Effects of vertical-layer structure and boundary conditions on CMAQ - v4.5 and v4.6 models

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1. Introduction

Due to computational constraints, air quality models are often run using fewer vertical layers than used in the meteorological model simulation (e.g. MM5). The Meteorology-Chemistry Interface Processor (MCIP), a component of the Community Multiscale Air Quality (CMAQ) model, has options for collapsing (averaging multiple vertical layers to a single vertical layer) and reducing the number of vertical layers aloft for meteorological inputs to the CMAQ model. This feature is often used for long-term simulation periods to reduce computational time, since additional vertical layers can significantly increase model runtime. However, the effect of collapsing vertical layers needs to be examined to determine whether the increased computational efficiency also comes with a degradation of model performance. Here, model performance refers to how well the model predictions compare to observations (i.e. model accuracy).

In addition to the effects that vertical-layer collapsing may have on the CMAQ model performance, boundary conditions can also have an impact on the model performance. Included with the CMAQ model code are "profile" initial and boundary conditions, which contain time-independent concentrations of chemical and aerosol species. While these profile concentrations were intended to estimate "background" concentrations, they are simple approximations. It has been anticipated that spatially and temporally varying boundary conditions from a global or coarser scale chemical transport model should be more realistic than these profiles. The GEOS-CHEM model (Bey et al., 2001), has been used to provide temporally and spatially varying boundary conditions to the CMAQ model for the past several years. The results that have accompanied CMAQ v4.4, v4.5 and now v4.6 utilized the GEOS-CHEM model for specifying the boundary conditions. CMAQ has historically had issues capturing the lowest observed concentrations (both hourly and daily 8-hr average maximum) of ozone (O_3). Increasing the number of vertical layers (by not collapsing layers) may improve predicted concentrations of ozone.

Therefore, this work is aimed at determining whether the increased vertical layers in CMAQ provides substantially improved model performance and assess whether using the spatially and temporally varying boundary conditions from GEOS-CHEM offer improved model performance as compared to the default profiles.

2. CMAQ Simulations

To address the points raised above, sensitivity simulations utilizing version 4.5 of the CMAQ model were performed at 36-km and 12-km grid resolutions for July 2001 using a combination of a collapsed 14 vertical-layer structure, an un-collapsed 34 vertical-layer structure, profile boundary conditions and GEOS-CHEM boundary conditions, resulting in total of eight different simulations for v4.5. These simulations are listed below, defined by the grid resolution, number of CMAQ vertical layers, and boundary conditions (BCs) used.

(i) CMAQ v4.5, 36x36-km horizontal grid, 14-vertical layers, profile BCs
(ii) CMAQ v4.5, 36x36-km horizontal grid, 14-vertical layers, GEOS-CHEM BCs
(iii) CMAQ v4.5, 36x36-km horizontal grid, 34-vertical layers, profile BCs

(iv) CMAQ v4.5, 36x36-km horizontal grid, 34-vertical layers, GEOS-CHEM BCs
(v) CMAQ v4.5, 12x12-km horizontal grid, 14-vertical layers, profile BCs
(vi) CMAQ v4.5, 12x12-km horizontal grid, 14-vertical layers, nested within 36-km with GEOS-CHEM BCs
(vii) CMAQ v4.5, 12x12-km horizontal grid, 34-vertical layers, profile BCs
(viii) CMAQ v4.5, 12x12-km horizontal grid, 34-vertical layers, nested within 36-km with GEOS-CHEM BCs

In addition to the CMAQ v4.5 simulations above, two simulations utilizing CMAQ version 4.6 for one month from each season of 2001 using 14 and 34 vertical-layer structures and GEOS-CHEM boundary conditions are also available for analysis. Aside from using a different version of the CMAQ model, these simulations differ from the v4.5 simulations by utilizing the new Carbon-Bond 05 (CB05) chemical mechanism and a new asymmetric convective mixing (ACM) scheme, while the v4.5 simulations used the CB-IV chemical mechanism and the eddy vertical mixing scheme.

3. Observational Data

Several observational datasets were used to assess the performance of the CMAQ model. The Air Quality System (AQS) was used to provide surface concentrations of hourly and daily maximum 8-hour average ozone. The observations were matched with model predictions using the Site Compare software available as a tool along with the release of CMAQ (as of v4.5). Upper-air concentrations of O_3 from ozonesondes from Huntsville, AL and Wallops Island, VA were also compared to modeled vertical profiles from the 12-km domain. Observations from the ozonesondes were matched to model predictions by extracting the O_3 concentration from each layer in the model for the grid cell containing the latitude/longitude of the launch site of each ozonesonde. Observations of aerosol concentrations (e.g. SO_4^{2-}, NO_3^-, NH_4^+) are provided by the Speciation Trends Network (STN), the Interagency Monitoring of Protected Visual Environments (IMPROVE) network and the Clean Air Status and Trends Network (CASTNet). These networks provide daily (STN, IMPROVE) and weekly (CASTNet) concentrations of various aerosol species.

