

MASS CONSISTENT ON-LINE AND OFF-LINE AIR QUALITY MODELING PARADIGMS: WRF LINKED WITH CMAQ

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1. INTRODUCTION

The Weather Research and Forecasting (WRF) modeling system represents culmination of various atmospheric modeling efforts and has potential not only to replace many of current operational and research weather forecasting models, but also to provide meteorological inputs that allow simultaneous on-line/off-line air quality modeling paradigms. Byun (1999a; 1999b) presented the need to have dynamically consistent formulations in meteorological and air quality models for multi-scale air quality studies and addressed the mass conservation issues while linking the meteorological and air quality models. WRF, which utilizes the set of fully compressible governing equations and the mass-flux based coordinate and grid systems as well as the highly accurate numerical algorithms, realizes a modeling framework with which establishment of both the on-line and off-line air quality modeling system is possible.

In this study, we demonstrate a mass-consistent off-line modeling paradigm by linking WRF with the EPA's Community Multiscale Air Quality (CMAQ) modeling system. Through the collaboration with the NCAR WRF development team, we have generated a set of the mass consistent meteorological flux fields from WRF for the CMAQ simulations. The WRF-CMAQ Interface Processor (WCIP) is constructed in such a way to have maximum compatibility between the two systems by passing through the mass consistent and physically compatible meteorological inputs for CMAQ (Kim and Byun, 2002). On-line modeling using the WRF and CMAQ systems will be possible by introducing coupled input/output application interface for the cooperating processors.

2. MASS FLUX VARIABLES FOR MASS CONSERVATION

Lee *et al.* (2004) compared effects of mass consistency errors in meteorological data for air quality modeling using the hydrostatic and nonhydrostatic versions of MM5. They showed that the hydrostatic MM5 introduce much less errors in the trace species transport in air quality simulations than the nonhydrostatic MM5 because of the better mass conservative characteristics of the hydrostatic formulations.

WRF, in the recent releases, utilizes mass coordinate dynamics, which will inherit the benefit of the hydrostatic MM5 formulations. Byun and Kim (2003) showed that WRF linked to CMAQ produced much better mass conservative characteristics than MM5 due to the use of complete governing set of fully compressible atmosphere as well as the better numerical algorithms implemented in WRF. The result clearly demonstrated benefits of using the dynamically consistent formulations between the meteorology and air quality models. However, the study also showed that mass correction was still needed for the off-line coupling between WRF and CMAQ.

Although use of different numerical advection algorithm in CMAQ from the one used in WRF was one of the reasons of the discrepancy, we suspected that there were more fundamental problems in linking WRF and CMAQ. In the present study, we hypothesize that the major mass consistency error originates from the use of instantaneous output of meteorological parameters from WRF. Skaramock, through personal communication in 2003, suggested that use of time-averaged mass flux variables would minimize the linkage problem in CMAQ. The idea was coherent with the temporal interpolation scheme for winds proposed by Byun (1999b). In the scheme, the contravariant components of a wind in the generalized vertical coordinate system at a time $t = (1-\alpha)t_n + \alpha t_{n+1}$ between the two consecutive meteorological output time steps t_n and t_{n+1} are determined by:

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$$(\hat{\mathbf{V}}_s)_\alpha = \frac{(\rho J_s \hat{\mathbf{V}}_s)_\alpha}{(\rho J_s)_\alpha}; (\hat{v}_s)_\alpha = \frac{(\rho J_s \hat{v}_s)_\alpha}{(\rho J_s)_\alpha} \quad (1)$$

where $\hat{\mathbf{V}}_s$ and \hat{v}_s are horizontal and vertical contravariant wind components, respectively, and ρ the density and J_s the vertical Jacobian in the generalized coordinate system. The Jacobian weighted density and wind components multiplied in the right hand side of Eq. (1) are interpolated linearly with the values at t_n and t_{n+1} . These are the mass flux variables responsible for maintaining the mass conservation characteristics of the off-line trace species transport.

One of the possibilities to suppress the mass inconsistency problems in the off-line modeling paradigm is to write out the averaged mass flux variables at each output time step. There are two possible ways to consider the averaged variables in Eq. (1): One is to separate the Jacobian weighted density from the contravariant wind components. In this case, the averaged contravariant wind provided by the meteorological model can be directly used for the Eq. (1). The other way is to calculate both the contravariant wind multiplied with the Jacobian weighted density and the Jacobian weighted density separately in WRF and then divide the wind with the density in CMAQ as shown in Eq. (1). In addition, with the mass-coordinate dynamics core supported by WRF, the vertical coordinates are time-dependent following the change in the hydrostatic pressure field. In such a system, similar temporal averaging must be applied for the hydrostatic pressure variables for defining the coordinate system in air quality modeling. In this study, we tested these two methods of handling the averaged mass flux variables used in the temporal integration of the continuity equation.

