P 154 # AN EVALUATION OF CMAQ'S PERFORMANCE IN THE PLANETARY BOUNDARY LAYER AND FREE TROPOSPHERE USING OZONESONDES

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1. INTRODUCTION

Because of both recent (Federal Register, 2008) and proposed (U. S. EPA Fact Sheet, 2009) revisions to the NAAQS for ground-level ozone (O_3), there has been an increased emphasis in the Community Multi-scale Air Quality (CMAQ) model's ability to accurately simulate the contribution of O_3 aloft to concentrations at the surface. Specifically, the modeling community needs to examine the contribution of transport aloft, whether it be regional, continental or even hemispherical; and the "background" or natural component of ozone, including ozone originating from stratospheric intrusions associated with tropopause folds and/or from lightning-generated NO_x emissions.

Unfortunately, the general lack of upper-air air quality measurements has limited the evaluation of CMAQ's ability to simulate ozone concentrations aloft. As a result most evaluations have historically focused on surface performance (Eder and Yu, 2006; Appel et al., 2007). These evaluations have taken advantage of extensive data sets offered by networks like CASTNet and EPA's AIRS-AQS.

While such analyses are essential in understanding and subsequently improving the model's performance, it is also important to examine the model's ability to simulate conditions aloft. Accordingly, this preliminary research utilizes data obtained from four ozonesonde sites (Trinidad Head, CA; Boulder, CO; Huntsville, AL and Wallops Island, VA) in order to evaluate the model's ability to simulate ozone concentrations as well as two meteorological parameters (temperature (^oC) and relative humidity (%)) in both the Planetary Boundary Layer (PBL) and the Free Troposphere (FT).

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2. CMAQ CONFIGURATION

This evaluation used a five-year (2002-2006) simulation of CMAQ (Version 4.7, released in the autumn of 2008). The modeling domain covered the contiguous United States (Fig. 1) using a 36 km x 36 km horizontal grid resolution (148 (columns) x 112 (rows) = 16,576 grid cells) and a 24-layer logarithmic vertical structure, extending from the surface to approximately 100 hPa.

The meteorological fields were provided from MM5, the Fifth-Generation Pennsylvania State University/National Center for Atmospheric Research (NCAR) Meso-scale Model (Grell, et al., 1994) and were processed using the Meteorological-Chemistry Interface Program (MCIP). This 5-year simulation used the CB05 gas-phase chemistry mechanism. Static, month specific, Lateral Boundary Conditions (LBCs) were derived from a 2002 simulation of GEOS-Chem (Bey et al., 2001).

The emissions, which were processed using the Sparse Matrix Operator Kernel Emissions (SMOKE) processor (Houyouz et al., 2000), were based on EPA's 2002 National Emissions Inventory (with year-specific fire, mobile (from MOBILE6), biogenic (from Biogenic Emission Inventory System (BEIS) v. 3.13 and point EGU data).

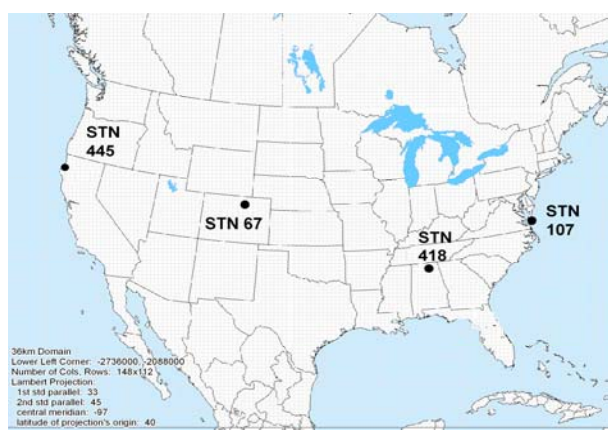

Fig.1 CMAQ domain and four ozonesonde sites.

3. OZONESONDE DATA

Site information for the four ozonesonde stations used in this analysis is found in Tab. 1, with their locations shown in Fig. 1. A comprehensive summary of each station, including climatological information can be found in Newchurch et al. (2003). For this analysis, the evaluation focused on sondes launched during the summers (June, July and August) from 2002-2006 and only during the afternoons. As a result between 37 and 135 sondes were used in the evaluation.

