2.16 Two-Way Coupled Meteorology and Air Quality Modeling

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Abstract A two-way coupled meteorology and air quality modeling system composed of the Weather Research and Forecasting (WRF) model and the Community Multiscale Air Quality (CMAQ) model is being developed to enable simulation of multiple interactions between meteorological and chemical atmospheric processes. The two-way WRF-CMAQ system allows frequent data exchange and chemical feedback to meteorological processes. This coupled system requires "in-line" computation of meteorology-dependent processes that have previously been pre-processed such as dry deposition velocity, biogenic emissions, and point source plume rise. The WRF-CMAQ system enables consistent and easily maintainable "off-line" (sequential WRF and CMAQ simulation) and "on-line" (coupled) capabilities. Initial tests show significant, but sporadic and isolated differences in ground level ozone fields between off-line and on-line runs. However, tests also show very little difference between the tightest coupling (WRF and CMAQ running at the same time-step) and looser coupling where CMAQ is called every four WRF time-steps.

Keywords CMAQ, coupled modelling, on-line, WRF

1. Introduction

The practice of sequential (i.e. off-line) modeling of meteorology-emissions-chemistry has significant limitations because chemical and aerosol processes have no impact on the meteorological simulation. For example, aerosol properties (mass concentration, size distributions, and composition) affect the optical scattering and absorption of short wave radiation. Aerosols also affect the microphysics of clouds through the properties of cloud condensation nuclei (CCN). In addition, as model grid resolution gets finer, the requirements for frequent data exchange between the meteorology and atmospheric chemistry components of the model system increase to impractical levels using disk I/O files. For example, Grell et al. (2004) estimated that for cloud resolving grid resolutions (<10 km) the meteorology input frequency to the air quality model should be at least as frequent as every 10 minutes. Thus, in recent years, coupled meteorology-air quality modeling systems have been developed

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to provide tighter temporal coupling between meteorology and air quality models as well as to provide feedback from the air quality simulation to the physical processes in the meteorology model.

Some combined meteorology and air quality models were developed by essentially adding atmospheric chemistry, along with source and sink processors, to established meteorology models. For example, MM5Chem and WRFChem (Grell et al., 2005) were outgrowths of the MM5 and WRF models. An advantage of such an approach is that transport processes, including advection, diffusion, and convective clouds, for chemical species can be handled identically to the meteorology tracers, i.e., water vapor and cloud microphysical species. A disadvantage of this approach is that air chemistry models often have different requirements for numerical integration such as strict mass conservation, positive definiteness, and greater computational efficiency than is commonly required for meteorology models. Other combined systems, such as the GATOR-GCMM (Jacobson, 2001), were designed and developed from the start with integrated meteorology and chemistry. This approach has been quite successful in research applications because it facilitates inclusion of cutting edge chemical, physical, and dynamical processes in a consistent and integrated system.

A third approach is to combine existing, well established meteorology and air quality models into a single executable program with time-step resolved meteorological and chemical data flow but with minimal modification to either model. An advantage of this approach is that the combined system builds on the many years of development, evaluation, and application that went into each model separately. Similarly, future developments in each model are easily assimilated into the combined system while maintaining equivalent one-way (off-line) capabilities, which is still required for many air quality policy studies. This approach also takes advantage of existing computational and numerical techniques in each model that have been optimized over many years for meteorology and air quality.

2. The WRF-CMAQ Two-Way Coupled System

The development of the two-way coupled WRF-CMAQ system involves three simultaneous efforts:

1. *The addition of capabilities to the WRF model that are particularly important for air quality applications.* These are mostly features that existed in the MM5 system and were used for off-line application with CMAQ. In particular, we have assisted in adding the Newtonian Nudging Four Dimensional Data Assimilation system to WRF (Deng et al., 2007), which is routinely used for retrospective air quality modeling studies. Also, we have added the Pleim-Xiu land surface model (PX LSM) (Xiu and Pleim, 2001), and the Asymmetric Convective Model version 2 (ACM2) (Pleim, 2007) to WRF. Preliminary testing of the WRF model including these new components is described by Gilliam et al. (2007)
2. *The incorporation of meteorology-dependent processes into CMAQ that have been previously computed in pre-processors.* To simplify the coupled system we

are removing the Meteorology-Chemistry Interface Processor (MCIP) so that meteorology data can be transmitted directly from WRF to CMAQ with no intermediate processor. All meteorology dependent processing, including biogenic emissions, point source plume rise, and dry deposition velocity calculations have been incorporated into the CMAQ model. This not only streamlines the system but also enables more sophisticated interactive modeling of biogenic emissions and surface fluxes. For example, the surface fluxes of some chemical species exhibit bi-directional behavior (e.g. mercury and ammonia). Bi-directional surface flux modeling for ammonia has already been developed and implemented in CMAQ.

