An Exploration of Model Concentration Differences Between CMAQ and CAMx

Brian Timin*, Karen Wesson, Patrick Dolwick, Norm Possiel, Sharon Phillips
U.S. Environmental Protection Agency, Office of Air Quality Planning and Standards, Research Triangle Park, NC, USA

1. INTRODUCTION

The majority of State Implementation Plan (SIP) modeling for the ozone and PM2.5 National Ambient Air Quality Standards (NAAQS) will be conducted with the CMAQ and CAMx air quality models. This paper explores the differences in base case concentrations predicted by the two models, given similar inputs.

Both models were run for a 2001 base case period using similar emissions and meteorological inputs. Significant differences were seen in the predicted model concentrations, especially for ozone and gaseous photochemical by-products. Several aspects of the modeling systems were explored to determine why the model predictions were dissimilar.

Among the inputs examined were vertical diffusion coefficients (Kv's), dry deposition velocities, photolysis rates, and cloud attenuation of photolysis rates. Several sensitivity runs were completed in an effort to further understand the cause of the concentration differences. The analyses uncovered fundamental differences between the two models and can qualitatively explain many of the concentration differences seen between the models.

2. OVERVIEW OF MODELING

CMAQ version 4.5 (Byun, 2006) and CAMx version 4.31 (Environ, 2006) were run for the July 2001 period (with a 10 day spin-up period at the end of June). Both models were driven with the same raw emissions and meteorological data. Both models were run with CB-IV chemistry. The emissions data were processed through SMOKE for both models. The CMAQ meteorological input data were processed through MCIP version 3.1 and the CAMx meteorological input data were processed through MM5CAMX. Both models used identical vertical structures. The 34 layer MM5 vertical structure was collapsed to 14 layers, with ~7 layers below the daytime boundary layer (less than 3100 meters). Both models had a 12km Eastern U.S. domain[1] nested inside of a 36km continental U.S. domain. All results shown are for the 12km nested domain.

2.1 Examination of CMAQ and CAMx Outputs

Comparisons of model output concentrations revealed large differences in predicted ozone concentrations. Figures 1 and 2 show the predicted layer 1 ozone concentrations at 2100 GMT on July 17th 2001.

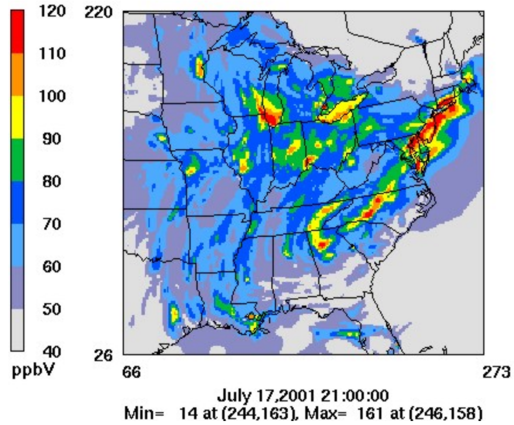

Fig. 1. CAMx 12km grid modeled ozone concentrations on July 17th, 2001 at 2100 GMT.

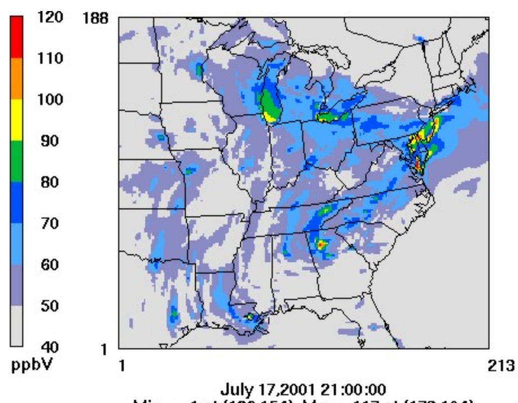

Fig. 2. CMAQ 12km grid modeled ozone concentrations on July 17th, 2001 at 2100 GMT.

As can be seen from figures 1 and 2, the predicted ozone concentrations in CAMx were significantly higher than those predicted by CMAQ. Afternoon peak ozone concentrations were often

**Corresponding author:*, Brian Timin, U.S. EPA, OAQPS, C431-01, RTP, NC 27711; e-mail: timin.brian@epa.gov .

[1] The CAMx 12km domain is larger (220 X 273) than the CMAQ 12km domain (188 X 212). The CAMx plots in this paper are cropped to produce approximately equal size plots.