Station	Lat. (° N)	Long. (° W)	Elev. (m asl)	#
Trinidad Head, CA *STN 445*	41.07	124.15	20	135
Boulder, CO *STN 67*	40.02	105.27	1743	98
Huntsville, AL *STN 418*	34.73	86.58	196	91
Wallops Island, VA *STN 107*	37.90	75.50	13	37

Tab. 1 Ozonesonde station information.

4. EVALUATION PROTOCOL

Observations from each of the four ozonesondes were assigned to the appropriate CMAQ grid cell and matched with the 24 layers using either: extrapolation to CMAQ layers where no observations were available (occurring most often in the lowest few layers); or weighted averaging when numerous observations were available within each CMAQ layer (occurring most often in the upper layers). Each data point represents the midpoint of the CMAQ layer. Only ozonesondes launched during the afternoons, when the PBL was more likely to be well mixed, were used in the calculation of the evaluation statistics.

A suite of performance metrics were calculated, including the Normalized Mean Error (NME) and the Normalized Mean Bias (NMB), which are the focus of this paper.

5. EVALUATION RESULTS

5.1 Ozone

Examination of Fig. 2 reveals that CMAQ varied in its ability to accurately simulate ozone concentrations throughout the PBL and FT at the four locations. CMAQ greatly over-predicts ozone throughout the lower PBL at the two coastal sites, especially at Trinidad Head. The model performs well throughout the most of the PBL at the two inland sites, especially at Boulder. CMAQ consistently and increasingly under-predicts ozone in the upper portions of the FT, especially near the tropopause.

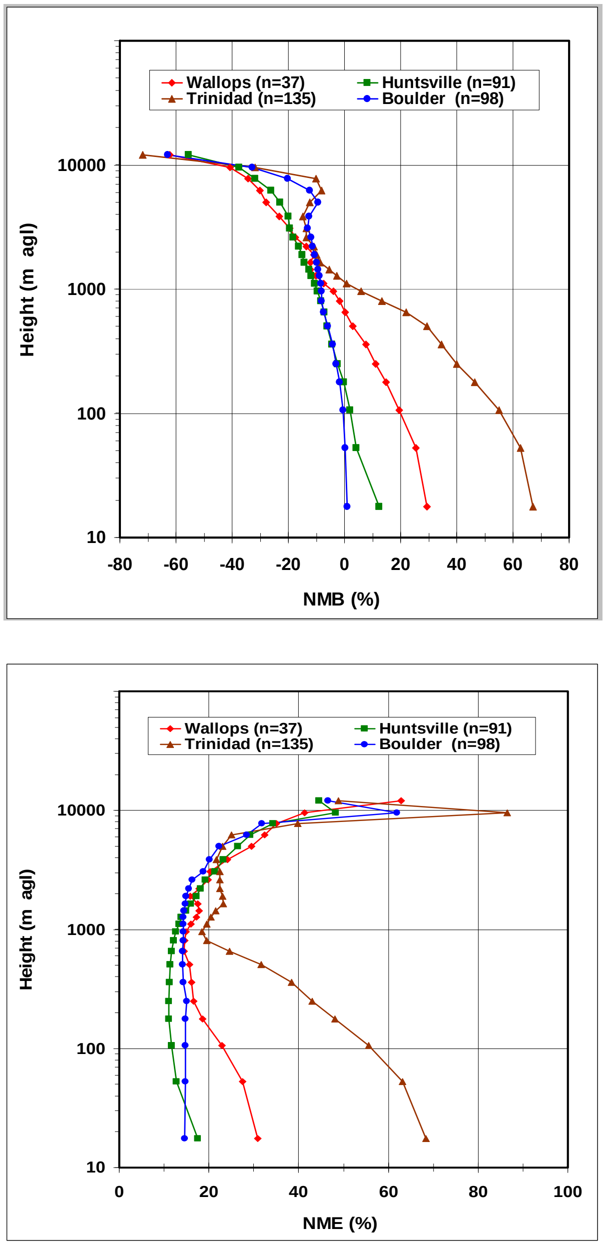

Fig. 2 Ozone NMB (%) top panel and NME (%) bottom panel associated with the four sites.

In order to better understand the model's performance at simulating O_3 at each of the four sites, we now exam them individually including the two meteorological parameters.

