REDUCING VERTICAL TRANSPORT OVER COMPLEX TERRAIN IN PHOTOCHEMICAL GRID MODELS

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1. INTRODUCTION

Annual photochemical grid modeling using the Comprehensive Air quality Model with extensions (CAMx; ENVIRON, 2009) for the Four Corners Air Quality Task Force (FCAQTF; Stoeckenius et al., 2009) and the Community Multiscale Air Quality (CMAQ; Byun and Ching, 1999) model for the Western Regional Air Partnership (WRAP; Mansell 2008) have resulted in large springtime ozone over predictions in the complex terrain of the Rocky Mountains. Figure 1 shows the 2002 WRAP CMAQ annual highest daily peak 8-hour ozone concentrations with corresponding observations. The highest predicted ozone values occur over the Rocky Mountains in the spring, most notably April and May. Comparison with 2002 observations shows that the WRAP modeling over predicted ozone levels in southwest Colorado by 20 ppb or more in these months.

The 2005 FCAQTF CAMx simulation also estimated the highest ozone concentrations in the spring (April) over the Rocky Mountains. The 2005 CAMx application used the same 19 layer vertical grid structure and 2002-based boundary conditions (BCs) as the 2002 CMAQ simulation. The FCAQTF performed numerous sensitivity tests that led to the realization that high ozone lateral BCs in the top-most CAMx layer (i.e., layer 19 spans approximately 8-15 km above sea level [MSL]), coupled with overly energetic vertical circulations above complex terrain, transport stratospheric ozone down to the ground resulting in springtime ozone overestimations. The lateral BCs for both CMAQ and CAMx were derived from a 2002 annual run of the Harvard GEOS-CHEM global chemistry model (Jacob et al., 2005). The maximum ozone BC from GEOS-CHEM occurs in the spring and exceeds 200 ppb in the topmost layer 19.

The CMAQ and CAMx models both diagnose vertical velocity internally from divergence in horizontal momentum in order to maintain mass conservation. Vertical velocity in each column is calculated by integrating the horizontal momentum divergence equation from the ground to the top of the model. When there is horizontal convergence, a positive (upward) vertical velocity increment is applied in order to conserve mass; the opposite occurs with horizontal divergence. Deviations from the meteorological model's (MM5 is this case) physics, coordinate system, and numerical methods lead to differences in vertical velocities in the air quality models from what is reported by the meteorological model. Furthermore, any numerical artifacts from the meteorological model will be transferred to the air quality models and possibly magnified.

Analyses of the most egregious vertical velocity profiles in CAMx FCAQTF modeling suggest that the low- to mid-tropospheric vertical velocities are actually well-behaved, and that the biggest problems are associated with "noisy" conditions in the uppermost layers. These problems do not appear to be related solely to the aggregation of multiple MM5 layers to bulky CAMx/CMAQ layers (e.g., CAMx/CMAQ layer 19 is a combination of 5 MM5 layers that span roughly the uppermost 8 km). Over the highest terrain, significant vertical transport is needed in only a shallow portion of the profile for the following reasons:

- The bottom of layer 19 is ~8 km MSL, approximately the minimum altitude of the wintertime tropopause (the top of the model is ~16 km);
- The top of the highest terrain is ~ 3 km MSL, requiring only 5 km of vertical transport from the bottom of layer 19 to reach the ground;

With deep afternoon mixing of 2-3 km above the highest terrain, vertical transport from the bottom of layer 19 would only need to extend downward 2-3 km before mixing would efficiently transport the ozone the rest of the distance to the surface.