20 to 30 ppb higher in CAMx (at the same time and location).

Additional species were examined to see if similar patterns existed, especially for ozone precursors.

While examination of species such as NO and NO_2 did not reveal any obvious differences, examination of CO revealed a very large systematic difference between the models. Figures 3 and 4 show the layer 1 CO concentrations for the two models for the same time period shown for ozone in figures 1 and 2.

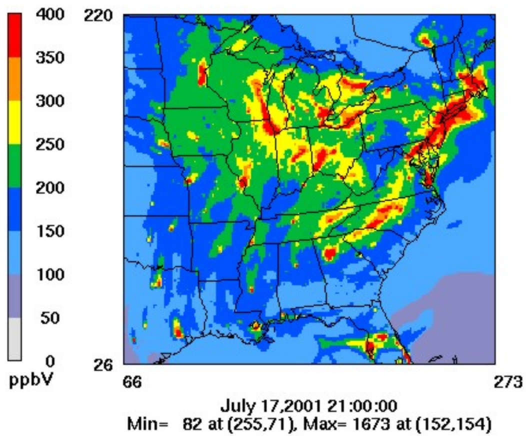

Fig. 3. CAMx layer 1 12km grid modeled CO concentrations on July 17th, 2001 at 2100 GMT

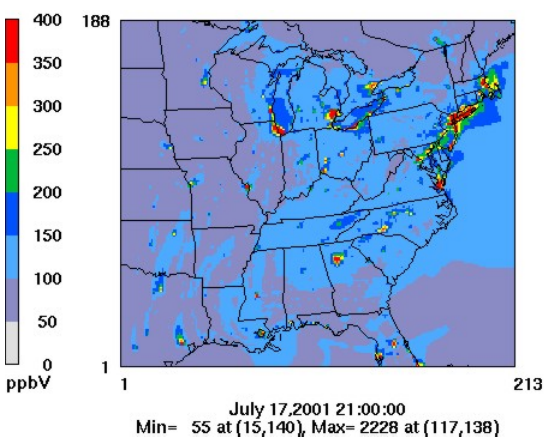

Fig. 4. CMAQ layer 1 12km grid modeled CO concentrations on July 17th, 2001 at 2100 GMT

The predicted CO concentrations are vastly different between the two models. The CO concentrations in CAMx are as much as twice the CMAQ CO concentrations in rural areas. However, in the largest urban areas, the concentrations are similar. The example plots only show one hour of one day, but the same pattern exists for all hours and all days during the simulation.

Additional species examined included formaldehyde (FORM), higher aldehydes (ALD2), hydrogen peroxide (H2O2), and various CB-IV VOC species (ISOP, PAR, OLE). In general, species with large secondary formation differed the most between the models. These include FORM, ALD2, and H2O2. Figures 5 and 6 illustrate the differences seen for formaldehyde (FORM).

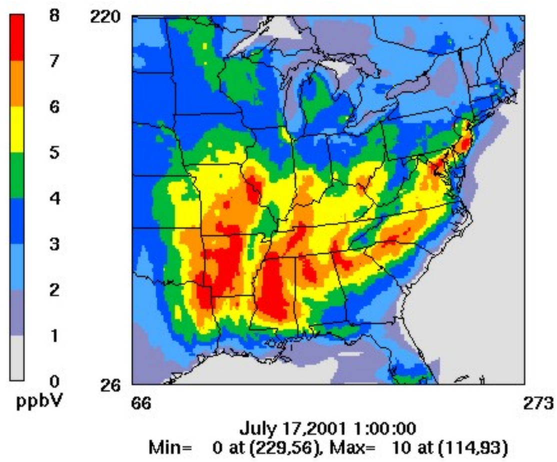

Fig. 5. CAMx layer 1 12km grid modeled FORM concentrations on July 17th, 2001 (24-hour average).