3. EXPERIMENTAL DESIGN

WRF Version 1.3 mass model and CMAQ Version 4.3 are used for the meteorological and air quality simulations, respectively, of an air quality episode over the Houston-Galveston area for the time period of 00 UTC 27-00 UTC 28 August 2000. WRF was run with a time step of 10sec. The horizontal domain of WRF consisted of 161×146 at 4 km resolution and the horizontal domain of CMAQ consisted of 90×90 grids inside the WRF domain. A stretching grid system was used for the vertical direction with 43 layers. The thickness of

the first layer was about 34 m and the model top was 50 hPa.

WRF physics options used include: 1) MRF PBL scheme, 2) OSU land-surface, 3) NCEP 3 class simple ice scheme and 4) Dudhia shortwave and RRTM long wave radiation scheme. The first guess and boundary conditions are from the NCEP Eta model on the Eta212 (AWIP 40 km domain).

The WRF registry was modified to add a few more time-averaged mass flux variables and a few lines of codes were added to compute the necessary time averaged, coupled variables as needed for the advection test in CMAQ.

4. MASS CONSISTENCY OF WIND IN ON-LINE/OFF-LINE COUPLING

Figure 1 shows the tracer advection results of uniform mixing ration field (IC=1.0 and BC=1.0) using the hourly MM5, WRF EM, and WRF EM with averaged mass flux variables. In this case, WRF EM is still better than MM5 in terms of mass consistency of wind field, but the difference is not large.

The result from the approach that uses time-averaged flux variables tested in this study is much better than the other method until the first 12-hour of simulations. An interesting feature that warrants a further study is the decrease in the deviation from 1.0 for the MM5 and WRF EM with the interpolated cases. There are no physical reasons that the discrepancy to decrease because the system resembles to a first order decay system. It is suspected that the apparent improvement of the results may be due to the compensating changes in the air density corresponding to the diurnal heating and cooling events of the system. This artifact in fact obscures the purpose of the present analysis.

Figure 2 shows that the vertically averaged IC1_BC1 tracer concentration fields at 2100 UTC August 27, 2000, for the three different cases. The spatial variation is much broader and the range of concentration is much more spread than the results of other cases. It must be noted that the results not necessarily indicate that the time-averaged mass flux approach is inappropriate when the data transfer of meteorological information to the air quality model is infrequent, i.e., 1 hour in this case. Further detailed study must be performed to resolve this somewhat incongruent result.

Another experiment is being prepared to verify the validity of this approach according to

the frequency of meteorological data transfer with the high frequency WRF output. For this, we have generated a pseudo on-line WRF-CMAQ modeling results by writing the WRF modeling output at the WRF numerical integration time steps and simulating CMAQ with the high frequency data. The results will be discussed at the conference.

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5. SUMMARY

In this study, we tested alternative approaches to maintain the mass consistency of wind field in off-line coupling between the WRF and CMAQ. For this, we introduced time-averaged mass flux variables in WRF and provide them as meteorological input for CMAQ. Preliminary results showed that the new method definitely slows down the degradation of tracer transport results, in particular during the first 12-hours of simulation. The apparent worse performance at a later times than others may be due to the inadequate implementation of the other testing cases, which unduly influenced the results by the changes in the air density corresponding to the diurnal warming and cooling events. Further study is needed to verify the validity of this approach with respect to the frequency of meteorological data transfer between the WRF and CMAQ systems.

6. REFERENCES

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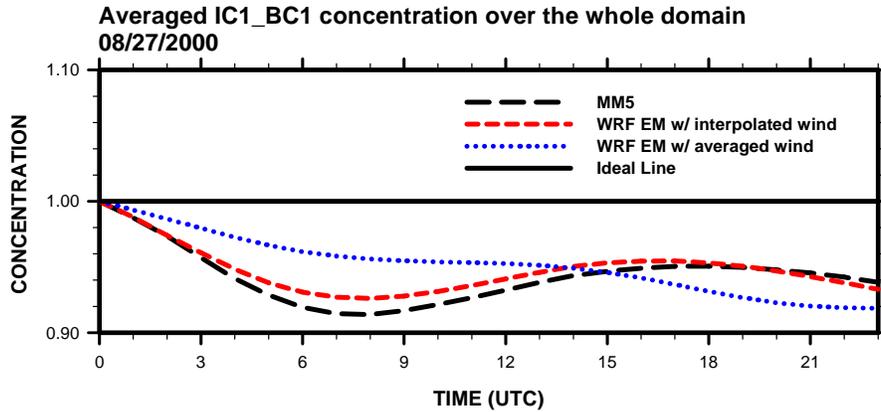