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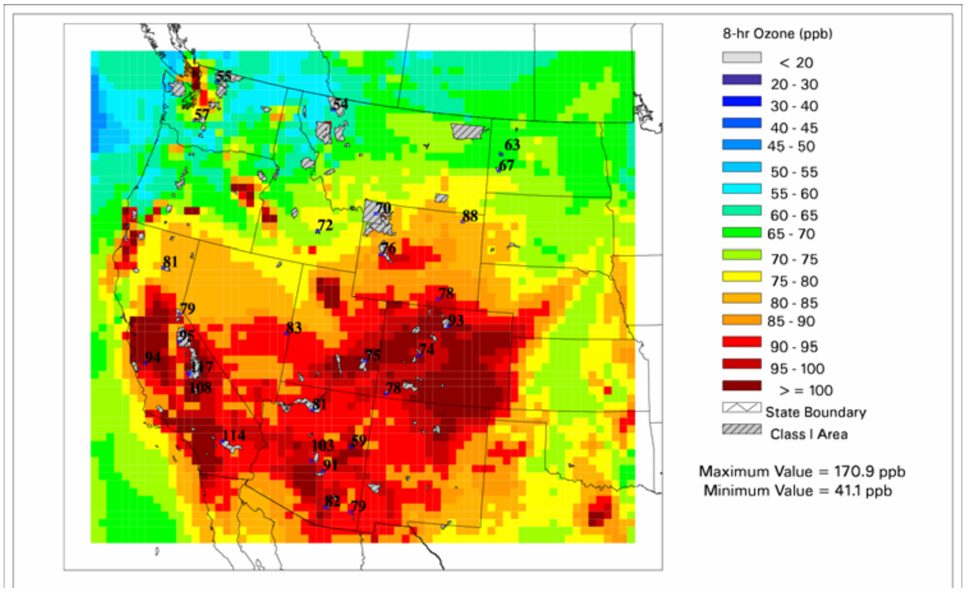

Fig. 1. Annual maximum daily peak 8-hr ozone concentrations (ppb) for the 2002 WRAP CMAQ 36-km regional grid with observations superimposed as numbers.

2. METHODOLOGY

Several strategies were investigated to determine a methodology that best reduces the deep vertical transport of high ozone from the CMAQ/CAMx top layer over elevated complex terrain. A CAMx test database was configured from the FCAQTF modeling application, which consisted of a single western U.S. 12-km regional grid with April-averaged BCs similarly generated from 2002 GEOS-CHEM global model output. The model was run for just the single month of April 2005 in inert mode to track ozone initial/ boundary conditions throughout the western U.S. We first investigated techniques for reducing the vertical velocities in the top most layers of CAMx through modification of the input horizontal winds:

- Use of a smoother-desmoother;
- Application of divergence minimization; and
- Use of a "mass filter".

These tests were also conducted with improved vertical resolution, which by itself was shown to be quite effective in reducing transport of stratospheric ozone to the surface. During the course of these investigations, we identified several other issues. First, the program used to process GEOS-CHEM model output to generate CMAQ/CAMx boundary conditions was improved to eliminate a high ozone bias in the top layers of CMAQ/CAMx. Second, an improved top boundary condition technique and an alternative vertical advection algorithm were implemented in CAMx. Results of these strategies are discussed sequentially below.

3. RESULTS

3.1 Smoother-Desmoother

The smoother-desmoother filter is described by Yang et al. (2008). CAMx sensitivity tests were performed using different smoothing factors and different numbers of layers and sweeps. Tests included smoothing just input horizontal wind fields, and smoothing input wind plus density fields (pressure and temperature). The smoother-desmoother filter helped reduce the magnitude of vertical velocity in upper layers with relatively little impact on horizontal wind fields. However, even with the most aggressive application of the smoother-desmoother technique, it could not adequately reduce the vertical transport of stratospheric ozone to the surface in CAMx. The largest reduction to the April-maximum ozone was much less than 10 ppb.

3.2 Divergence Minimization

A divergence minimization scheme was obtained from CALMET version 5.87 (Scire et al., 2000) and adapted to the CAMx grid structure. The algorithm first computes three-dimensional wind divergence in each grid cell. If the absolute value of the wind divergence within any grid cell exceeds a specified threshold, divergence minimization is applied in a series of passes. This process is repeated until the absolute value of wind divergence falls below a specified threshold in all grid cells in a particular layer, or until the process is repeated a set number of iterations, whichever comes first.