5.2 Trinidad Head, CA

CMAQ's performance in the PBL at this west-coastal location is by far the poorest of any site (Fig. 3). Values of NMB and NME for O_3 exceed 60% near the surface and average over 30% within the remainder of the PBL. Its performance in the FT is comparable with the other locations as it slightly underpredicts (NMB: -10%) between 1 - 9 km and then greatly underpredicts (NMB: -60%) nearer the tropopause (10 – 11 km). Examination of the simulated meteorological parameters at this location is revealing in that temperature is overpredicted (up to 20% near the surface) and relative humidity is underpredicted (-10%) throughout the PBL. This warm, dry bias indicates that MM5-CMAQ has done a poor job in simulating the cool, moist influence of the marine-PBL that dominates at this west coast location. This is not surprising, however, given the 36 km resolution used by the models.

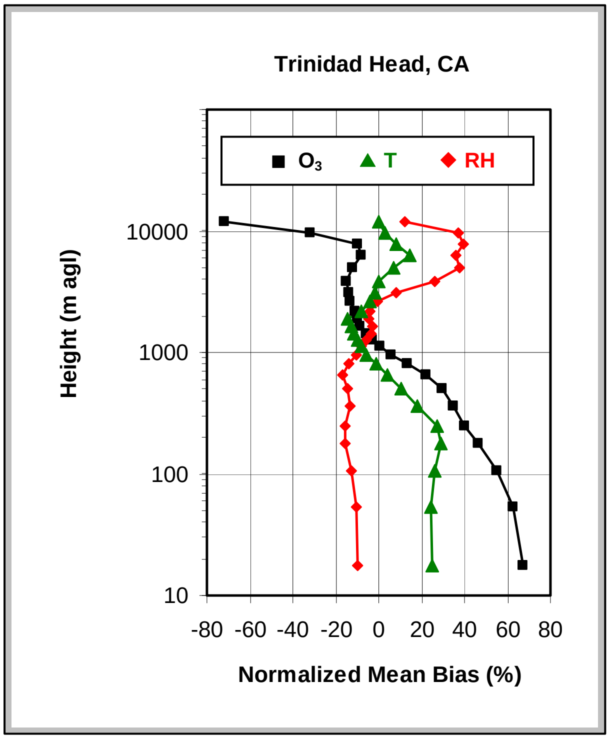

Fig. 3. NMB associated with CMAQ's simulation of O_3, Temperature and Relative Humidity for Trinidad Head, CA (STN 445).

The underprediction in the FT, while not as large as the overprediction in the PBL is still a concern and may be attributable to the lateral boundary conditions (LBC) used in the model. Currently, LBC values are provided by GEOS-Chem (Bey et al., 2001), and though they represent an improvement over previously used static LBCs, they may still be too low. As seen in Fig. 4, the western LBC values in the FT average near 50 ppbv and never exceed 60 ppbv, even near the tropopause. Recent suggests these values should be considerably higher, due in large part to inter-continental transport from Asia (Cooper et al., 2010).

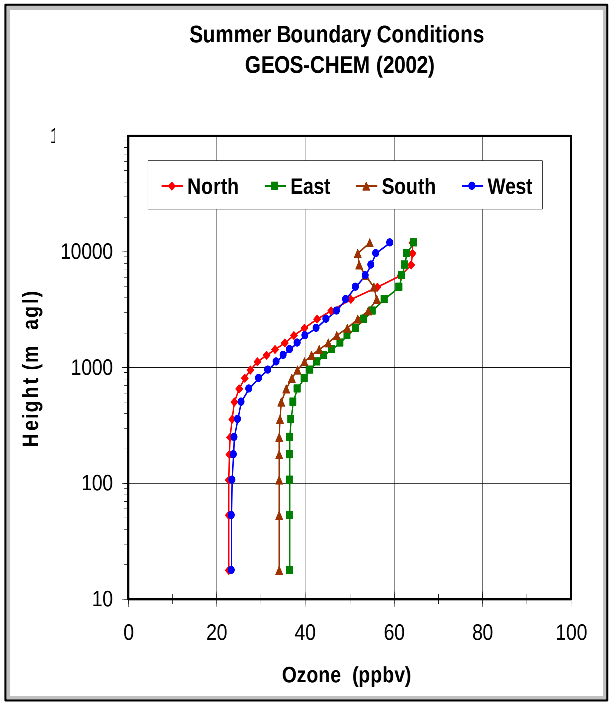

Fig. 4. Summer averaged O_3 concentrations for each of CMAQ's Lateral Boundaries.