4. Summary

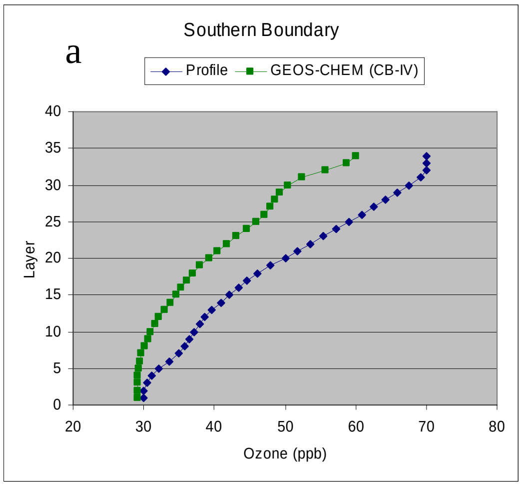
Table 1 shows the CMAQ model layer and the corresponding height above the ground of the top of each model layer for 14- and 34-layer vertical structures.

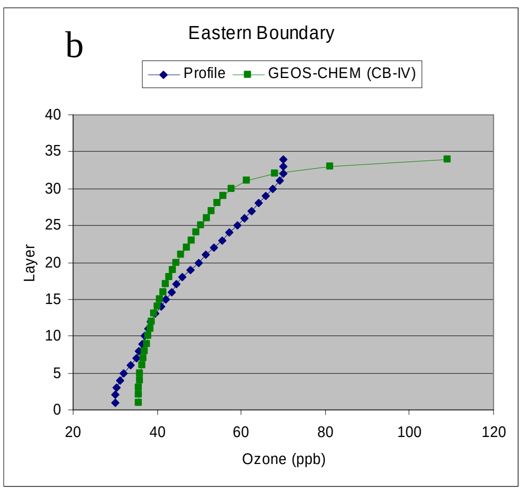
Table 1. Approximate heights of the top of each CMAQ vertical layer.

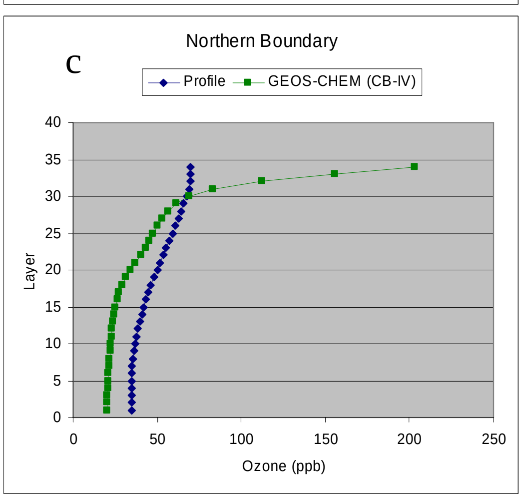
14 Layer		34 Layer	
Layer	Height (m)	Layer	Height (m)
1	36	1	36
2	72	2	72
3	145	3	108
4	290	4	145
5	435	5	217
6	660	6	290
7	1050	7	365
8	1535	8	440
9	2045	9	515
10	2870	10	590
11	3880	11	670
12	5640	12	745
13	8710	13	900
14	13700	14	1060
		15	1220
		16	1385
		17	1550
		18	1810
		19	2070
		20	2440
		21	2910
		22	3410
		23	3940
		24	4500
		25	5100
		26	5750
		27	6440
		28	7200
		29	8025
		30	8950
		31	9990
		32	11195
		33	12625
		34	14410

The 14-layer vertical structure contains 10 layers below 3km, while the 34-

layer vertical structure contains 21 layers below 3km. The 34-layer vertical structure also contains several more layers near the top of the troposphere, which should result in a better representation of the tropopause.







