbed (AMT)* that streamlines the process of testing and evaluating refined aerosol process modules over a wide range of spatial and temporal scales. The *AMT* will consist of a modular and user-friendly version of WRF-chem, and a suite of tools to evaluate the performance of aerosol process modules via comparison with a wide range of field measurements. The primary tasks associated with the *AMT* include: 1) improving the coding of aerosol process modules (where needed) to facilitate evaluations; 2) developing a series of test simulations, archived field data, and analysis tools suitable for systematically evaluating aerosol process modules; 3) utilizing WRF-chem and analysis tools on various computer platforms to ensure platform portability; and 4) implementing, testing and evaluating new aerosol treatments in collaboration with the aerosol modeling community.

A modular model will enable various treatments of specific aerosol processes to be systematically compared, while all other atmospheric processes (e.g. other aerosol processes, emissions, gas chemistry, meteorology) remain the same. Examples of specific aerosol processes that require further refinements include aerosol-cloud interactions, secondary organic aerosol formation, aerosol optical properties, new particle formation, representation of the aerosol size distribution, and treatments for emissions (e.g. dust, sea-salt). Our activities will be coordinated within the WRF-chem working group so that the version used in the *AMT* will contain the latest updates available from the publicly distributed version of WRF-chem.

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 the community of users.

2. Modularity

WRF-chem (Grell et al. 2005; Fast et al. 2006) is a multi-scale model; consequently, aerosol treatments can be tested both at the local scale where the predictions can be directly evaluated using field measurements as well as at large scales compatible with those used by global climate models. To evaluate 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 the same. WRF-chem in its current form does not fully meet this requirement; therefore, we will remove many of these dependencies so that the aerosol processes will be more modular. This will include creating generic aerosol process modules that can be employed by multiple aerosol mechanisms. Modularity is an on-going issue that is also being addressed by WRF-chem developers (e.g. NOAA).

3. Data Sets and Toolkits

This task consists of assembling a series of test simulations and analysis tools. The test simu-

Corresponding author: Jerome D. Fast, PNNL, jerome.fast@pnl.gov, 509-372-6116.

lations will be a combination of idealized and real-world cases that have extensive field campaign measurements. Several cases are needed because some field campaigns obtain measurements primarily on aerosol aging during clear-sky conditions, while other campaigns obtain measurements related to cloud-aerosol interactions. Aerosol field campaigns are typically up to about a month in duration, but longer simulation periods will be employed for some cases to evaluate predictions over a wider range of meteorological conditions.

The beta-version of the *AMT* that is being developed this year will utilize measurements made during the 2006 MILAGRO field campaign (Fast et al. 2007). This field campaign was chosen because of the wide range of particulate measurements that were made over multiple spatial scales to account for aerosol evolution over several transport days. The second test case to be developed next year will involve cloud-aerosol interactions. Ultimately the *AMT* will employ data from several field campaigns and will evolve as new field campaigns are conducted.

A set of tools will be developed that extracts model output, read the observational data, generates various qualitative comparisons, and computes statistical performance parameters. The tools will be developed using software commonly used by atmospheric modelers. We envision an "analysis toolkit" that compares model predictions with all available measurements using statistics and graphical methods. Similarly, an "inter-comparison toolkit" compares the performance of WRF-chem using various aerosol treatments. Running the model and analyzing the output will be controlled by a script file, as depicted in Fig. 1.

A history of model simulations will be archived as user-accessible data sets, thereby making it easier for investigators to evaluate new aerosol process modules and quantify/document the improvements. This 'encyclopedia' approach is needed to systematically record model performance, a capability that has been lacking. Our intent is to expand the types of inter-model evaluations presented in McKeen et al. (2007) that utilizes data from the ICARTT/NEQAS 2004 field campaign. In contrast to McKeen et al. (2007), the *AMT* will focus more on specific aerosol processes and will utilize only WRF-chem so that the meteorology, emissions, and trace gas chemistry are treated the same.

By creating the data sets and tools, redundant work for future model evaluations will be eliminated so that the time needed to test new aerosol process models will be reduced.

4. Computational Aspects

Aerosol treatments require hundreds to thousands of additional scalars in WRF that pose computational challenges, including compilation, load balancing, and scalability (Gustafson et al. 2005).

For idealized cases and modest real-world cases, WRF-chem can be run on traditional computer clusters with ~64 processors or less. But some simulation cases will require significant computational resources. The 'encyclopedia' approach of saving all comparison simulations, will also require large amounts of output that will not be suitable for traditional FTP downloads to user's home institutions. For example, the output from a single simulation using WRF-chem with a modest number of nodes and nested domains that also saves most of the 3-D chemistry scalars can easily be as large as a terabyte. The 'encyclopedia' will need petabytes of storage.

