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) one of the main issues faced in using fewer vertical layers than used in the meteorological simulation (e.g., RMM) is 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.
- The GEOS-CHEM model (Bey et al., 2003) has been used to provide temporally and spatially varying boundary conditions to CMAQ for the past several years.
- 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 has been used to provide temporally and spatially varying boundary conditions to CMAQ for the past several years.
- The results which have accompanied CMAQ v4.5 and v4.6 utilize 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 32 km grid resolution for July 2001.
- These simulations were performed using a combination of a collapsed 14 vertical-layer structure, as well as MSL 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 grid, 34 vertical layers, profile BCs
  - (ii) 12x12-km horizontal grid, 34 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
- Other 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 structure 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 condition were performed.

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 same temporal and spatial resolution of the GEOS-CHEM data, and this means that the x-km scale is different for the northern boundary plot.

Observational Data and Statistics
- Surface ozone observations provided by the Air- Quality System (AQS).
- The composite 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 of the 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 Trend Network (STN)
  - Interagency Monitoring of Protected Visual Environments (IMPROVE)
  - Clean Air Stakes and Trend Network (CASTNet)
- Several statistics are included on some of the figures:
  - Peak of Daily Maximum (PDM) measure of how free the predictions are of a single observed peak.
  - Mean Bias (MB) and Max Error (ME)
  - Systematic Root Mean Square Error (RMSSE)
  - Unsystematic Root Mean Square Error (RMSSEu)
- The time series plots show that the use of GEOS-CHEM boundary conditions improved ozone predictions (both upper and lower concentrations), which is a better representation of the observations.

Comparison with Ozonesondes
- Vertical-layer collapsing and boundary conditions had little effect on model accuracy.
- Of all the simulations analyzed here, the simulation utilizing CMAQ v4.6, 34-vertical layers and GEOS-CHEM boundary conditions had 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 underestimated in CMAQ models.
- 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 eastern domain boundary, but have a much smaller impact on predictions along the western 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 PM2.5 predictions.
- Of 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:

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