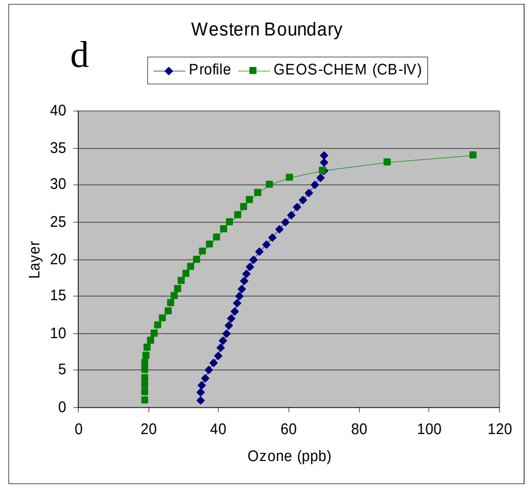
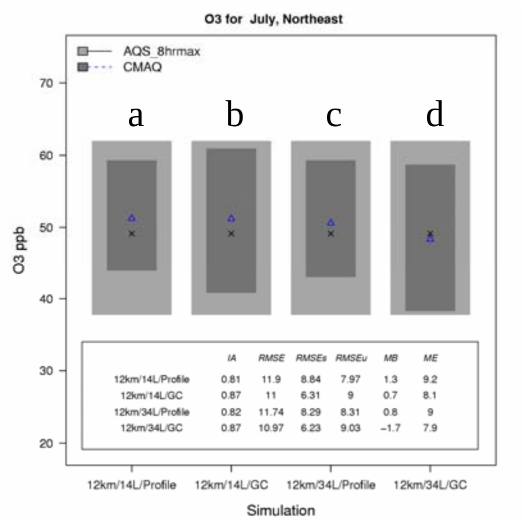


Figure 1. 34-layer vertical ozone concentrations in the profile boundary conditions (blue) and GEOS-CHEM boundary conditions (green) for a) southern boundary b) eastern boundary c) northern boundary and d) western boundary.

The GEOS-CHEM boundary conditions vary temporally (every three hours) and also vary spatially across each boundary. For the purpose of this analysis, each GEOS-CHEM boundary has been averaged temporally (monthly average for July 2001) and spatially along each boundary. Fig. 1 shows a comparison of the 34-layer O_3 vertical profile for the profile boundary conditions and the temporally averaged GEOS-CHEM boundary conditions for each of the four lateral boundaries. With the exception of the eastern boundary, the concentration of O_3 for the lowest level is lower with GEOS-CHEM than with profile boundary conditions. The concentration of O_3 at the top layer is higher in GEOS-CHEM than in the profile boundary conditions, except for the southern boundary, where the tropopause is higher than along the other boundaries. The GEOS-CHEM boundary conditions have the highest concentrations in the upper layers for the northern boundary where the tropopause is the lowest, while the profile boundary condition O_3 concentrations are the same or smaller for the northern boundary than the other three boundaries.

Fig. 2 shows an example of how CMAQ O_3 predictions are influenced by the GEOS-CHEM boundary conditions. The figure shows the observed and predicted median daily maximum 8-hour average O_3 for July 2001 for the (v), (vi), (vii) and (viii) simulations for the Northeast. The

Northeast region is the same as that presented in Lehman et al. (2004). The shading represents the 25% to 75% quartile range of the data. Summary statistics for each simulation are given below each box plot. Note that for the simulations that use profile boundary conditions (Figs. 2a and c), the model quartile range is narrower than that of the observations, suggesting the model not capturing the range of observed O_3. The simulation utilizing a 14-layer vertical structure and GEOS-CHEM boundary conditions (Fig. 2b), the predicted quartile range is broader, indicating the model did better capturing the range of observed concentrations. However, the model still falls short of capturing the entire observed range of concentrations. The simulation utilizing 34-vertical layers and GEOS-CHEM boundary conditions (Fig. 2d) does better than the other simulations at capturing the lower range of observed concentrations. However, there is little improvement in the upper range as compared to simulation (v).



	IA	RMSE	RMSEs	RMSEu	MB	ME
12km/14L/Profile	0.81	11.9	8.84	7.97	1.3	9.2
12km/14L/GC	0.87	11	6.31	9	0.7	8.1
12km/34L/Profile	0.82	11.74	8.29	8.31	0.8	9
12km/34L/GC	0.87	10.97	6.23	9.03	–1.7	7.9

Figure 2. Box plots daily maximum 8-hour average O_3 for July 2001 for 12x12-km horizontal grid CMAQ v4.5 simulations using a) 14-layer vertical structure and profile boundary conditions; b) 14-layer vertical structure and GEOS-CHEM boundary conditions; c) 34-layer vertical structure and profile boundary conditions; and d) 34-layer vertical structure and GEOS-CHEM boundary conditions. The shading represents the 25% to 75% quartile ranges of the data for the observed concentrations (light gray) and predicted concentrations (dark gray), while the points represent the median (black cross – obs; blue triangle – CMAQ). Summary statistics of Index of Agreement (IA), Root Mean Square Error (RMSE, ppb), systematic RMSE ($RMSE_s$, ppb), unsystematic RMSE ($RMSE_u$, ppb), MB (ppb) and ME (ppb) are included.