5.3 Boulder, CO

CMAQ's simulation of O_3 throughout the PBL at this high elevation site is the best of the four sites as the NMB ranges from 0 to -10% (Fig. 5) and the NME averages near 15% (not shown). The model's performance in the FT over Boulder is very similar to that of Trinidad Head (i.e. NMB averages -10% between 1 and 9 km and then greatly increases to -60% near the tropopause around 10 – 11 km.) Although farther removed from the western domain boundary, the influence of the LBC may still be impacting concentrations at this location.

Unlike the Trinidad location, examination of the meteorological performance is not immediately enlightening, as both the temperature and humidity are underpredicted throughout most of the PBL, resulting in average NMB of about -10%.

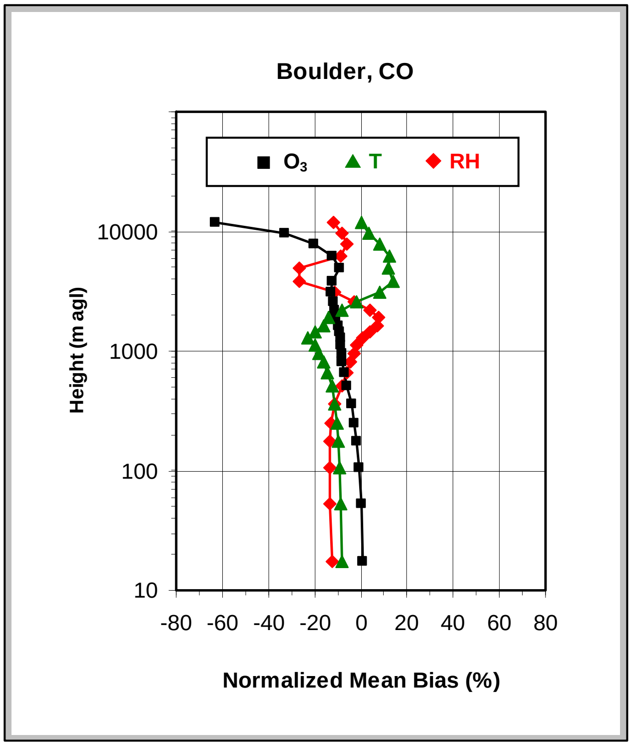

Fig. 5. NMB associated with CMAQ's simulation of O_3, Temperature and Relative Humidity for Boulder, CO (STN 67).

5.4 Huntsville, AL

When considering the overall performance, (i.e. including the meteorological parameters) CMAQ's simulation at this inland, low elevation is better when compared to the other three (Fig. 6). Both temperature and relative humidity are within ± 10% NMB through the PBL and well into the FT. CMAQ's simulation of O_3, while better than the west-coast location, is, surprisingly, not as good as the Boulder location, especially at the surface and in the middle portions of the FT (from 2 to 9 km). Though somewhat speculative at this stage of the investigation, a portion of the large underprediction found here (and at Wallops Island, as seen in Section 5.5) may be attributable to the exclusion of NO_x generated lightning in the emissions inventory. Of the four sites, only Huntsville and Wallops Island are dominated by maritime tropical air and the associated convection during the summer. Recent studies have indicated that NO_x emissions from lightning may contribute any where from 10 (DeCaria, et al., 2005) to 24 ppb (Cooper et al., 2006) of O_3 in the FT over the eastern U.S.

