# Triumphs and Tribulations of WRF-Chem Development and Use

William I. Gustafson Jr., Jerome D. Fast,
Richard C. Easter, and Steven J. Ghan

Pacific Northwest National Laboratory, Richland, WA

In order to address scientific questions related to aerosol chemistry and meteorological-aerosol-radiation-cloud feedbacks at the urban to regional scale, scientists at the Pacific Northwest National Laboratory (PNNL) have made substantial contributions to the chemistry version of the Weather Research and Forecasting model (WRF-Chem) during the past one and a half years (Fast et al. 2005). These contributions include an additional gas-phase chemistry mechanism, a sectional aerosol module, an additional photolysis module, feedbacks between aerosols and radiation, and extending the nesting capability of WRF to include the chemistry scalars. During the development process, a number of limitations in WRF have been identified that complicate adding all the desired chemistry capabilities as originally planned. These issues will be discussed along with changes that have been made to help mitigate some of them. Features currently in development will also be discussed including comprehensive treatment of cloud-aerosol interactions and a secondary organic aerosol (SOA) mechanism for the sectional aerosol module.

## 1. Fully implemented contributions

The original chemistry framework within WRF was designed by Georg Grell and his team at the Forecast Systems Laboratory (Grell et al. 2005), to which the following process modules have been added. The additional gas phase chemistry mechanism added to WRF-Chem is CBM-Z (Zaveri and Peters 1999), which is based on the CBM-IV carbon bond mechanism. CBM-Z extends CBM-IV by including reactive long-lived species and their intermediates. For organic species and reactions it uses a lumped-structure approach based upon similar carbon bonds. The version in WRF-Chem treats isoprene, $SO_2$, and (optionally) DMS chemistry.

Corresponding author: William I. Gustafson Jr., William.Gustafson@pnl.gov

A new aerosol mechanism called the Model for Simulating Aerosol Interactions and Chemistry (MOSAIC) (Zaveri et al. 2005a; 2005b; 2005c) that employs a sectional treatment of aerosol size distribution has been added to WRF-Chem. This mechanism compliments the modal aerosol mechanism currently in WRF-Chem, MADE-SORGAM (Ackermann et al. 1998; Schell et al. 2001), allowing more detailed aerosol calculations to be made when specific research needs demand them. MOSAIC uses either a moving center or two-moment approach to solve the dynamic equations for mass and number. Each size bin includes nine particulate species plus two variables used to track the aerosol water content and hysteresis effect.

The photolysis mechanism added to WRF-Chem is Fast-J (Barnard et al. 2004; Wild et al. 2000). Fast-J uses the aerosol number, refractive index, and wet radius for each aerosol size bin to calculate the corresponding aerosol optical depth, single scatter albedo, asymmetry factor, and extinction via a spherical Mie code. These in turn, are used to calculate the photolysis rates. Additionally, the optical properties returned by the Mie code are used to couple aerosols with the Goddard Space Flight Center shortwave radiation code (Chou and Suarez 1994) in WRF. This enables WRF-Chem to simulate direct aerosol-radiation feedbacks associated with the predicted evolution of primary and secondary particulates.

To fully take advantage of the newly added mechanisms for research on the regional scale, the nesting capability of WRF has been extended to include the chemistry scalars. This permits the use of higher resolution in regions with high emissions where, for example, point source plumes need to be resolved to properly simulate the chemistry. Through inter-grid feedbacks, the improved chemistry from the fine domain(s) is interpolated to the coarser domain(s) where it is advected to the surround-

