Mass Conservative Coupling of MM5 with CMAQ

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The inconsistency of meteorological data from MM5 may lead to mass conservation errors in CMAQ. We have applied the method of adjusting the vertical wind component to make CMAQ strictly mass conservative. Simulation results prove that this method is an effective technique. Recently a coding error was discovered in the vertical advection module of CMAQ. Results also show that any CMAQ run prior to fixing this error may be subject to severe mass conservation errors especially over complex terrain. The fix reduces the error but does not completely eliminate it therefore vertical wind adjustment is still recommended.

1. INTRODUCTION

Air quality models (AQMs) such as CMAQ are expected to maintain a uniform mass mixing ratio field for an inert tracer after transport with the winds produced by the meteorological models (MMs) such as MM5. This expectation could only realize if the two models used the same discretization, i.e., grid, time step, and finite difference forms. In many present day applications CMAQ and MM5 share the same grid structure however finite difference forms used for advection in AQMs are usually different from those in MMs. Also, since the outputs of the MMs are stored less frequently than the AQM time step, the input variables cannot be reconstructed exactly at the desired instants. Therefore, the wind components and the air density do not satisfy the discrete continuity equation in AQMs even though they may have done so in MMs. This is referred to as the inconsistency of the meteorological fields (Byun, 1999; Odman and Russell, 2000; Lee et al., 2004). As a result of this inconsistency, uniform mass mixing fields are perturbed. The perturbation is usually more pronounced with data from non-hydrostatic MMs than with data from hydrostatic MMs for the same domains. If left untreated, the perturbation may grow in time and generate instabilities in AQM solutions.

Odman and Russell (2000) showed that some attempts to establish consistency and produce stable results in AQMs sacrifice mass conservation of pollutant species. Ideally, there should be no mass conservation error in AQMs that establish source receptor relationships for the design of emission control strategies.

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2. ADJUSTING VERTICAL WINDS

Some widely used AQMs including CMAQ adopted an approach where a uniform tracer is transported along with other species and the concentrations are renormalized using the deviation of the tracer from uniformity as the norm. As a result the uniform mixing ratio field is maintained. However, the approach overlooks that non-linear advection schemes are used in AQMs for high accuracy. These schemes would affect pollutant fields of different distribution differently. Most species of interest, especially the emitted ones, have spatial distribution far from being uniform. Therefore, renormalizing the concentration of a species based on the perturbation of a uniform field can increase or decrease its mass artificially. We found that the mass conservation errors introduced by this approach can be very large.

Species mass conservation is not sacrificed if the consistency of meteorological fields is established through the continuity equation. To satisfy the discrete continuity equation in the AQMs, wind or density fields (or both) from MMs must be adjusted. Lu et al. (1997) prefer adjusting the density field, while Odman and Russell (2000) adjust either the vertical wind component or the vertical flux.

The inverse donor cell method described in Odman and Russell (2000) was applied in CMAQ to satisfy the discrete continuity equation by adjusting the vertical winds. This method requires advection of air in addition to all the species and the use of the donor cell scheme for vertical advection.

$$c_k^{n+1} = c_k^* - \frac{\Delta t}{\Delta z_k}\left(w_{k+1/2}c_k^* - w_{k-1/2}c_{k-1}^*\right) \quad (1)$$

First, we apply horizontal wind components to the air density field, r^n, to obtain an intermediate field r^*. Piecewise parabolic method (Collela and Woodward, 1984) is used for horizontal advection. Then, we require that the density after the vertical advection operator is applied to r^* be equal to r^{n+1}. The latter is calculated from the MM data by using linear interpolation in time. Thus, we need to calculate a new value for vertical velocity that would yield the desired value of density. Substituting concentrations with air densities, Equation (1) is solved for $w_{k+1/2}$ as

$$w_{k+1/2} = \frac{1}{r_k^*}\left(\frac{\Delta z_k}{\Delta t}\left(r_k^* - r_k^{n+1}\right) + w_{k-1/2}r_{k-1}^*\right) \quad (2)$$

Since $w_{1/2} = 0$, Equation (2) can be used starting from the surface layer ($k = 1$) and moving to the top, each time using the vertical velocity computed for the previous layer. The winds at the top of the model will usually have a vertical component. The vertical velocities computed from Equation (2) must be used in Equation (1) to advect all other pollutant species. Note that the horizontal advection operator must always be applied before the vertical. Also, since the donor cell scheme is subject to the Courant stability condition, the case when the Courant number exceeds unity requires special treatment.

3. TESTING CMAQ: RESULTS AND DISCUSSION

Applying the method described above to CMAQ, we simulated an imaginary tracer experiment using meteorological data generated for the Fall-line Air Quality Study (FAQS). In this experiment inert tracers were released from different locations in the Tennessee Valley. These locations were chosen specifically to increase the potential of transport over complex terrain. All releases started at 8:00 UTC and ended at 14:00 UTC. The total amount of inert tracers released at each location is 24 kg. Starting two hours before the release of inert tracers and using the meteorological fields generated by MM5, we ran the model for 42 hours. The CMAQ grid covered the FAQS domain with 75x66 cells of 12-km size. It had 13 layers vertically, with 7 layers in the lowest kilometer and the surface layer having a thickness of 18m. During the simulation we followed the tracer concentrations and calculated the total mass of the tracers within the entire domain.

The same simulation was conducted with two more versions of CMAQ. First we used the original CMAQ version 4.3 (released September 12, 2003). Recently, Dr. Daewon Byun's group at the University of Houston discovered a coding error in the vertical advection routine of this version of CMAQ. The problem was that the original CMAQ code inadvertently assumed uniform grid but the vertical layer spacing is non-uniform. This error was corrected in the second version.