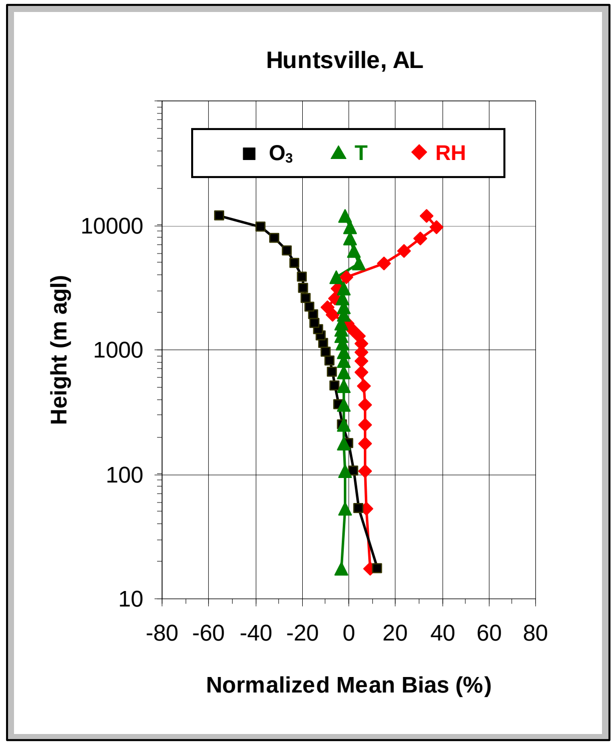

Fig. 6. NMB associated with CMAQ's simulation of O_3, Temperature and Relative Humidity for Huntsville, AL (STN 418).

5.5 Wallops Island, VA

Though not as poor as the west-coast site, CMAQ's simulation of O_3 in the PBL at this east-coast location is still poorer than the inland sites (Fig. 7). Values of NMB and NME exceed 30% near the surface and average over 15% within the remainder of the PBL. As just noted, CMAQ's performance in the FT is comparable to that of Huntsville and somewhat poorer than either Trinidad Head or Boulder.

Examination of the meteorological parameters at this location is less revealing than the other coastal site in that the temperature is simulated quite well throughout both the PBL and FT (NMB within ± 10%). The RH exhibits some positive bias near the surface and in the upper portions of the FT.

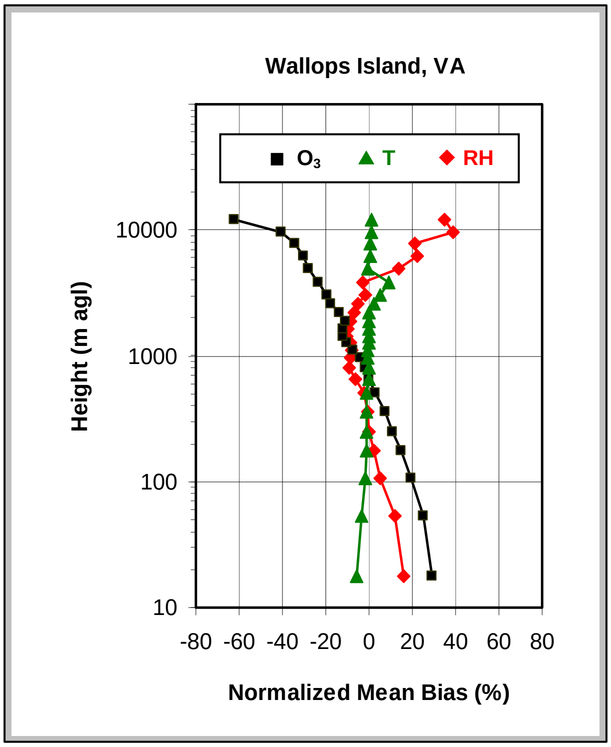

Fig. 7. NMB associated with CMAQ's simulation of O_3, Temperature and Relative Humidity for Wallops Island, VA (STN 107).

6.0 SUMMARY

This preliminary evaluation of CMAQ reveals that the model varies in its ability to accurately simulate O_3 concentrations in the PBL and FT at four ozonesonde locations. CMAQ greatly over-predicts O_3 throughout the lower PBL at the two coastal sites, especially at Trinidad Head, CA. This can be attributed to the model's inability to accurately resolve marine boundary layers at a 36 km scale. CMAQ performs considerably better throughout most of the PBL at the two inland sites, especially at Boulder, CO.

Within the FT, the model tends to under-predict at all sites. This is likely attributable, in part, to insufficient LBCs at the two western locations and the lack of lightning generated NO_x emissions at the two eastern locations. And finally, CMAQ greatly and consistently under-predicts ozone in the upper portions of the FT, especially near the tropopause, at all four locations. This is likely due to the model's omission of ozone originating from stratospheric intrusions associated with tropopause folds.

Ongoing research is addressing each of these deficiencies so that future releases of CMAQ will better simulate O_3 concentrations aloft and their potential contribution to concentrations at the surface.

7.0 REFERENCES

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