Evaluation of CMAQ with FAQS Episode of August 11th-20th, 2000

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We have applied MM5/SMOKE/CMAQ to the FAQS episode of August 11th-20th, 2000 in Georgia's metro areas. The sensitivity of CMAQ predictions to the minimum vertical eddy diffusivity has been tested with the cutoff value as 1.0, 0.3, 0.1, 0.03 and 0.0001 m^2/s. The evaluation of CMAQ was made by comparing the predictions with the measurements from AIRS, PAMS, SEARCH and ASACA datasets for 29 matched species. Further analyses were made based on the results of evaluations.

1. INTRODUCTION

The Fall line Air Quality Study (FAQS) is a study to assess urban and regional air pollution, to identify the sources of pollutants and pollutant precursors, and to suggest cost-effective controls to improve air quality in the metro areas lying along Georgia's "fall line"- the line dividing the Piedmont region from the coastal plain. The FAQS episode of August 11th–20th is a serious ozone pollution episode with extremely stable weather conditions during its worst days: On 15 August a surface ridge axis extended southward towards the Gulf Coast, while the upper level ridge held firm over the Central Plains and upper Mississippi Valley; On 16 August the surface ridge and stable conditions intensified; On 17 August, subsiding and stable conditions continued.

We applied MM5/SMOKE/CMAQ (version 4.2.2) (EPA, 1999) to this FAQS episode, and found poor model performance for both ozone and NO during the night: ozone was overestimated and NO was underestimated, suggesting excessive vertical mixing. Reproducing the meteorological parameters of nocturnal stable boundary layer is difficult. A factor of 3 was estimated as the uncertainty range for the UAM-V input variable of vertical diffusivity especially at night between 7pm and 7am (Hanna et al., 2001).

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We tested the impact of the minimum vertical eddy diffusivity (Kzz) calculated from MM5, by resetting the minimum cutoff of Kzz as 0.3, 0.1, 0.03 and 0.0001 m^2/s respectively. The original default was 1.0 m^2/s in the CMAQ release.

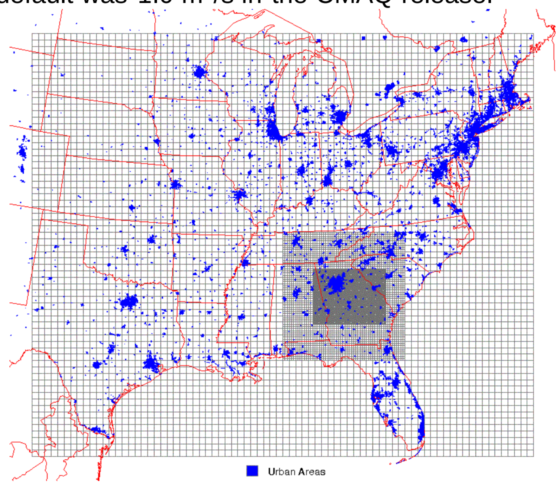

Fig. 1 FAQS modeling domain and subdomains.

Here, we discuss the:(1) Application of MM5/SMOKE/CMAQ in this FAQS episode and the evaluation methodology of CMAQ results and (2) Effects of the minimum cutoff Kzz used in CMAQ.

2. APPLICATION AND EVALUATION OFCMAQ TO THE AUGUST 11th-20th, 2000 FAQS EPISODE

2.1 Model Setup and Parameters

FAQS modeling used a triple-nested domain (Fig.1), including a 36-km resolution in the horizontal with 78x66 cells (FAQS36), a 12-km resolution with 57x60 cells (FAQS12), and a 4-km resolution with 102x78 cells (FAQS4). All of the FAQS grids have a 13 layers vertically, with 7 layers in the lowest kilometer. However, when we were generating meteorological fields, we ran MM5 with grids that are 3 cells lager on each side than the corresponding FAQS grids and with a 34 layers vertically with the top at 70mb. All of the grids use Lambert Conformal

Projection with parameters of 30°N, 60°N and 90°W. We used NCEP ETA data and ADP observational data in MM5 modeling, with one-way nesting, surface FDDA only for winds and gridded FDDA (no FDDA with finest grid), and OSU land-surface scheme and MRF physics parameterization schemes (Grell, 1994).

We applied SMOKE to generate the CMAQ-ready emissions fields for FAQS grids with the FAQS2000 inventory for Georgia (Unal et al. 2003) and NET99 inventory (EPA website) projected to 2000 by applying the projection factors obtained from EGAS 4.0 for other states, as well as hourly CEM data for large EGU point sources. The spatial surrogate parameters were developed based on 2000 census data (http://www.census.gov) of urban definitions, roads, population and housing. SAPRC99 was used in both SMOKE and CMAQ. Mobile6 was used to generate the mobile emission factors for applying the VMT inventory. We applied BEIS3 with BELD3 database to generate the biogenic emissions.

Default initial and boundary conditions from CMAQ were used for FAQS36 and then the initial and boundary conditions for FAQS12 and FAQS4 were obtained from FAQS36 or FAQS12 concentration outputs respectively.

We then applied CMAQ using SAPRC99 gas-phase mechanism to the August 11-20, 2000 episode using the FAQS grid. After the simulation with the original release of CMAQ, additional CMAQ simulations were also conducted by resetting the minimum Kzz cutoff at 4 different values: 0.3, 0.1, 0.03, and 0.0001 m^2/s respectively.

2.2 EVALUATION METHODOLOGY

Model results were evaluated using data from AIRS, PAMS, SEARCH and ASACA datasets.

