The Application of MM5/WRF Models to Air Quality Assessments

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1. Introduction

In light of the rapid development of the Weather Research and Forecast (WRF) model and the eventual replacement of MM5 by the WRF model, some discussion of the needs of the air quality modeling community as it pertains to mesoscale meteorological modeling is warranted. Accurate simulations of the transport, diffusion, dry and wet deposition, and chemical transformations for airborne chemical species, aerosols and particulate matter are largely dependant on data sets than can properly resolve the spatial and temporal evolution of the meteorological fields on a wide range of scales. In recent years, the use of three-dimensional high frequency mesoscale data sets derived from dynamical models such as MM5 to drive air quality simulation models has been growing. This trend will continue as computational power increases and improvements in physics and numerics of dynamical models proceed. Additionally, relatively simple air quality models requiring only limited meteorological inputs are being replaced with more advanced numerical models capable of utilizing three-dimensional meteorological fields.

The objective of this paper is to provide information on how MM5 is used to drive air quality models. This information we hope can help guide decisions regarding the future development and implementation of the WRF model so this model can become the primary mesoscale meteorological model for the air quality modeling community. A more comprehensive overview of meteorological modeling issues related to air quality modeling studies is given by Seaman, 2000.

2. Air Quality Simulation Modeling

Recently, the National Oceanic and Atmospheric Administration (NOAA) has placed emphasis on the development of real-time air quality forecast models with the objective being an operational national air quality forecast system. Such an air quality modeling system will likely be directly coupled to the WRF model.

Air quality impact assessments for regulatory permitting applications, siting studies, visibility impact studies and studies of emissions control strategies do not involve real-time forecasts, but instead, rely on historical meteorological data sets as input to air quality simulation models. Such studies vary in complexity from assessing the impacts of emissions from a single industrial facility to emissions from many complex sources over large areas. Air quality modeling domains vary largely in spatial dimensions from domains as small as 10 x 10 kilometers to as large as 600 x 600

kilometers. Air quality models consist of photochemical grid models or source-receptor models. Photochemical grid models use the meteorological grid directly to compute concentrations while source-receptor models compute concentrations at very dense networks of specific grid points called receptors. Many averaging periods are typically examined, ranging from hourly averages to annual averages. The averaging periods are mostly determined by specific pollutant standards such as the National Ambient Air Quality Standards and the Prevention of Significant deterioration increments.

Air quality model simulations in most applications involve multiple iterations in order to test source configurations and emissions scenarios and at times perform source attribution analysis. Individual emission sources or groups of sources with similar characteristics are often included within a single simulation for the full modeling period and the total pollutant concentrations computed using post-processing software to vield total predicted concentration fields. Thus a single air quality assessment may require many air quality model simulations. For this reason, for most air quality assessments, it is not practical to directly couple MM5 or WRF with an air quality model. Models like MM5 and WRF are computationally too expensive to run multiple times during an air quality analysis. As a result MM5 and ultimately WRF model simulations must be performed independently from an air quality model to develop the mesoscale meteorological data sets required. In fact, many air quality modelers are never involved in conducting such simulations. Only a specific number of private sector companies, the United States Environmental Protection Agency, and the National Park Service typically perform data assimilation simulations using MM5.

These three dimensional mesoscale data sets are used as a front end to air quality or diagnostic meteorological models. Meteorological data sets used for air quality models usually contain one full year of data but multi-year data sets are used as well in many studies.

3. Developing Three Dimensional Meteorological Fields for Dispersion Modeling Using MM5

Early dispersion models typically used hourly observations at a single meteorological station and were not capable of simulating pollutant transport and diffusion within spatially variable meteorological fields. More recent and advanced air quality modeling systems such as the CALMET/CALPUFF modeling system (Scire et al, 2000a,b) have this capability, but the success of such models is dependant in part on having

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meteorological data sets that can adequately resolve the synoptic, mesoscale, and planetary boundary layer structures. In most applications observational data is limited and can not adequately resolve details of the meteorological fields. Dynamical models have the ability to realistically simulate mesoscale meteorological fields not completely resolved by observations alone.

It is important to point out that the meteorological regimes important for air quality simulations are different from those emphasized in operational forecasting applications. In operational forecasting applications of the MM5 and WRF models, emphasis is placed on meteorological situations involving strong synoptic or mesoscale forcing where issues of severe weather and heavy precipitation events are important. For air quality applications, the reverse is true. Large air quality impacts typically occur during meteorological situations involving weak forcing (Zhang and Rao, 1998) where light winds and large diurnal changes in boundary layer stability occur. The ability to resolve the spatial and temporal evolution of diurnal terrain forced circulations is critical to simulations of pollutant transport and diffusion and ultimately to the prediction of ground level concentrations of chemical species and particulate matter.

