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

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Motivation and Background

Vertical-Layer Collapsing

- Due to computational constraints, air quality models (e.g. CMAQ) are often run using fewer vertical layers than used in the meteorological simulation (e.g. MM5)
- The effect of collapsing vertical layers needs to be examined to determine whether the increased computational efficiency comes with a degradation in model accuracy

Boundary Conditions

- In addition to the effects of vertical-layer collapsing, boundary conditions can have a significant impact on model accuracy
- Included with the CMAQ model code are "profile" boundary conditions which are time independent and do not vary spatially (however values are different for each of the four boundaries)
- These profile concentrations are simple approximations that are intended to represent "background" concentrations
- It has been anticipated that temporally and spatially varying boundary conditions 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 CMAQ for the past several years
- The results which have accompanied CMAQ v4.4, v4.5 and now v4.6 utilized the GEOS-CHEM model for boundary conditions
- The effect of using GEOS-CHEM boundary conditions as opposed to the profiles needs to be examined

CMAQ Simulations

- Sensitivity simulations were performed using CMAQ v4.5 at 36-km and 12-km grid resolutions for July 2001
- Simulations were performed 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
- The result is eight different simulations using CMAQ v4.5 (July 2001):
  - (i) 12X12-km horizontal grid, 14 vertical layers, profile BCs
  - (ii) 12X12-km horizontal grid, 14 vertical layers, GEOS-CHEM BCs
  - (iii) 12X12-km horizontal grid, 34 vertical layers, profile BCs
  - (iv) 12X12-km horizontal grid, 34 vertical layers, GEOS-CHEM BCs
- 36km simulations were performed with consistent specifications, and these provide boundary conditions for the 12km simulations
- Additionally, two simulations utilizing CMAQ v4.6 using 14 and 34 vertical-layer structures and GEOS-CHEM boundary conditions are also available for analysis
- However, the v4.6 simulations differ from the v4.5 simulations by utilizing the new Carbon-Bond 05 (CB05) chemical mechanism, a new asymmetric convective mixing (ACM) scheme, as well as some other changes to the model chemistry
- Only the difference between vertical-layer structure can be examined with the v4.6 simulations, since no simulations using v4.6 with profile boundary conditions were performed

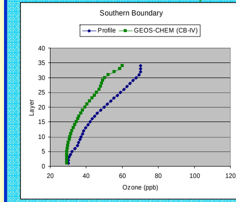
Observational Data and Statistics

- Surface ozone observations provided by the Air Quality System (AQS)
- Site Compare software (available as a tool with the CMAQ release) was used to match observations and predictions in time and space
- Upper-air concentrations of ozone were available from ozonesondes launched from Huntsville, AL, Wallops Island, VA and Boulder, CO.
- Observations from the ozonesondes were matched to model predictions by extracting ozone from each all layers in the model at grid cell containing the lat/lon of the launch site of each sonde
- Observations of aerosol concentrations (e.g. Sulfate, Nitrate, Ammonium) are provided by:
  - Speciation Trends Network (STN)
  - Interagency Monitoring of Protected Visual Environments (IMPROVE)
  - Clean Air Status and Trends Network (CASTNet)
- Several statistics are included on some of the figures:
  - Index of Agreement (IA): measure of how free the predictions are of error (Willmott, 1981)
  - Mean Bias (MB) and Mean Error (ME)
  - Systematic Root Mean Square Error (RMSEs): portion of error due to systematic model errors
  - Unsystematic Root Mean Square Error (RMSEu): portion of error due to random errors in the model or model inputs

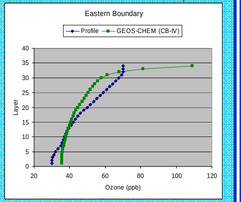
Profile and GEOS-CHEM Boundary Conditions

Note that GEOS-CHEM values shown below represent average ozone concentrations for July 2001 for the entire boundary. The CMAQ simulations utilized the entire temporal and spatial resolution of the GEOS-CHEM data. Also note that the x-axis scale is different for the northern boundary plot.

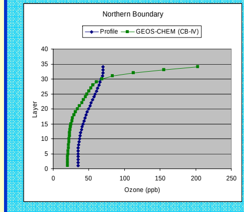
Southern Boundary



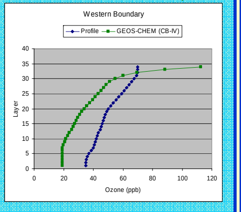
Eastern Boundary



Northern Boundary

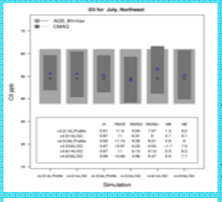


Western Boundary

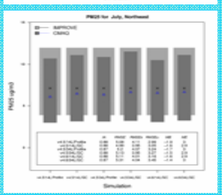


Comparison to Surface Networks

The figures below show the 25% to 75% quartiles (observation – light shading; CMAQ – dark shading) and the median concentration (observation – black x; CMAQ – blue triangle) for the various 12-km simulations for the Northeast (as determined by Principle Component Analysis). Summary statistics for the domain are included on each figure for each simulation. The first four simulation (from the right) utilize CMAQ v4.5, while the last two simulations utilize CMAQ v4.6.