The computational expense and disk storage will require that a version of the *AMT* be made publicly available on a supercomputer for users to access for free. We will also be exploring alternative approaches so that users can download portions of the *AMT*. For example, the files created by the "analysis toolkit" and "inter-comparison toolkit" will be smaller and size and may be suitable to download.

5. Collaborative Activities

Once the overall framework of the *AMT* has been established, it will be made available to the atmospheric sciences community. The long-term success of the *AMT* depends upon aerosol scientists viewing it as a useful tool in streamlining their research, developing new aerosol process modules, and providing new scientific insights. A workshop and electronic survey will be conducted in the near-future to get input from the scientific community. A web page will be created later this summer. Those interested in participating in the *AMT* should contact the principal investigator.

The project is currently supported by PNNL during the first phase. DOE will be considering whether to provide for the continued development and maintenance of the infrastructure. We envision that during the initial stages of this project, a "top-down" approach is needed to put together the core infrastructure. Then, a more "bottom-up" approach of the *AMT* guided by a larger community will be adopted that could include support from other agencies.

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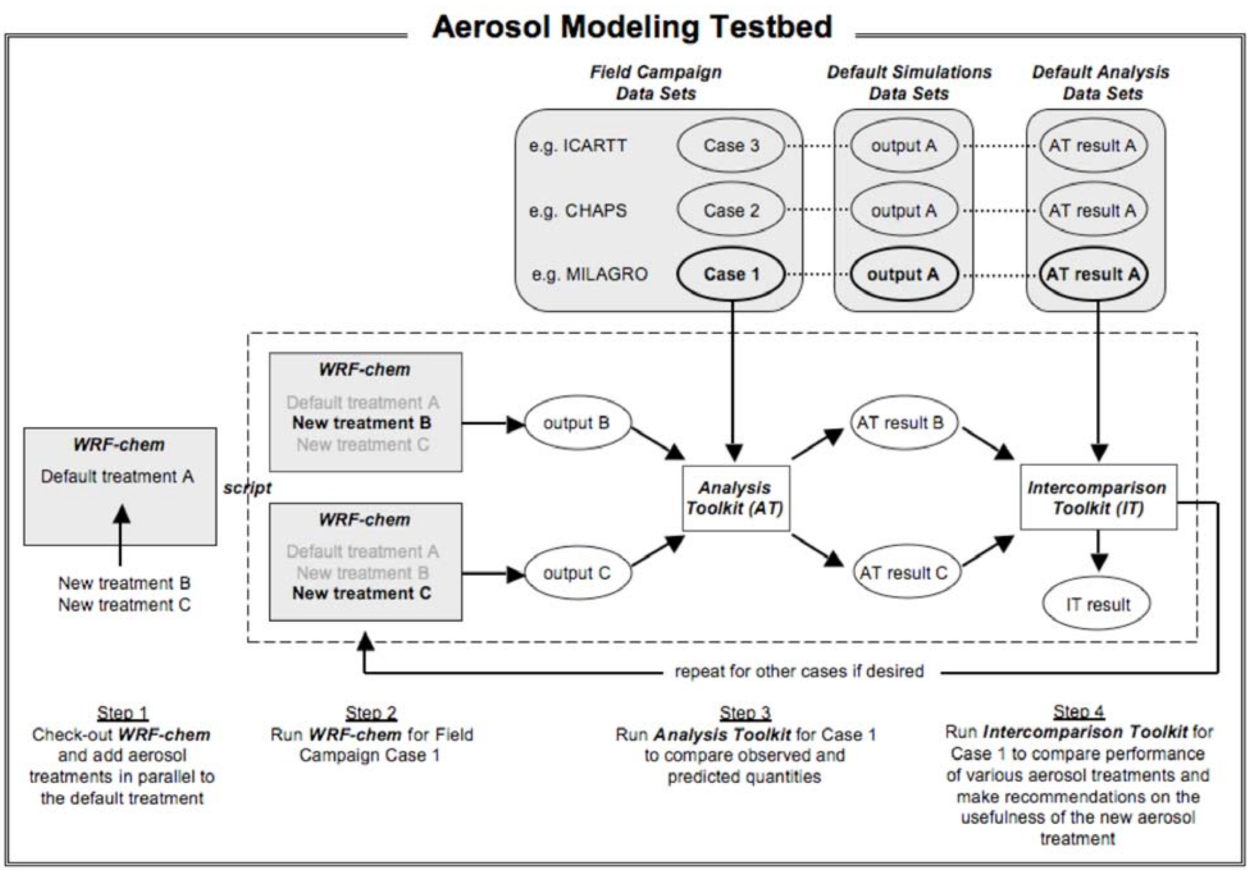

Figure 1. Schematic diagram depicting the concept of the *Aerosol Modeling Testbed* and how it would be used to test one type of aerosol treatment.