The MM5 model has proven to be a powerful tool for the air quality modeling community due to its wide availability and its grid nesting and four dimensional data assimilation (FDDA) capabilities. Since most air quality modeling applications involve fine grid resolution, the MM5 model's grid nesting capability has allowed high-resolution data sets to be developed over limited areas with manageable computational requirements. Performing MM5 simulations with FDDA using Newtonian nudging (Stauffer and Seaman 1990, and Stauffer et al 1991) can be used to restrain the model's solutions from deviating too strongly from observations or from a gridded analysis. MM5 with FDDA can be used to develop realistic three-dimensional fields that are completely suited as inputs to air quality or diagnostic meteorological models. Modeling studies (Seaman et al 1995) have shown FDDA has the ability to improve the simulations of wind, temperature, moisture and mixed layer depth and they concluded that modeling with FDDA can produce spatially consistent solutions without degrading the important dynamical processes.

For applications to air quality modeling, multiple MM5 simulations are typically performed using FDDA with the length of each simulation typically not extending beyond a five-day period. Grid nesting is always used since the objective is to obtain meteorological fields with a horizontal resolution of 5 km or less. Enough MM5 simulations are performed to complete a full one-year three-dimensional data set of meteorological fields. Figure 1 shows a schematic of how MM5 simulations with FDDA are conducted to develop a three-dimensional mesoscale data set for air quality modeling. Up to 74 separate MM5 simulations are required to build a one-year data set of meteorological fields.

Analysis nudging is the most common technique used. The nudging is typically performed on the large scale coarse domain and sometimes on the intermediate nest depending on the quality of the analysis and the grid resolution. Analysis nudging is almost never performed on the fine scale nest due to inadequate gridded analyses. In some cases, if suitable observational data are available, observational nudging will be performed on the fine scale nest. However, in most air quality modeling applications, observational data is either not available or is unsuitable for use in MM5. Studies (Stauffer and Seaman 1994) have suggested that assimilating unsuitable observations into the simulation (e.g. assimilating meso-alpha scale observations into a meso-beta scale simulation) can degrade the quality of the simulation. Thus many MM5 simulations will not use nudging at all on the finest scale nests unless it is determined that suitable observational data is available. The three dimensional meteorological fields from the fine-scale nested grids are the objective and these fields are used as the input to air quality models or a diagnostic meteorological model.

4. Use of MM5 Meteorological Fields in Diagnostic Meteorological Models.

In most air quality modeling studies air quality impacts must be assessed in environments that have very significant and small scale terrain features as well as sharp gradients in land surface characteristics that are less than the typical resolutions used in MM5 simulations. The result is that the effects of the terrain and land surface characteristics, on the meteorological fields is not always resolved in the MM5 simulations alone.

Thus MM5 generated meteorological fields are often used to drive a diagnostic meteorological model that can be run at finer resolutions than is operationally practical with MM5. Such diagnostic models have the potential to use the important information contained in the MM5 data to resolve the effects of the finer scale terrain on the meteorological fields and thus resolve meteorological structures forced by the terrain, such as terrain channeling and gravity driven slope flows. Experiments with MM5 and the CALMET diagnostic model (Robe and Scire, 1998) have demonstrated that improvements in meteorological fields are evident by blending MM5 simulations with a suitable diagnostic meteorological model.

Figures 2 shows a schematic of a modeling grid configuration for MM5 and the CALMET/CALPUFF modeling system that would be typical of an air quality assessment. The CALMET meteorological model uses the MM5 meteorological fields as a first guess. The CALMET model then adjusts the meteorological fields to reflect the higher terrain and land use data. Optionally, the resulting meteorological fields can be enhanced by directly incorporating observations into the CALMET simulations.

4. Applying the WRF Model to Air Quality Assessments

Conceptually the WRF model can easily be used in place of MM5 for air quality modeling applications. Currently the 3DVAR assimilation technique is being developed for implementation into the WRF model and a version of MM5

with 3DVAR capability has recently been released. The implementation of 3DVAR capability will likely lead to the eventual implementation of 4DVAR into the WRF model.