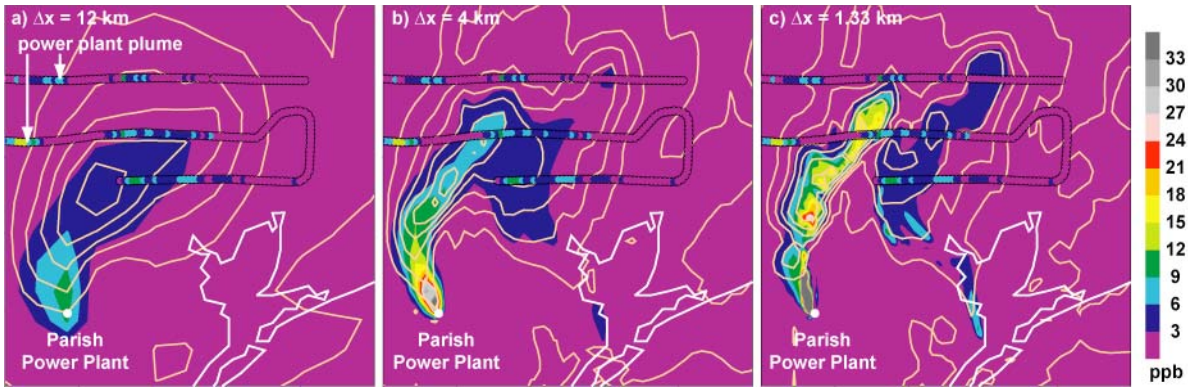



**Figure 1** Plots of $SO_2$ (shaded) and $PM_{2.5}$ (contoured with an interval of 2 μg $m^{-3}$) for the Houston area on 28 August 2000 21UTC at ~600 m AGL. Each plot shows the resolved gas and particulate amount for a simulation with (a) 12 km grid spacing (single grid), (b) 4 km grid spacing nested inside a 12 km grid, and (c) a 1.33 km grid doubly nested in 12 and 4 km grids. Aircraft observations of $SO_2$ are overlaid along the flight path.

ing region. Figure 1 demonstrates the effect of increased resolution on simulating $SO_2$ and $PM_{2.5}$ that is possible via nested grids. Panel (a) represents a single domain simulation, (b) a two domain simulation, and (c) a three domain simulation with the highest resolution possible from each simulation shown.

## 2. Contributions in development

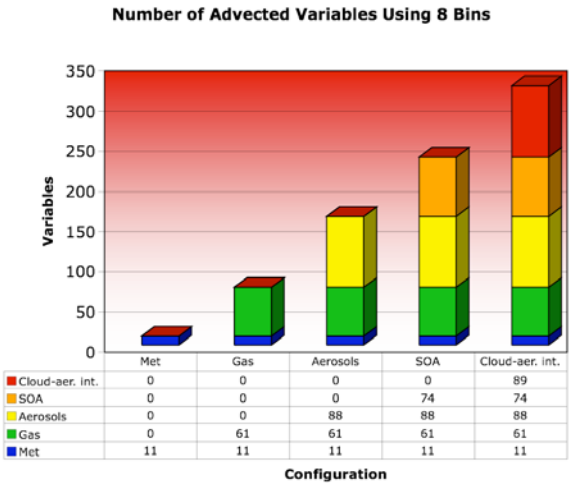
Two additional features are currently being added to WRF-Chem and should be fully tested this year. The first involves a comprehensive treatment of cloud-aerosol interactions. Aerosols can act as cloud condensation nuclei and alter the dynamics within the cloud (Abdul-Razzak and Ghan 2002; Easter et al. 2004; Ghan et al. 2001). This is done by coupling MOSAIC with the Lin et al. microphysics scheme (Lin et al. 1983; Rutledge and Hobbs 1984) and providing conversion pathways between interstitial and cloud-phase aerosol via supersaturation based activation and via evaporation. Aerosol scavenging by precipitation is also treated. Activated (cloud-phase) aerosol number and mass species and cloud droplet number are treated explicitly. A cloud chemistry module treats trace gas uptake and aqueous reactions in cloud droplets. Uptake and wet removal of trace gases by precipitation is also treated in a limited fashion. When completed, this will provide the capability to simulate both direct and indirect aerosol radiative forcing within the WRF framework, and will be a powerful tool for research investigating the effects of aerosols on regional climate.

The second feature in development is a SOA mechanism for MOSAIC. This will allow more detailed studies of aerosols in regions with high amounts of volatile organic compounds. It will also allow more direct comparisons to be made between MOSAIC and MADE-SORGAM since the latter already has an SOA mechanism built into it.

These added features are facilitated by the introduction of a generalized chemistry array pointer, which is indexed by aerosol composition, size, type, and phase. This permits a variety of aerosol configurations, including both internal and external mixtures, sectional and modal size distributions, and interstitial, cloud, rain, snow, and graupel phases of the aerosol.