Figure 1. 24 hour time series of averaged tracer concentration with IC (initial condition)=1.0 and BC (boundary condition)=1.0 for MM5 (long-dashed), WRF EM with interpolated wind (short-dashed), and WRF EM with averaged wind (dotted).

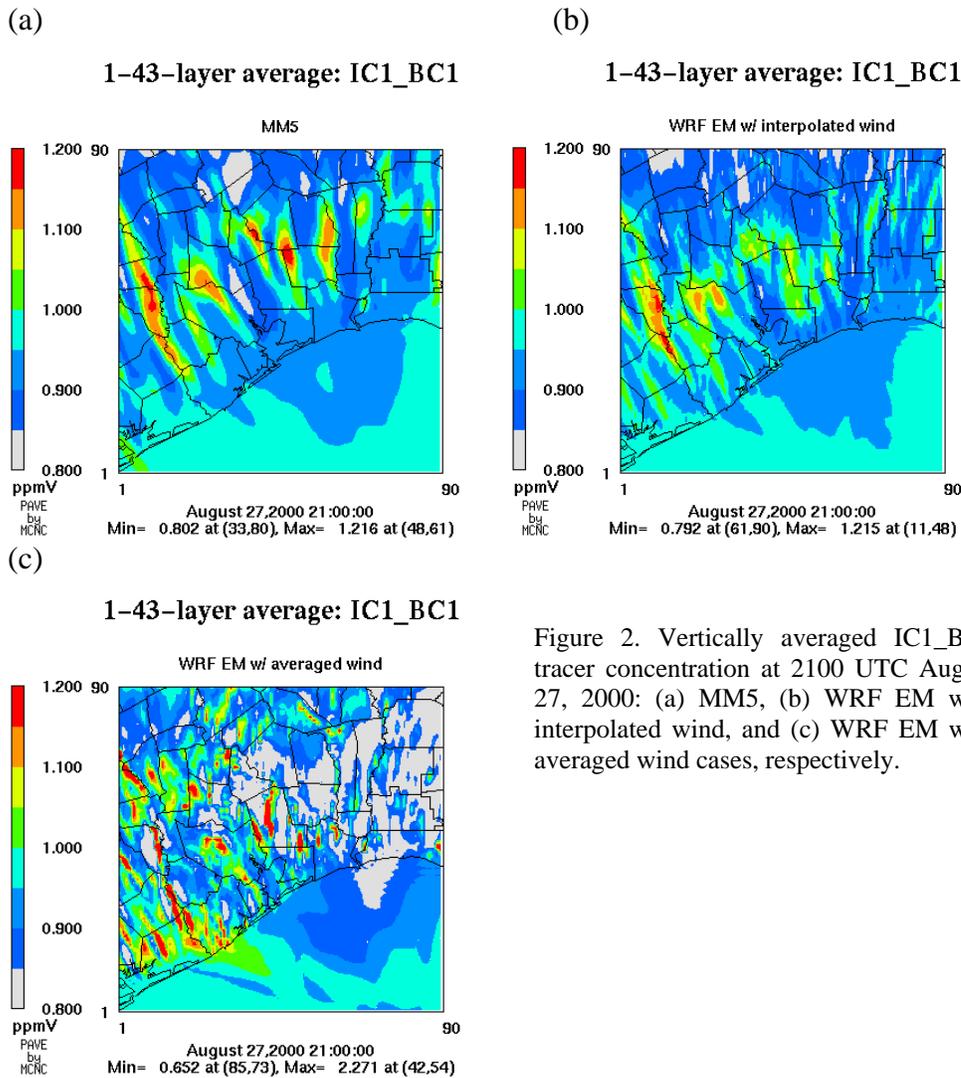


Figure 2. Vertically averaged IC1_BC1 tracer concentration at 2100 UTC August 27, 2000: (a) MM5, (b) WRF EM with interpolated wind, and (c) WRF EM with averaged wind cases, respectively.