Both vertical-layer structure and boundary conditions have an impact on ozone predictions. The use of GEOS-CHEM for boundary conditions improves the range (both upper and lower) of ozone predictions, resulting in an improvement in the bulk statistics. Collapsing of the vertical layers results in a slight degradation of model accuracy for the v4.5 simulations. For the v4.6 simulations, collapsing of the vertical layers results in a much greater degradation in model performance. This is likely due to several of the changes in CMAQ v4.6, particularly the new asymmetric convective module (ACM), which affects vertical mixing within CMAQ.



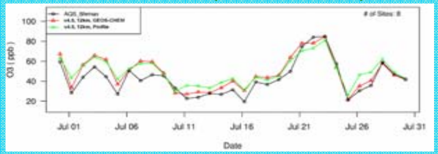
The effects of vertical-layer structure and boundary conditions on $PM_{2.5}$ predictions is much smaller than that on ozone predictions. Statistically, all the simulations (including the v4.6 simulations) are very similar. The mean bias is highest with the 14-layer simulation using profile boundary conditions and lowest with the CMAQ v4.6 34-layer simulation using GEOS-CHEM boundary conditions. The other statistics are nearly identical for each simulation. The use of GEOS-CHEM for boundary conditions appears to increase predictions of $PM_{2.5}$ slightly, while collapsing the vertical layers results in slightly lower predicted concentrations of $PM_{2.5}$.

Time Series Plots for Select Regions

Shown below are time series of observed 8-hr maximum O3, along with predictions from a simulation using boundary conditions provided by GEOS-CHEM (red) and one using profile boundary conditions (green).

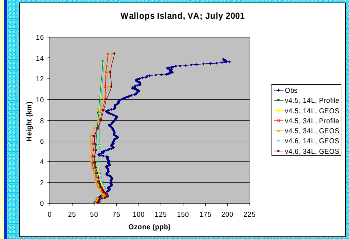
Central California Sites (36km Simulations)

Northeast Sites (36km Simulations)

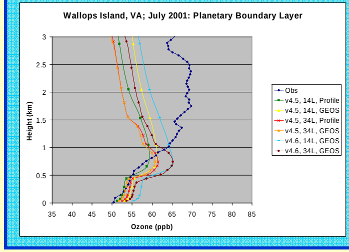


Houston, TX Sites (12km Simulations)

Comparison with Ozonesondes



Ozonesonde data for Wallops Island, VA (average of sondes released on July 3, 11, 18 and 26) plotted with CMAQ predicted average ozone concentrations from the same days and times. All the simulations under-estimate ozone above one kilometer, regardless of the vertical-layer structure or boundary conditions used.



Predicted ozone concentrations in the lowest one kilometer are predicted fairly well. Interestingly, the simulation using profile boundary conditions and 14 vertical layers most closely agrees with the observations near the surface. The simulation using CMAQ v4.6, 14 vertical layers and GEOS-CHEM boundary conditions has the highest ozone concentrations throughout the lowest 3-km.

Summary

- Neither the vertical structure or boundary conditions have much effect on predictions of ozone throughout the troposphere. Ozone is consistently under-predicted above 1-km.
- Collapsing of vertical layers results in a decrease in predicted ozone concentrations, especially at low concentrations.
- The use of GEOS-CHEM boundary conditions results in a larger range in ozone predictions (both upper and lower concentrations), which is a better representation of the observations.
- The time series plots show that the use of GEOS-CHEM boundary conditions significantly improves model predictions along the western domain boundary, but have a much smaller impact on predictions along the eastern domain boundary. The impact of the boundary conditions on the 12km simulation results was minimal for the example shown (Houston, TX).
- Vertical-layer collapsing and boundary conditions had little effect on model accuracy for $PM_{2.5}$ predictions.
- Of all the simulations analyzed here, the simulation utilizing CMAQ v4.6, 34-vertical layers and boundary conditions from the GEOS-CHEM model had the greatest accuracy (in terms of operational performance).
- For this limited analysis, it appears that operational model performance (at least for ozone) is improved by using GEOS-CHEM for boundary conditions. Collapsing of the vertical layers does seem to degrade model accuracy slightly, particularly when utilizing CMAQ v4.6.
- Further analysis needs to be performed (including analysis of other months) to determine the full impact of boundary conditions and vertical-layer collapsing.

References:

Willmott, C.J., 1981. On the validation of models. Physical Geography, 2, 184-194.

Acknowledgements: The authors would like to thank Lucille Bender, Nancy Hwang and Ruen Tang with CSC for performing the majority of the simulations used in this study. Thanks to Rob Pinder with NOAA/ARL/ASMD for reviewing this material and providing helpful comments.