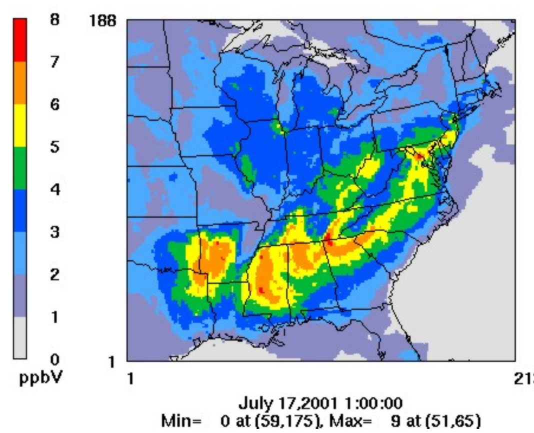

Fig. 6. CMAQ layer 1 12km grid modeled FORM concentrations on July 17th, 2001 (24-hour average).

Again, the CAMx concentrations were significantly higher than those seen in CMAQ for the same location and time period.

As a result of these findings, additional analyses and sensitivity studies were completed in an effort to better understand the large differences between the two models.

3. SENSITIVITY STUDIES

Several avenues were explored in the analysis of the model concentration differences. First, existing information and studies were examined to look for clues to differences in the models. Both models were run with CB-IV chemistry. However, the implementation of the chemistry in the models is somewhat different. Some differences between the models include: 1) CAMx version 4.31 was run with "Mechanism 4" which contains additional reactions beyond the base CB-IV mechanism. 2) Both models use different pre-processors to calculate photolysis rates. 3) Both models use different schemes to calculate the attenuation of photolysis by clouds.

Upon review of each of these differences, it was found that none were likely the cause of the large differences in ozone, CO, and secondary gases. This is discussed below.

3.1 Chemical mechanism

Additional CMAQ runs were completed with a newer version of CMAQ (v4.6) which contained the CB-05 mechanism (Yarwood, 2006). CB-05 contains many of the same "additional" reactions as CAMx "Mechanism 4" ("CB-IV+" mechanism). The CB-05 mechanism was expected to produce higher ozone (~5 ppb) in CMAQ and it did. But, given that this change in chemical mechanisms (going from CB-IV to CB-05) gave a relatively modest increase in ozone, we believe it is unlikely that the additional reactions in CAMx CB-IV+ were a major cause of ozone concentration differences between CAMx (CB-IV+) and CMAQ ("standard" CB-IV).

3.2 Photolysis rates

The clear skies photolysis rates were examined in both models. The CAMx CB-IV rates for NO2 and ozone photolysis were slightly higher than the CMAQ CB-IV rates, but the CMAQ CB-05 rates were higher than the CAMx CB-IV rates. Since the increase in ozone concentrations from CMAQ CB-05 was not nearly as large as the difference in ozone concentrations between the models, it is not likely that the differences in photolysis rates are a major cause of concentration differences between the two models.

3.3 Cloud attenuation of photolysis rates

The differences in cloud attenuation between the models have previously been explored in (Dolwick, 2007). The study found that there tended to be less attenuation of UV radiation in CAMx, which caused small areas of higher ozone in CAMx. However, the overall ozone differences were constrained to small areas and did not account for the large regional ozone differences between the two models.

4. SENSITIVITY RUNS

Several additional model runs were completed in order to test differences in vertical mixing and dry deposition. For vertical mixing, we implement two different vertical mixing schemes in CAMx and compare the results to CMAQ. These tests help us understand the impact of vertical mixing on model concentrations. For the deposition sensitivity tests, we explore the different schemes used by the two models. Our CAMx run used a "Wesely" based dry deposition scheme (Wesely, 1989), while CMAQ was run with a more up to date dry deposition scheme called "M3Dry".

4.1 Vertical mixing

CAMx uses vertical diffusion coefficients (Kv's) as an input to the model. The Kv's are generated in the postprocessing of the MM5 meteorological data (using the MM5CAMX program). There are two options for generating CAMx Kv's: an O'Brien scheme and a "CMAQ-like" scheme. The "CMAQ like" scheme is designed to replicate the CMAQ methodology[2] for generating Kv's. The initial version of CAMx was run with the O'Brien vertical mixing scheme.