3. *The coupling of WRF and CMAQ at the model time step level is accomplished by adding CMAQ as a subroutine called from WRF's solver routine.* Meteorology data is transferred from WRF to CMAQ via a virtual data file in CMAQ's IO/API format. Thus, no alteration of CMAQ's I/O system is needed. Chemical data (aerosol concentrations and properties) are transferred back to WRF via another virtual data file. Figure 1 shows a schematic representation of the coupled system.

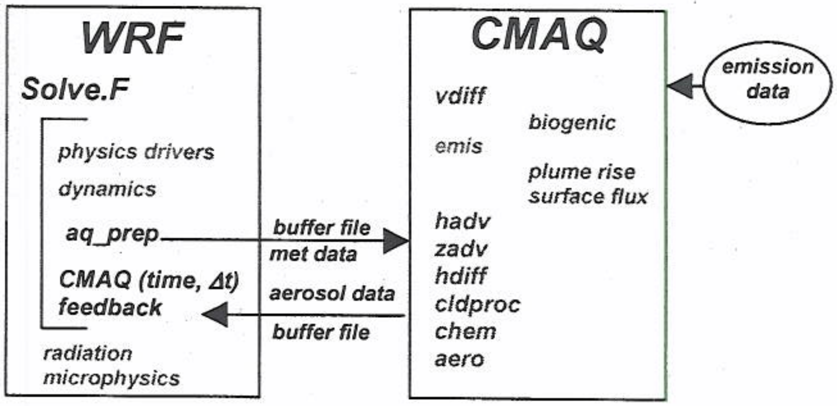

Fig. 1 Schematic of two-way coupled WRF-CMAQ system. The subroutines in black type (aq_prep, CMAQ, and feedback) are added to WRF for two-way capability

3. Testing the Two-Way System

Preliminary tests of the coupled WRF-CMAQ system have been made in one-way mode. One-way means that meteorology data is transferred from WRF to CMAQ every time CMAQ is called but the feedback of chemical data (aerosol information) back to WRF from CMAQ is not yet implemented. We have tested both 1:1 and 1:4 WRF to CMAQ time-step ratios. The tests were one-day, 12 km grid resolution simulations for the eastern US with a 1 minute WRF time-step. Hence, the 1:1 test means that CMAQ is also running at a 1 minute process integration time-step. Note that 1 minute is much shorter than off-line CMAQ simulations would use at 12 km grid resolution. Therefore, we also tested the 1:4 ratio where CMAQ is called every fourth WRF time-step. Both simulations are compared to an off-line simulation, where WRF and CMAQ are run sequentially with meteorology data written to disk files hourly and subsequently read into CMAQ. Note that whatever the frequency of meteorology data for either off-line or coupled configuration, the meteorology data is temporally interpolated to the model time.