Initially the divergence minimization procedure showed promise in reducing estimated ground-level ozone concentrations. Peak April ozone concentrations were reduced by 10-15 ppb. However, further investigation revealed that divergence minimization generated spurious and troublesome numerical artifacts at the top of the model, such as directional reversals and strong accelerations in the vertical velocity fields. These numerical artifacts, in combination with the CAMx time-and space-invariant ozone top boundary conditions (set to 70 ppb in this case to represent time- and space-averaged conditions over the domain and year) resulted in a strong dilution of ozone in the top layer. Obviously, the constant 70 ppb top ozone BC is inconsistent with the GEOS-CHEM ozone estimates for that season and height (~15 km MSL).

To address this inconsistency, a “zero-gradient” top BC concentration approach was implemented in CAMx, whereby the top BC is internally derived instead of directly input to the model: concentrations above the top layer are assumed to be the same as in the concentrations in the top layer each time step. This change actually resulted in a strong increase in the simulated ground-level ozone concentrations (~10 ppb) due to the lack of artificial dilution at the top, but the zero-gradient approach is more scientifically defensible.

3.3 Improved Vertical Resolution

Other tests with CAMx demonstrated that using all available (34) vertical layers from the meteorological model output (i.e., no layer aggregation/collapsing) significantly reduced surface ozone concentrations compared to using 19 layers, at the cost of doubling the computational requirements. An alternative 22 layer model configuration, which added more vertical resolution in the upper portion of the domain, produced comparable results to the full 34 layer model with only a modest (~10%) increase in computer time over the 19 layer model configuration (Figure 2).