The 3DVAR and 4DVAR techniques have the significant advantage of allowing many different types of data to be assimilated more easily when compared to other schemes. Examples of such data include satellite radiance measurements, reflectivity and radial winds derived from Doppler radars, aircraft observations and data from wind profilers. However, an important issue for air quality applications related to the 3DVAR/4DVAR method is the The 3DVAR technique computational requirements. currently is computationally intensive to run when compared with the current Newtonian nudging scheme used in MM5. Many iterations are required to achieve the desired balanced analysis field. This may not be an issue for initializing the WRF model over relatively short periods for a forecast simulation, but may be a determining factor in whether the WRF model with 3DVAR can be practical for long-term continuous data assimilation as required by air quality Since meteorological fields derived from modelers. dynamical models require continuous assimilation over specified time windows, the 4DVAR approach may be more desirable for developing meteorological data sets for air quality models. However, the 4DVAR method is even more computationally expensive compared to 3DVAR. For a typical sequence of MM5 FDDA simulations with Newtonian nudging for the purpose of developing a full one-year mesoscale data set of three dimensional meteorological fields, using three MM5 domains, about two months of CPU time is typically required on a two processor DEC workstation. This is very manageable for most air quality assessments. However, to this author's knowledge we don't yet know what the CPU requirements would be for continuous data assimilation simulations with 3DVAR or 4DVAR to produce a one-year mesoscale data set.

5. Summary and Recommendations

The MM5 model has proven to be a powerful tool for developing three-dimensional high-resolution meteorological fields for air quality assessments. The key components of MM5 that have allowed this are its grid nesting and FDDA capability with Newtonian nudging. The MM5 model is typically run with FDDA for at least a full year and the resulting meteorological fields are used as direct input to an air quality model or to a diagnostic meteorological model.

Ultimately, over time the WRF model will replace MM5 as the primary community mesoscale model. A key issue with the WRF model as it pertains to its use for air quality modeling studies is how FDDA will be implemented. While 3DVAR and 4DVAR techniques have the advantage of being able to assimilate a wide variety of meteorological data simultaneously, there is concern that these techniques may be computationally too expensive to run for long-period data assimilation simulations typically performed by the air quality modeling community.

It is recommended that more studies be conducted to test the 3DVAR and eventually the 4DVAR schemes both in MM5

and later in the WRF model to assess the benefits and disadvantages of these methods when developing threedimensional meteorological fields for air quality assessments. It is also recommended that a Newtonian nudging scheme be implemented in the WRF model at least until further studies are completed to test the practicality and utility of using 3DVAR and 4DVAR for long period data assimilation simulations. Newtonian nudging schemes although not perfect, are operationally practical and have provided reasonable results for air quality applications. We feel that over time, the 3DVAR/4DVAR approach will prove to be the desired approach for developing mesoscale data sets for air quality modeling applications. However, we feel currently, that the Newtonian nudging approach should only be abandoned when the more advanced 3DVAR/4DVAR methods have been proven as a practical and effective tool for air quality modeling applications.

6. References

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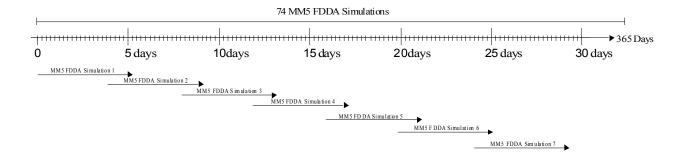


Figure 1. Schematic showing how MM5 simulations are conducted with continuous four dimensional data assimilation to develop a one-year three dimensional mesoscale meteorological data set for air quality modeling. The small tick marks show where 6-hourly analysis nudging takes place throughout the simulations. Each simulation overlaps the previous periods simulation to account for model spin-up time.

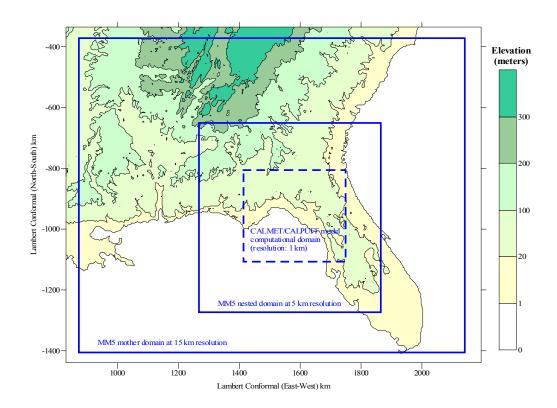


Figure 2. Schematic showing a typical grid configuration for an air quality modeling study. The CALMET meteorological model and the CALPUFF dispersion model both share the same computational domain with a resolution of 1 km. The CALMET model is nested within the MM5 inner 5 km resolution nest and uses the MM5 winds as a first guess.