The ozonesonde data in Fig. 3 shows the range of vertical O_3 concentrations between the various 12x12-km horizontal grid simulations and the observed data. The simulations are closely clustered near the surface (within 5 ppb of each other), with simulation (v) having the lowest O_3 concentration at the surface (closet to the surface O_3 observation) and the simulation using CMAQ v4.6 having the highest concentration at the surface. The model largely under-predicts O_3 concentrations aloft, especially above 1 kilometer.

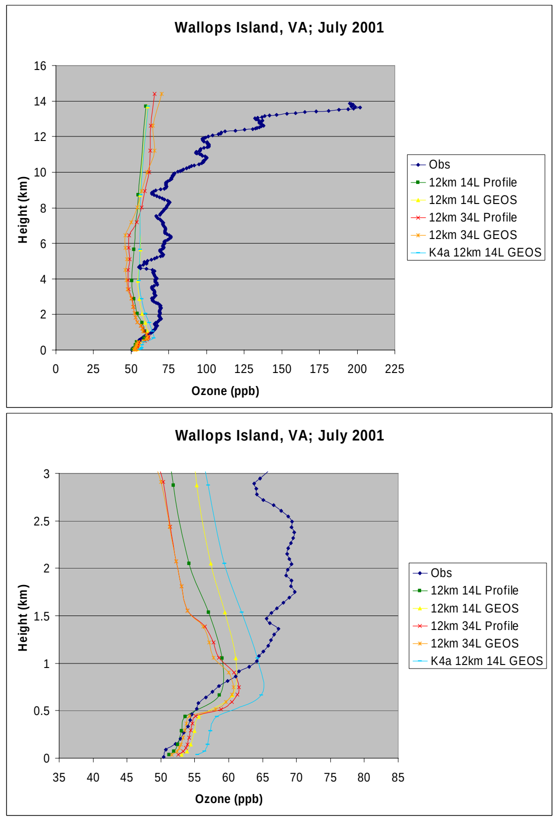


Figure 3. Ozonesonde data for Wallops Island, VA for July 2001 (average of sondes released on July 3, 11, 18 and 26) plotted along with vertical ozone concentrations from the various 12x12-km horizontal grid resolution sensitivity simulations. O_3 concentration (ppb) is plotted along the ordinate and height (km) is plotted along the abscissa. The full extent of the model vertical profile is plotted above, while only the lowest 3 kilometers (roughly the boundary layer) is plotted below.

There is little difference between the predicted O_3 concentrations aloft, with O_3 concentrations between the various simulations generally within 10 ppb of each other. Even though O_3 concentrations near the top of the troposphere were much higher in the GEOS-CHEM boundary conditions than the profile boundary conditions, the predicted concentrations near the tropopause are only slightly higher using 34-vertical layers and GEOS-CHEM boundary conditions than those using the profile boundary conditions.

Preliminarily results suggest that O_3 performance can be improved with the use of GEOS-CHEM boundary conditions in place of the default profile boundary conditions, while the use of an un-collapsed, 34-layer vertical structure may results some improvement in O_3 performance for low concentrations. More analysis is needed to quantify any improvement in CMAQ O_3 predictions. Predictions of O3 aloft (above 1km) are poor when compared to ozonesonde data. More analysis is needed to determine the full impact both boundary conditions and vertical-layer structure on CMAQ model performance. Additional analysis will be done to include the effects of boundary conditions and vertical structure on fine particulate aerosol species.

DISCLAIMER

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References

Bey, I., D.J. Jacob, R.M. Yantosca, J.A. Logan, B.D. Field, A.M. Fiore, Q. Li, H.Y. Liu, L.J. Mickley and M.G. Schultz, 2001. Global modeling of tropospheric chemistry with assimilated meteorology: Model description and evaluation, Journal of Geophysical Research, **106**, 23073-23096.

Lehman, J., K. Swinton, S Bortnick, C. Hamilton, E. Baldridge, B. Eder and B. Cox, 2004. Spatio-temporal characterization of tropospheric ozone across the eastern United States. Atmospheric Environment, 38, 4357-4369.