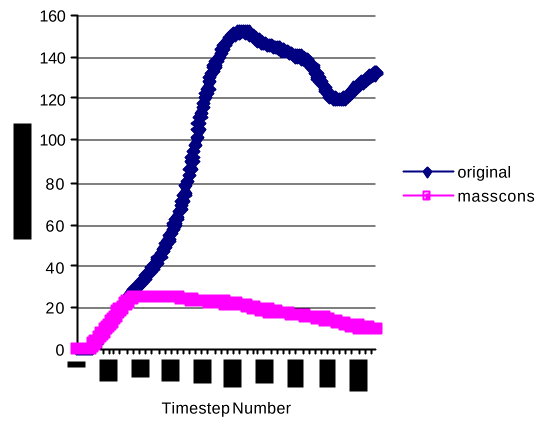

Fig.1 Evolution of total mass of Tracer-1 as predicted by the original and mass conservative versions of CMAQ. Tracer-1 was released from the location of the Eastman Chemical Co., TN.

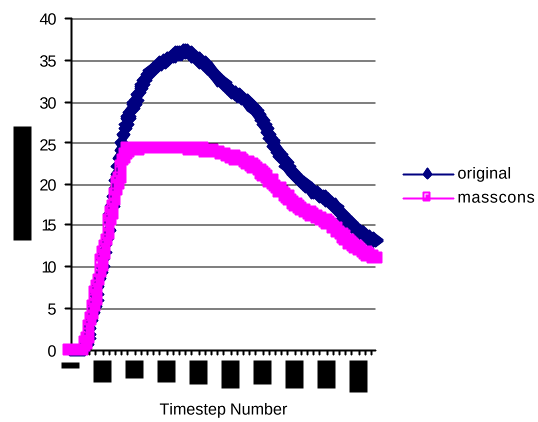

Fig.2 Evolution of total mass of Tracer-2 as predicted by the original and mass conservative versions of CMAQ. Tracer2 was released from the location of TVA's John Sevier Plant, TN.

Figure 1 and Figure 2 show time series of the domain-wide total mass of Tracer-1 and Tracer-2, respectively, as predicted by original CMAQ and the version of CMAQ that uses vertical wind adjustments. If the model is mass conservative, the simulated total mass of Tracer-1 and Tracer-2 should be kept at 24 kg until it starts to decrease when the tracers are transported out of the domain. CMAQ is mass conservative when it uses the adjustment of vertical wind method but the original CMAQ Version 4.3 is creating mass. The amount of erroneous increase in tracer mass is large especially for Tracer-1: the total mass was artificially increased by about 5 folds.

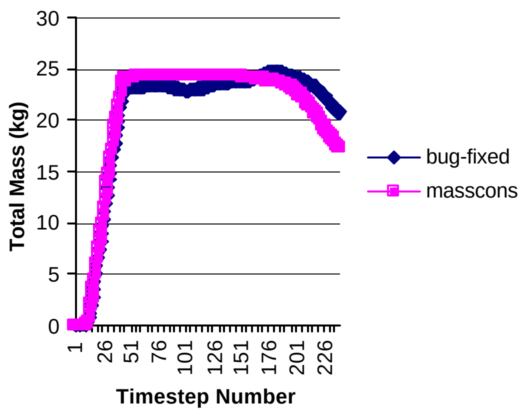

Fig.3 Evolution of total mass of Tacer-2 as predicted by the corrected CMAQ and mass conservative version of CMAQ. Tracer-2 was released from the location of TVA's John Sevier Plant, TN.

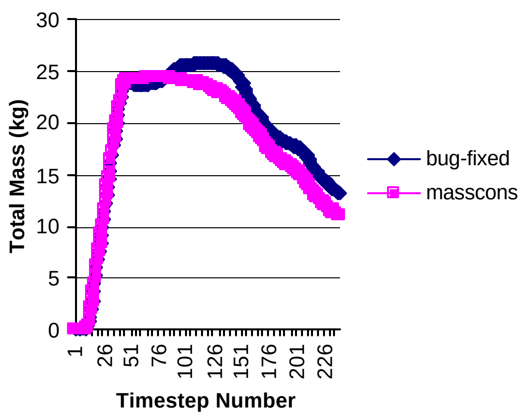

Fig.4 Evolution of total mass of Tracer-3 as predicted by the corrected CMAQ and mass conservative version of CMAQ. Tracer-3 was released from the location of TVA's Bull Run Plant, TN.

Figure 3 and Figure 4 show time series of the total mass of Tracer-2 and Tracer-3, respectively, as predicted by CMAQ with corrected vertical advection and CMAQ with vertical wind adjustments. After correcting vertical advection the mass conservation errors are reduced significantly. However, mass is still artificially increased, after an initial decrease, both for Tracer-2 and Tracer-3. In contrast to the fluctuations in the mass predicted by the corrected CMAQ, mass conservative CMAQ with vertical wind adjustment kept total mass constant before the tracers were transported out of the domain.

4. CONCLUSIONS

Any CMAQ run prior to correcting the coding error in vertical advection may be subject to severe mass conservation errors over complex terrain. The correction reduces the mass conservation errors but it does not completely eliminate them.

Adjusting vertical winds proved to be an effective method to conserve mass in CMAQ. We recommend the use of vertical wind adjustment in future versions of CMAQ.

5. REFERENCES

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