We ran CAMx for the July 2001 period with the "CMAQ-like" Kv's in order to estimate the impact of differences in vertical mixing between the models. The "CMAQ-like" Kv's almost always were higher than the O'Brien Kv's, and therefore generated more vigorous daytime mixing.

Figure 7 shows an example of the vertical Kv patterns between the schemes. The plot is for hour 2000 GMT on July 19th for a grid cell over Atlanta. The differences between O'Brien and "CMAQ-like" Kv's in this plot are typical of an afternoon peach hour for most areas in the domain. The "CMAQ-like" Kv's are always higher than O'Brien throughout the mixing layer. And the O'Brien Kv's usually begin to fall off at a lower layer than the "CMAQ like" Kv's. This indicates less vigorous mixing (to a lower height) in CAMx with O'Brien Kv's.

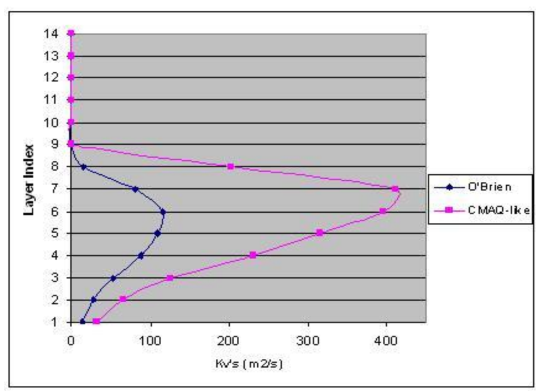

Fig. 7. Vertical Kv profile (layers 1-14) in CAMx for a grid cell over Atlanta on July 19th, 2001 at 2000 GMT. The pink profile is for the "CMAQ-like" Kv's and the blue profile is for the O'Brien Kv's.

---

[2] We have examined the actual Kv's from a CMAQ model run to see how they correspond to the "CMAQ like" Kv's produced by CAMx. The two sets of Kv's were very similar.

We would expect the increased mixing with the "CMAQ-like" Kv's to produce less ozone compared to the O'Brien Kv's. This was verified with the CAMx sensitivity run. Figure 8 shows the ozone differences in CAMx for the two Kv schemes. The differences are shown for the same hour that is plotted in figure 7 and show a mixture of ozone increases and decreases. In general, ozone went down (with "CMAQ-like" Kv's) by up to 10-15 ppb in areas with high ozone in the O'Brien case. Ozone went up in areas that were oxidant limited and therefore, increased mixing led to less titration of ozone and higher concentrations. This pattern is typical of most late afternoon hours on most days.

This sensitivity run clearly shows that CAMx run with the O'Brien mixing scheme produces more peak ozone compared to the CMAQ scheme. This likely accounts for at least part of the higher ozone seen in CAMx compared to CMAQ.

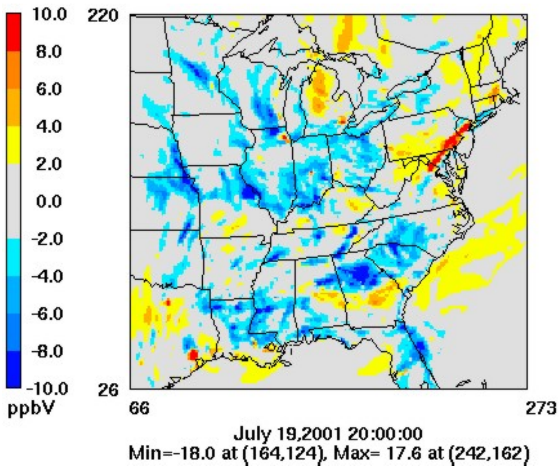

Fig. 8. One hour average ozone difference between CAMx run with O'Brien and "CMAQ like" Kv's (CMAQ-like – O'Brien) on July 19th, 2001 at 20Z. Negative values are ozone reductions due to "CMAQ like" Kv's.

4.2 Dry Deposition

CAMx uses a Wesely based dry deposition scheme (Wesely, 1989) that has been used in photochemical models for over 15 years. A similar scheme is available in CMAQ, called the RADM dry deposition scheme. CMAQ model runs over the last ~4 years have generally used a more recent dry deposition scheme called M3Dry (Pleim, 2001). M3Dry contains many improvements over previous schemes. M3Dry has updated resistance values based on more recent literature and field studies and it is also closely coupled with the Pleim-Xiu land surface model (used in MM5). M3Dry is able to use leaf area index and meteorological information to estimate canopy wetness, and it uses canopy wetness information to enhance dry deposition velocities for soluble gases (when surfaces are wet).