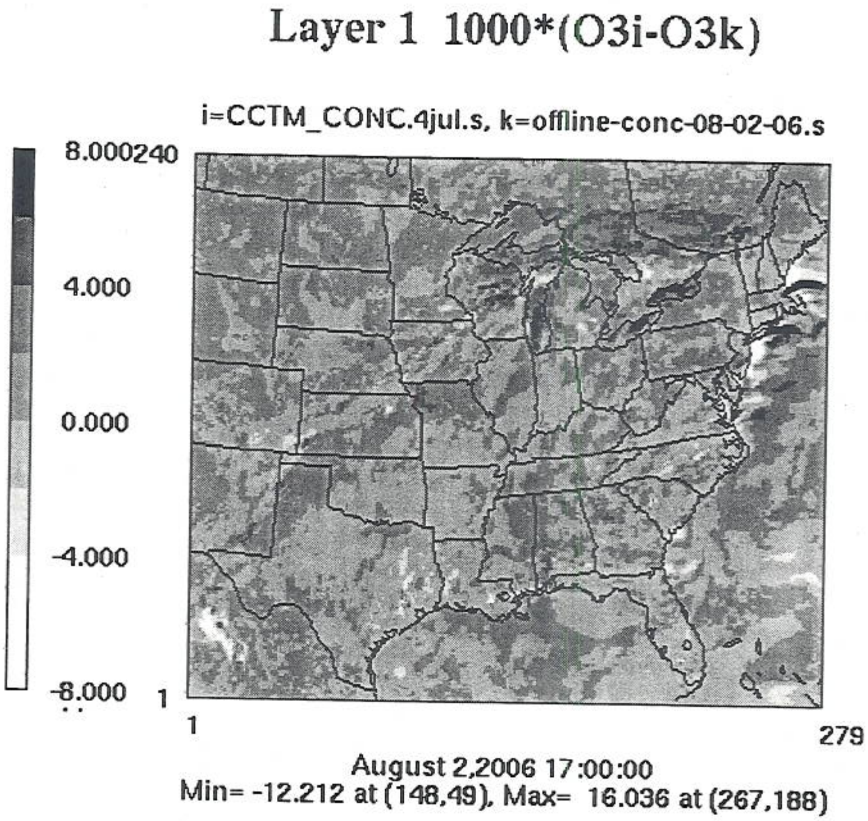

Fig. 2 The difference in ground-level ozone (ppb) between the off-line run and the 1:1 coupled run at 17 UT on August 2, 2006

Figure 2 shows the difference between the off-line run and the 1:1 coupled run for ground level ozone at 17 UT on August 2, 2006. Note that the greatest differences are in the Great Lakes region in an area of extensive cloudiness associated with a storm system. Thus, differences in photolysis rates caused by temporal inter-polation of cloud cover can produce significant differences between off-line and 1:1 coupled simulations. There are also large differences in plumes blowing offshore along the northeast coast that may be caused by slight differences in the interpolation of wind fields.

The flexibility of the frequency with which the CMAQ is called allows for investigation of the trade-offs between run-time and accuracy. Figure 3 shows the difference in ground level ozone between the 1:1 run and the 1:4 run, which means that CMAQ is running at a 1minute synchronization time-step for the former and 4 minutes for the latter. Clearly, the difference between these runs is far less than between the offline and the 1:1 run (Figure 2).

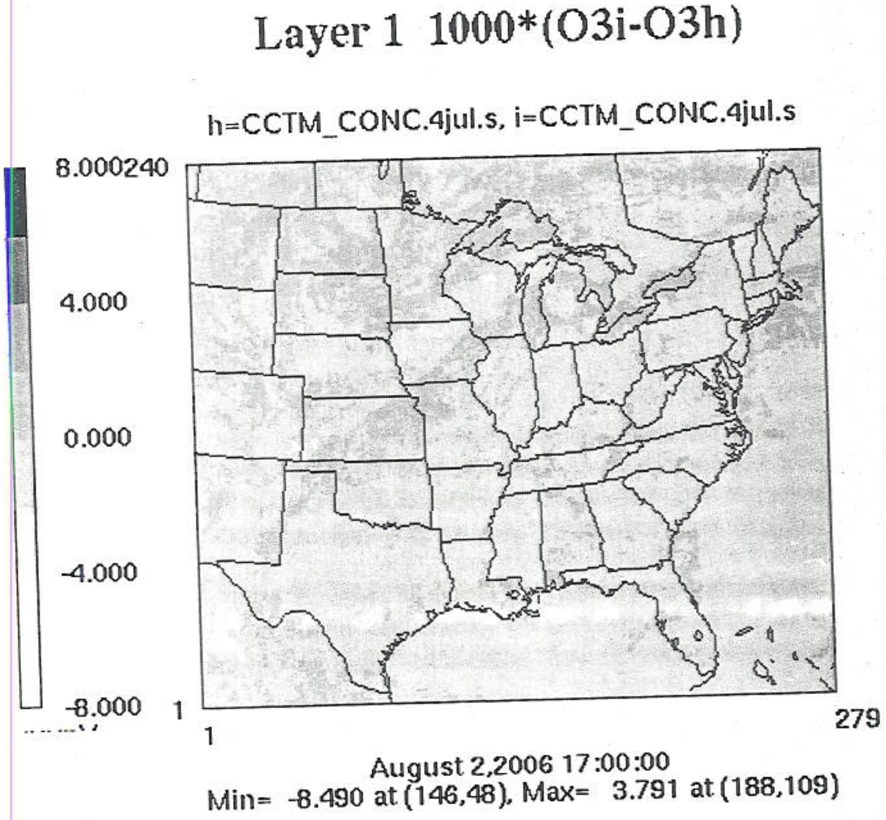

Fig. 3 The difference in ground-level ozone (ppb) between the 1:1 coupled run and the 1:4 coupled run at 17 UT on August 2, 2006

The run time statistics for each of these 24 hour runs on a 16 processor SGI Linux cluster are 2:15:23 for the WRF run alone, 4:52:07 for the 1:4 run and 9:02:52 for the 1:1 run. Thus, for this case, the 1:4 run seems to represent a reasonable compromise that gives almost identical results to the 1:1 run at a little more than half the run time.