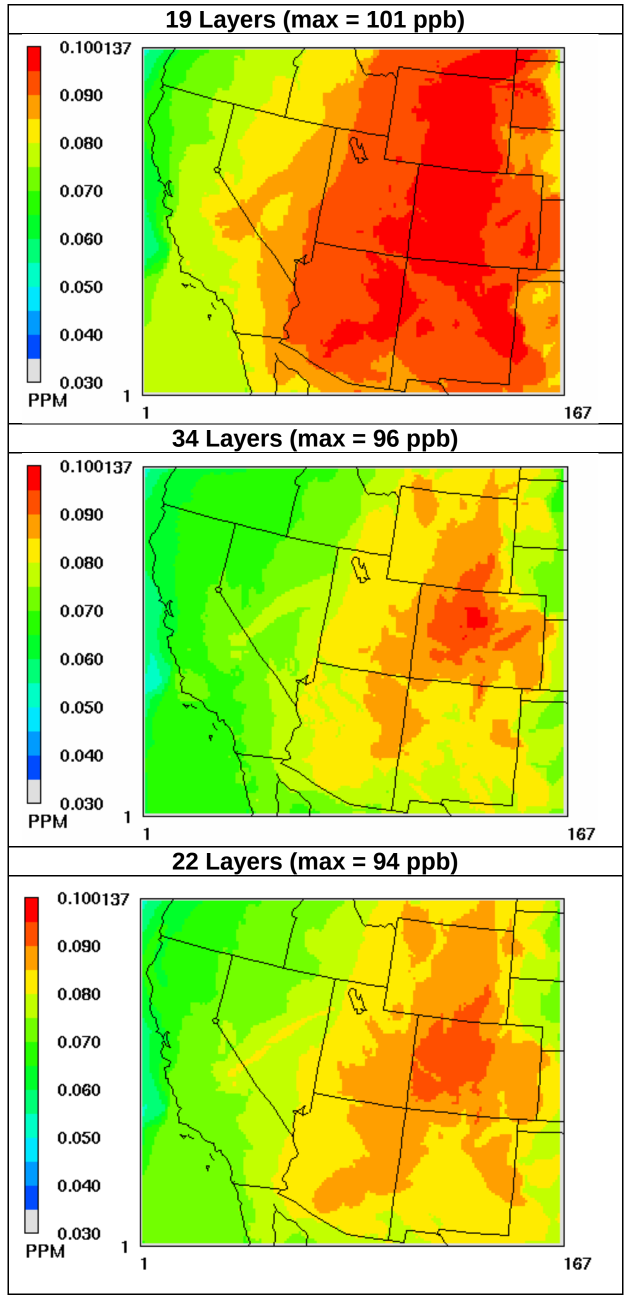

Figure 2. April 2005 CAMx inert maximum ozone concentrations (ppm) using “zero-gradient” top boundary conditions and the original 19 layer vertical structure (top), the full 34 layer vertical structure (middle) and the intermediate 22 layer vertical structure (bottom).

3.4 Improved Boundary Conditions

New 2005 GEOS-CHEM outputs were obtained and used to generate day-specific diurnally varying BCs for the FCAQTF April 2005 test database. The resulting BCs were significantly higher than the April-averaged 2002 BCs and generated enormous surface ozone concentrations (reaching nearly 300 ppb). We reviewed the interface program used to process the GEOS-CHEM output to CMAQ/CAMx BC inputs and identified a bias in the layer interpolation scheme that over stated ozone at the top of the model when low-resolution layer structures were employed. The GEOS-CHEM BC interface program was revised and used with new 2005 GOES-CHEM dataset. CAMx simulations using the improved day-specific April 2005 BCs resulted in up to half the surface ozone of the unfixed 2005 BCs, but remained much higher than the results using the original 2002 April-averaged BCs (Figure 3).

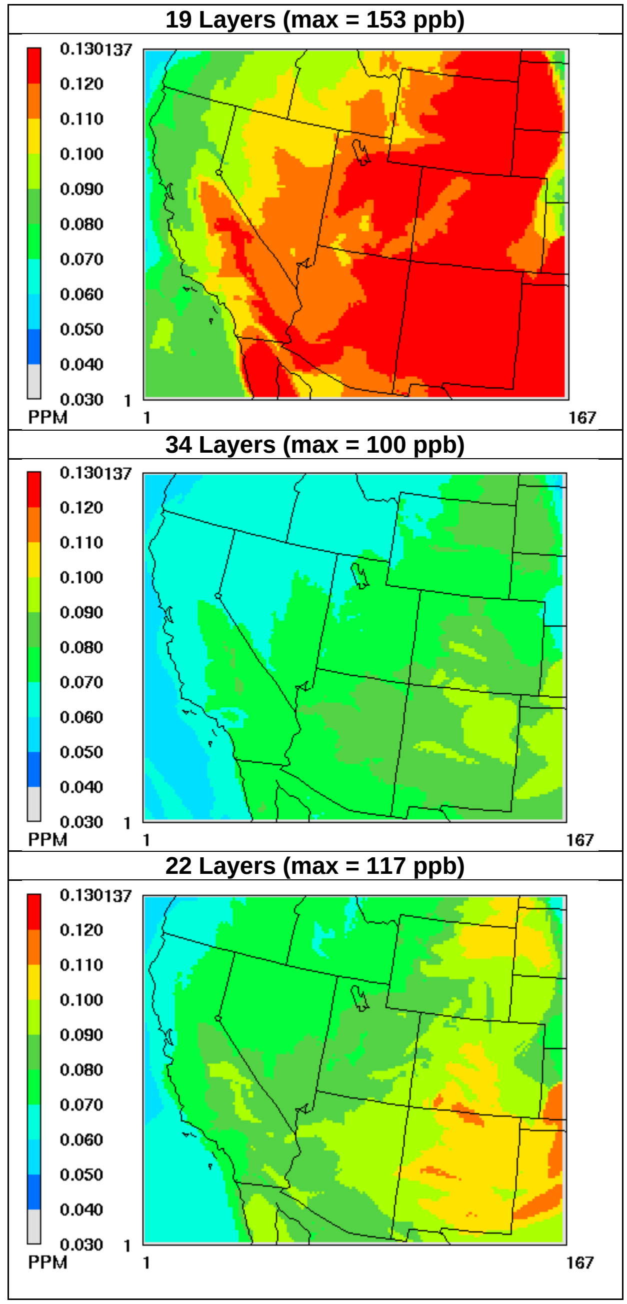

Figure 3. April 2005 CAMx inert maximum ozone concentrations (ppm) using "zero-gradient" top boundary conditions, the improved 2005 day-specific lateral boundary conditions, and the original 19 layer vertical structure (top), the full 34 layer vertical structure (middle) and the intermediate 22 layer vertical structure (bottom).