4.2.1 Dry deposition velocities

Dry deposition velocities (Vd) in CMAQ and CAMx were compared for several species to determine if major differences existed between the models. Among the species examined, large differences were noted for CO and NO, and smaller (but significant) differences were seen for other species including ozone, formaldehyde, NO_2, and hydrogen peroxide. In general, CMAQ deposition velocities were always higher than those seen in CAMx.

There are several differences that were seen. For CO and NO, CMAQ deposition velocities (using M3Dry) were 2-4 orders of magnitude higher than CAMx. For non-soluble gases, CMAQ deposition velocities were generally 20-100% higher than CAMx. For soluble gases (NH3, formaldehyde, etc.), CMAQ deposition velocities were several times higher than CAMx when modeled surfaces were wet.

Figures 9 and 10 show the deposition velocities for CO from CAMx and CMAQ on July 17th at 1600 GMT. This represents typical peak early afternoon deposition velocities. As can be seen in the figures, the CO Vd in CAMx is near zero while the CMAQ Vd (using M3Dry) ranges from 0.4-1.4 cm/s.

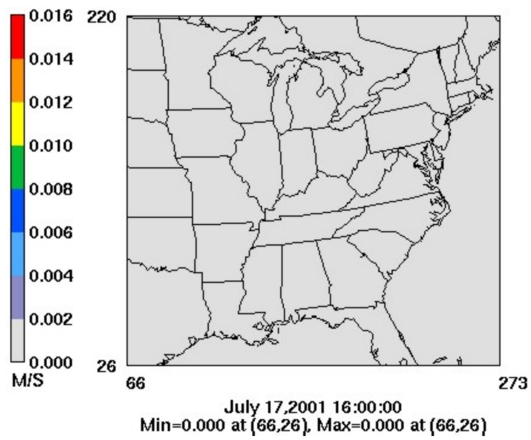

Fig. 9. CAMx 12km grid deposition velocity (Vd) for CO on July 17th, 2001 at 1600 GMT.

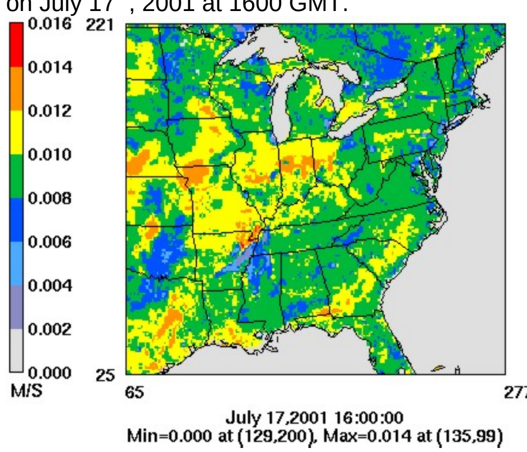

Fig. 10. CMAQ 12km grid deposition velocity (Vd) for CO (M3Dry) on July 17th, 2001 at 1600 GMT.

Figures 11 and 12 show ozone deposition velocities for the same time period. The CMAQ Vd values are generally 20-50% higher than those seen in CAMx.

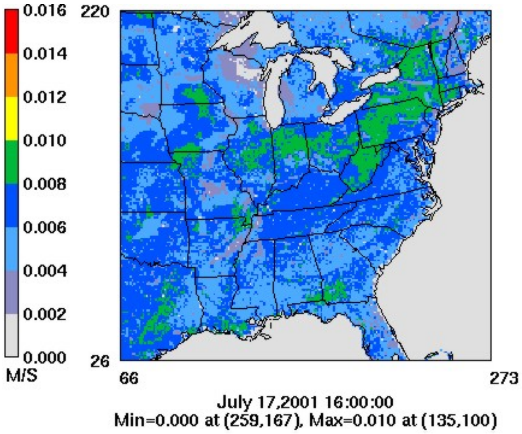

Fig. 11. CAMx 12km grid deposition velocity (Vd) for O3 on July 17th, 2001 at 1600 GMT.