4. Next Steps

We are currently working on the feedback of aerosol information from the CMAQ back to WRF. As with the meteorology data transfer from WRF to CMAQ, the aerosol data is transferred from CMAQ to WRF via an in-memory buffer file. The aerosol information, including size distribution, chemical composition, and mass concentration, will be read into WRF and processed to compute single scattering albedo, extinction coefficient, and asymmetry factor for each wavelength band used in the WRF radiation model. Once in place, the WRF-CMAQ system will include the direct effects of aerosols on radiation. We will also implement the indirect effects of aerosols on CCN and cloud microphysics. A beta version of the WRF-CMAQ system that includes the direct aerosol feeback effects is targeted for release in October 2008.

5. Conclusions

The CMAQ modeling system is being further developed in several ways. The WRF-CMAQ coupling will enable integration of aerosol effects into WRF physics processes, such as radiation and cloud microphysics. Furthermore, online WRF-CMAQ coupling will facilitate much more frequent data flow between meteorological and chemical components, which is particularly important at cloud-resolving grid resolutions ($\Delta x < 10$ km). This approach seems to be the best way to achieve the benefits of simultaneously integrated meteorology and chemistry while maintaining consistency with the WRF and CMAQ systems that both have large communities of users and are continually being advanced. The WRF-CMAQ coupled system is currently in development with the first beta release scheduled for October 2008.

As part of the effort to develop the two-way coupled system the dry deposition, biogenic emission, and plume rise models are now contained within the CMAQ model thus enabling more sophisticated treatment of surface exchange processes including bi-directional flux modeling. Initially, bi-directional algorithms are being developed for ammonia and mercury. In both cases the models are being developed as the science is being discovered through field experimental research.

Initial tests of the coupled WRF-CMAQ system have successfully reproduced off-line simulations but with substantial differences in some areas. We attribute these differences primarily from differences in interpolated cloud and wind fields between the off-line system that interpolates between hourly meteorology inputs and the on-line system that gets updated meteorology every minute (for the 1:1 run). The comparison between the 1:1 run and the 1:4 run, however, show very little difference, which suggests that less frequent calls to CMAQ (every 4 minutes in this case) may be a reasonable way to achieve greater computational efficiency without significant loss of accuracy.

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Discussion

J. Kushta:

After including the aerosols feedback into radiation and microphysics of cloud, could a secondary correction in photolysis rates (j-values) be necessary (in the same time step)? (Especially when the timestep of CMAQ routine is multiple to the meteo time step).

J. Pleim:

The next release of CMAQ (version 4.7 in October 2007) will include the effects of aerosols on photolysis rates.

A. Baklanov:

First of all I like that CMAQ is also moving now from offline to the online coupling approach. However, two questions: Are the comparisons online vs offline simulations based only on the different meteorology reading, not considering any feedback mechanism? In you two-way coupling the "online access" approach is using, when models are running separately and exchanging data on each time step. Why you do not try to realise other way of "full online integration", when CMAQ will be implemented inside WRF (e.g. like in WRF-Chem)? In this case you'll save computation time for the buffer files treatment and can avoid other important problem in offline integration when cloud water and chemical species and treated by different advection schemes.

J. Pleim:

The results shown here do not include feedback effects of aerosols on the radiation or microphysics in WRF. We are currently working on these feedbacks which will be included in the Beta system to be released in October 2008. I think there are plusses and minuses to the two-way coupled approach versus the "full online integration". An advantage of the coupled method that we use is that almost the same CMAQ code can be run "online" or "offline". Considering our large user community, much of which uses the system for air quality control policy development, consistency between online and offline configurations is very important. Another advantage of this approach is the flexibility to run CMAQ at a longer integration time step than for WRF. This saves a lot of CPU time with very little effect on results. On the other hand, as the questioner points out, there can be important inconsistencies such as between WRF's advection of microphysical species and CMAQ's advection of chemical species. However, these inconsistencies can be minimized by using the same advection scheme in both models. For example, the PPM advection scheme is now available in both WRF and CMAQ. Note that our method of data exchange between WRF and CMAQ, via in-memory buffer files, does not add any significant run time to the system.