## 3. Impediments and work-arounds in WRF-Chem

During development of WRF-Chem, in addition to typical issues related to using a beta version of the code, a more significant difficulty has occupied much of our time: simulations using the sectional aerosol approach require a large number of variables. Figure 2 demonstrates this by showing the number of advected variables within the model as the complexity is increased from a basic meteorology setup to a fully coupled meteorology-trace gas-aerosol-cloud interacting model. The basic meteorology




| | Met | Gas | Aerosols | SOA | Cloud-aer. int. |
|---|---|---|---|---|---|
| Cloud-aer. int. | 0 | 0 | 0 | 0 | 89 |
| SOA | 0 | 0 | 0 | 74 | 74 |
| Aerosols | 0 | 0 | 88 | 88 | 88 |
| Gas | 0 | 61 | 61 | 61 | 61 |
| Met | 11 | 11 | 11 | 11 | 11 |

**Figure 2** Number of advected variables in WRF-Chem as the complexity is increased. The table lists the number of variables used for the following model mechanisms: meteorology, gas-phase chemistry, aerosol chemistry, secondary organic aerosol mechanism, and cloud-aerosol interactions. Eight size bins are assumed for the sectional aerosol model.

model advects up to eleven variables, depending upon the moist physics setting, whereas the full model advects 323 variables, assuming eight size bins are used within MOSAIC. Some research applications will require more size bins, possibly doubling the number of aerosol variables. Additionally, MOSAIC is being used with an internal mixture assumption. If the code is modified in the future to use external mixtures, the number of aerosol variables could possibly increase by another factor of four or five. The net result is that the WRF model infrastructure needs to handle two to three orders of magnitude more variables than in a typical meteorology setup.

Handling this number of variables is computationally expensive in terms of both cycles and memory. For example, the ratio of wall time to simulation time for a three domain configuration with 12/4/1.33 km grid spacing and grid points of 89x89x57, 73x73x57, and 91x91x57 respectively, is roughly 3:1 on a 16 node, dual processor Pentium4 cluster with Myrinet.

Due to memory limitations, a typical Linux cluster can only run domains with roughly 100 grid points or less per side when nested with two to three domains. This, in turn, limits the scalability of the model to roughly 32 processors due to the larger percentage of the grid points that must be passed during halo communications compared to larger domains. In order to complete a nested simulation for the Houston area, with domain sizes of 89x89, 73x73, and 91x91 with 57 levels, we upgraded our Pentium4 Linux cluster to have 3 Gb of memory per dual-processor node and we replaced the Gigabit Ethernet communications with a 2 Gb $s^{-1}$ Myrinet configuration. With the original configuration of 1 Gb of memory per node, we could not run the third domain concurrently with domains one and two. Using Myrinet increased our simulations speeds by roughly 30%. At the conference, more information on the distribution of CPU time between advection, I/O, and within the chemistry modules will be given.

The additional chemistry variables also cause difficulties with compiling. For a typical 8-bin MOSAIC setup (without SOA or cloud-aerosol interactions) the longest include file generated by the Registry in our version of the model is over 44,000 lines long. Both the Portland and Intel compilers could not handle the code without making modifications. To date, we still have not been able to successfully use WRF-Chem with the Intel compiler. This prevents running the model on the Itanium cluster at the Environmental Molecular Sciences Laboratory (EMSL) co-located with PNNL. Ultimately, if this problem cannot be overcome, the domain sizes we can use will be limited by the addressable memory limits of 32 bit architectures. (Note that we do not have access to an Opteron system so we do not know how well the available compilers for that architecture work.)

The large number of chemistry variables also complicates coding of nesting. To reduce the number of lines of code by several thousand in solve_em.F, John Michalakes modified the handling of boundary arrays so that a new 5-D array type is generated by the Registry that combines the functionality of the 4-D and boundary field types. In addition to simplifying the code, this infrastructure improvement has the secondary benefit of reducing the memory requirements of WRF-Chem by 12%.

## 4. Discussion

WRF-Chem will eventually be a powerful tool that can be used to study many aspects of aerosol chemistry and climate feedbacks. While computational limitations currently limit large domains and long time integrations, specific case studies are within the current computer capabilities available within many university and government laboratories. Through judicious selection of model options, the model can be customized to meet specific research goals and computer limitations.

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