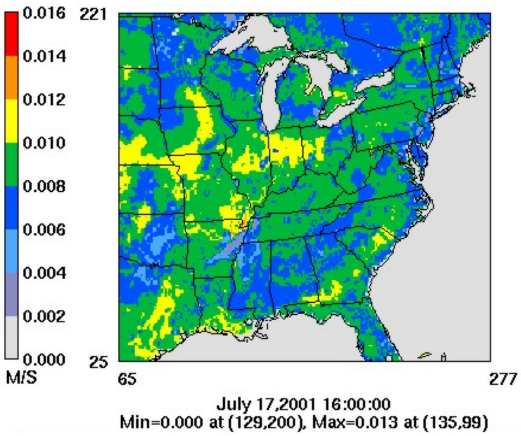

Fig. 12. CMAQ 12km grid deposition velocity (Vd) for O3 (M3Dry) on July 17th, 2001 at 1600 GMT.

4.2.2 Dry deposition sensitivities

Two CMAQ sensitivity runs were completed in order to examine the ozone response to dry deposition schemes. Both sensitivity runs were completed for a short time period with a more recent CMAQ platform. The platform used CMAQ v4.6 with CB-05 chemistry and 2002 emissions and meteorology. We ran CMAQ for the August 1-15th, 2002 period, with a 7 day ramp-up period. There were several high ozone episodes in the East during this period.

The first sensitivity run investigated the CO, NO, and NO_2 deposition velocities in order to better understand the differences between CMAQ and CAMx. The second sensitivity run looked at CMAQ ozone using the older RADM dry deposition scheme, in an effort to emulate the dry deposition scheme in CAMx. We then compared the ozone predictions in CMAQ using RADM back to the concentrations from the M3Dry model run.

4.2.2.1 Mesophyll resistance sensitivity

In our first sensitivity test of deposition, it was found that the Vd values for CO, NO, and NO_2 (especially CO and NO) were too high in M3Dry. A resistance value was added to M3Dry to represent mesophyll resistance for these three species and this resulted in CO and NO Vd values which were ~2 orders of magnitude lower than the original values in M3Dry. The rural CMAQ CO concentrations went up by a large amount and compared better to what was predicted by CAMx. We concluded that the mesophyll resistance values had a large impact on CO concentrations. The impact on ozone concentrations was small. Daily peak ozone concentrations went up by 1 or 2 ppb in many areas in the East.

4.2.2.2 RADM dry deposition sensitivity

Substituting the RADM dry deposition scheme for the M3Dry scheme in CMAQ had a large impact on modeled concentrations. The RADM deposition velocities were generally lower than M3Dry. The spatial patterns and magnitude of the RADM deposition velocities looked qualitatively similar to the deposition velocities from CAMx. This was expected, due to the common origin of both schemes (Wesely).

Figure 13 shows the 8-hour average ozone maximum on August 5th, 2002 from the base CMAQ v4.6 model run (using M3Dry). Figure 14 shows the increase in ozone on the same day as a result of switching to the RADM dry deposition scheme (everything else in the model runs were held constant). Ozone concentrations increased by 8-24 ppb (8-hour average) over large portions of the domain. Ozone increases were largest where peak values were seen in the base case.

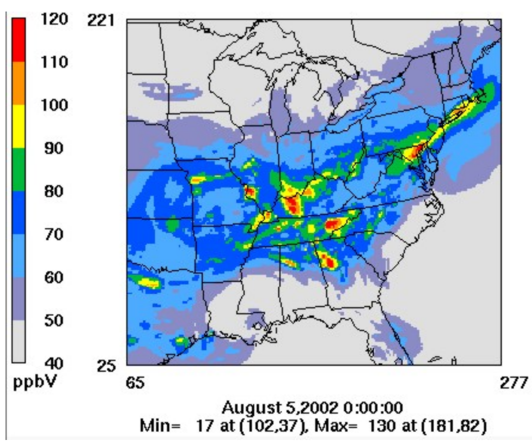

Fig. 13. CMAQ layer 1 12km grid modeled ozone concentrations on August 5th, 2002 (8-hour average).