3.5 Mass Filter

Rotman et al. (2004) have developed a mass filter for the Lawrence Livermore National Laboratory IMPACT global chemistry model. IMPACT is run on global observational analyses fields; the interpolated wind and density fields are not self-consistent and thus can include dynamic inconsistencies among the meteorological variables that can produce spurious results, including excessive vertical velocities. The mass filter helps to eliminate these dynamic inconsistencies in the IMPACT model, so we expected that its application on the CAMx input meteorological fields could help reduce the excessive vertical transport as well.

The mass filter was adapted to the grid structure and variable staggering used in CAMx, and applied to the FCAQTF 12 km modeling database using varying levels of adjustments. Note that these tests used the improved 2005 GEOS-CHEM lateral BCs and zero-gradient top BCs on the 19-layer configuration. Application of the most aggressive configuration of the mass filter reduced the April maximum surface ozone concentrations by 10-20 ppb (Figure 4). However, this reduction was not sufficient to reduce the excessive surface ozone in these inert tests to observed levels.

3.6 Revised Vertical Transport Algorithm

Given the limited success in reducing the excessive vertical transport in the CAMx FCAQTF test modeling database through alterations of the horizontal wind fields, alternatives to the CAMx vertical transport algorithm were then investigated.

The diagnostic vertical velocity algorithm and associated upstream backward Euler vertical advection solver were found to possess a downward bias. The vertical velocity method was

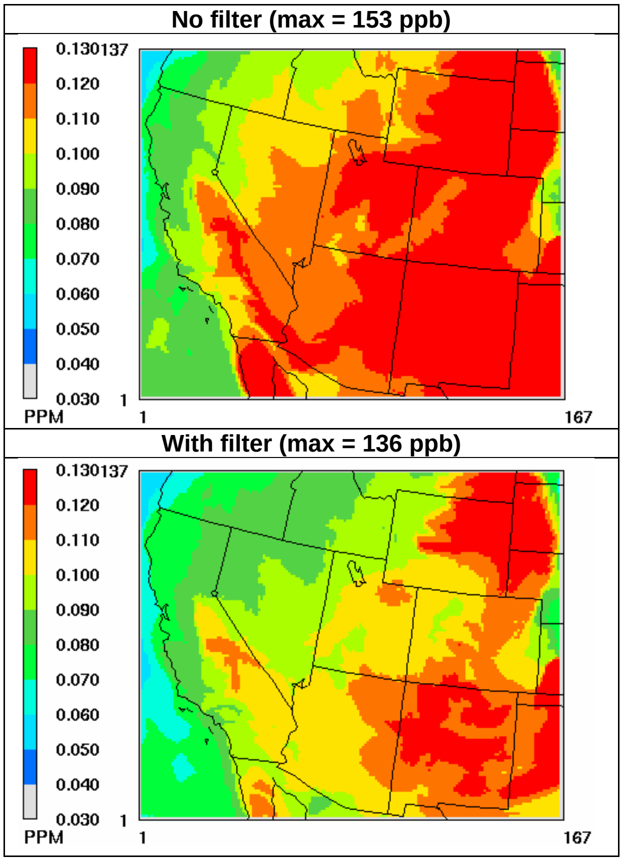

Figure 4. April 2005 CAMx inert maximum ozone concentrations (ppm) using "zero-gradient" top boundary conditions, the improved 2005 day-specific lateral boundary conditions, and the original 19 layer vertical structure. Original meteorology (top) and after application of the mass filter (bottom).