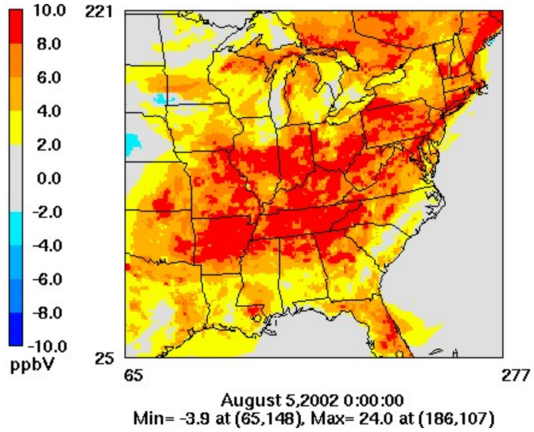

Fig. 14. 8-hour average ozone difference between CMAQ with RADM dry and M3Dry (RADM – M3Dry) on August 5th, 2002. Positive values are ozone increases due to RADM dry deposition.

5. CONCLUSIONS

Through sensitivity testing of CAMx and CMAQ we were able to account for most of the major concentration differences between the two models. We concluded that the largest difference in ozone concentrations in the two models is due to differences in the dry deposition schemes. Ozone increased by 10-20 ppb when a dry deposition scheme similar to the CAMx scheme is used in CMAQ. There were also problems identified in the CO and NO deposition velocities in M3Dry in CMAQ. Adding a value for mesophyll resistance for CO has a large impact on CO concentrations in CMAQ, though a somewhat small impact on daily ozone concentrations.

Sensitivity testing of vertical mixing schemes within CAMx revealed that inserting a "CMAQ-like" mixing scheme in CAMx leads to increased mixing and generally lower peak ozone concentrations (by up to 15-20 ppb).

Although difficult to precisely quantify, the combined effects of vertical mixing and dry deposition differences in CAMx and CMAQ likely account for the vast majority of the ozone concentration differences between the two models. These model formulation issues also account for differences in predicted concentrations of secondary aerosols (e.g. sulfate) and other photochemical precursors and by-products.

6. RECOMMENDED FOLLOW-UP

Further work is needed to examine the vertical mixing and dry deposition schemes in both CAMx and CMAQ. Vertical mixing in the models should be compared to mixing height observations to determine which scheme is most appropriate. Dry deposition velocities should be compared to published literature and fields studies to determine potential deficiencies in the current schemes. We stress that the models should not be compared to observed ozone concentrations to determine the appropriate mixing and deposition schemes. Conclusions based solely on an operational evaluation for ozone can lead to and/or perpetuate compensating errors in the modeling system.

7. REFERENCES

Byun, D., and K. L. Schere, 2006: Review of the governing equations, computational algorithms, and other components of the Models-3 Community Multiscale Air Quality (CMAQ) modeling system. *Appl. Mech. Rev.*, **59**, 51–77.

Dolwick, P., 2007: The effects of cloud attenuation on air quality: A comparison of model treatments. Presented at the 87th AMS Annual Meeting, San Antonio, TX.

ENVIRON International Corporation. User's Guide Comprehensive Air Quality Model with Extensions (CAMx) Version 4.30; ENVIRON International Corporation: Novato, CA, 2006. www.camx.com

Pleim, J. E., A. Xiu, P. L. Finkelstein, and T. L. Otte, 2001: A coupled land-surface and dry deposition model and comparison to field measurements of surface heat, moisture, and ozone fluxes. *Water Air Soil Pollut.* Focus, 1, 243–252.

Wesely, M. L., 1989: Parameterization of surface resistances to gaseous dry deposition in regional-scale numerical models. *Atmos. Environ*., **23**, 1293–1304.

Yarwood, G., S. Rao, M. Yocke, and G. Whitten, 2005: Updates to the carbon bond chemical mechanism: CB05. Final report to the US EPA, RT-0400675. Available at www.camx.com

8. ACKNOWLEDGEMENTS

We want to thank CSC for running CMAQ and CAMx; Jon Pleim for assistance on dry deposition issues (including recommendations for mesophyll resistance values); Environ for CAMx help and Kirk Baker of LADCO for CAMx assistance.