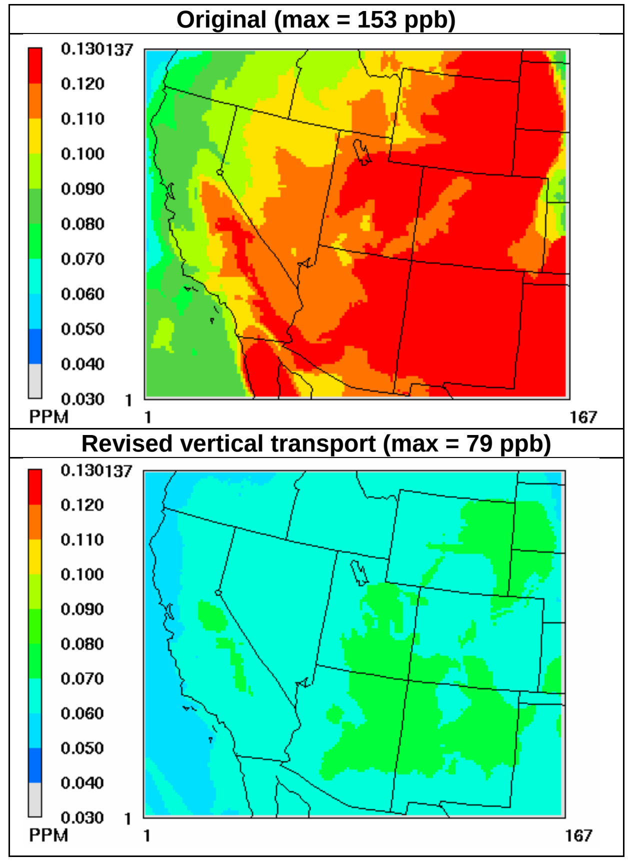

Figure 5. April 2005 CAMx inert maximum ozone concentrations (ppm) using "zero-gradient" top boundary conditions, the improved 2005 day-specific lateral boundary conditions, and the original 19 layer vertical structure. Original model configuration (top) and the revised vertical advection algorithm (bottom).

modified and the vertical solver was replaced with a new centered difference algorithm to be consistent. The modified version of CAMx was run for the FCAQTF April 2005 inert ozone test case with the following:

- 19 vertical layers;
- Improved lateral BCs from 2005 GEOS-CHEM; and
- Zero-gradient top BC.

Figure 5 compares the daily maximum ozone concentrations for the April test run using the original and revised vertical transport algorithms. Using the original vertical transport algorithm, maximum April ozone concentrations in excess of 100 ppb occur throughout the Rocky Mountain States and over the Sierra Nevada Mountains with a peak ozone value of 153 ppb (as seen in Figures 3 and 4). With the new vertical advection algorithm the maximum April ozone concentrations are in the 50-80 ppb range with a peak of 79 ppb. The CAMx modification results in simulated ozone that is more comparable with the observed values. The revised CAMx model was subjected to sensitivity tests to assure it remains mass consistent and mass conservative.

4. SUMMARY AND CONCLUSIONS

Excessive vertical transport in the CMAQ and CAMx models over high terrain have been shown to be the cause of overestimated ground level ozone concentrations in the spring. Both CMAQ and CAMx possess similar vertical velocity algorithms and solvers. Several techniques were investigated to reduce the vertical velocities by applying smoothers/filters and divergence minimization to the horizontal wind fields. Although these helped reduce the magnitude of vertical transport of ozone, they were insufficient to eliminate the springtime ozone overestimation bias. However, improved vertical resolution and revised vertical velocity and vertical advection algorithms were implemented in CAMx that eliminated the excessive downward transport of ozone from the top layers of the model while continuing to be both mass consistent and mass conservative.

The next step is to test the revised CAMx model using full photochemistry on the FCAQTF 36/12/4 km nested-grid modeling database and to conduct a model performance evaluation. We will also conduct an investigation into whether a similar approach can be implemented in the CMAQ model.

5. ACKNOWLEDGEMENTS

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