For O_3, CO, SO_2, NO, NO_2 and isoprene, direct comparison was conducted; for other reactive odd nitrogen species except NO and NO_2 (e.g. NO_x, NO_y and NO_z), the modeled species were summed up to match the corresponding observation species; for nonmethane organic compounds besides isoprene and particulate matter species, the observed species were summed up correspondingly to the modeled species; for TNMOC and PMSHC, both the observations and the modeled species were developed for comparison.

Among the statistical measures used in the evaluation are Mean Bias Error (MBE), Root Mean Square Error (RMSE), Mean Normalized Bias (MNB), Mean Normalized Error (MNE), Mean Observed Concentration (MOC), Mean Error (ME), Normalized Mean Bias (NMB), Normalized Mean Error (NME), Fractional Bias (FB), Fractional Error (FE) (Odman M. T. et al., 2002), and the measures from Least Squares Fitting (Kenney and Keeping, 1962): Correlation Coefficient (r^2), Regression Coefficient (b) and the intercept (a).

The above statistical measures were calculated using corresponding pairs of observations and measurements. For each FAQS grid, the different statistical groups include overall measures or the measures for each episode day, for each monitoring site, for each hour, for each sub day period, for each landuse category of station locations and/or for each classification according to the height difference between the station elevation and the terrain height of the corresponding grid cell.

The 4 landuse categories used to do the statistical calculations are urban, forest, agriculture and other rural.

3. ANALYSIS OF THE EVALUTION RESULTS: FINDINGS

3.1 Artificial Surface Ozone Values

With simulations found high levels of ozone at night when the default ($1m^2/s$) Kzz cutoff was used. Reducing the Kzz cutoff to $0.0001m^2/s$ led to localized, aberrantly high ozone peaks during the day in a few locations (e.g. Fig.2, 3).

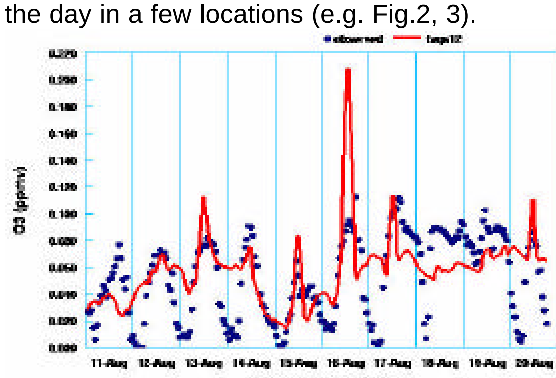

Fig.2 Time Series Plot of Simulated and Observed Surface Ozone Concentrations in Santa Rosa County, FL, using a minimum Kzz of $10^{-4}m^2/s$ in CMAQ.

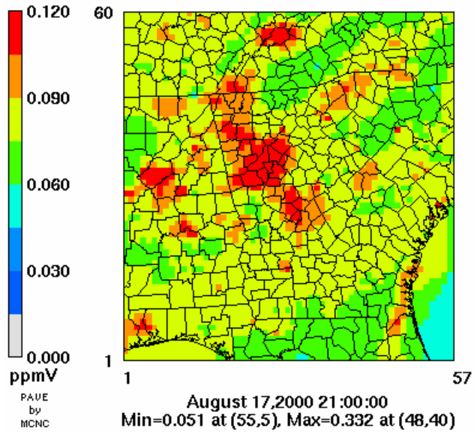

Fig.3 Late Afternoon Surface Ozone Concentrations on August 17th, 2000 in the FAQS 12-km Grid using a Minimum Kzz of $10^{-4}m^2/s$.

Further investigation indicated that all of the grid cells, having artificially high surface ozone concentrations, had a common feature in that they all had mixed landuse within the grid cell but in the mixtures water is the majority (e.g. costal grid cells and the grid cells over larger lakes). The OSU Land Surface Model of MM5 treated these grid cells entirely as water (Fig.4). Since the strong cooling effect of the water surface, much lower vertical diffusion is simulated over water during the day. On the other hand, the actual vertical diffusion would not be inhibited so much since a sizable fraction is over land. Land-based emissions (e.g. from roads and trees) are emitting into the grid cell and are simulated as being trapped very near the surface, where photochemistry rapidly produces ozone. This artificial trapping of large emissions of NOx and reactive VOCs leads to simulating very high levels of ozone during the daytime.

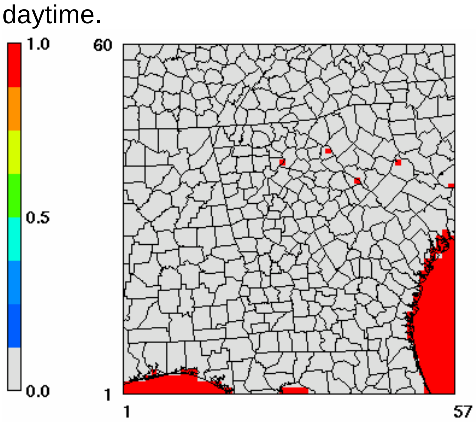

Fig.4 Gridded fractions of USGS water in the FAQS 12-km grid, re-assigned by MM5 with OSU LSM (1.0 was assigned when USGS water is the major USGS landuse inside the grid cell, if not 0.0 was assigned)

Aggregating surface meteorological parameters from the fractional landuse for each grid cell in the meteorological modeling would be one solution to this problem, which not only will solve the problem which happens in the grid cells over the mixed landuse with water, but also will improve the simulations in all other grid cells which is over any mixed landuse. An alternate solution is smoothing the Kzz in CMAQ for those grid cells over the mixed landuse with water by averaging the Kzz of this grid cell with its surrounding grid cells by assuming that the averaged vertical eddy diffusivity from the adjacent grid cells would be closer to the reality than the one derived from taking the whole grid cell as over purely water.

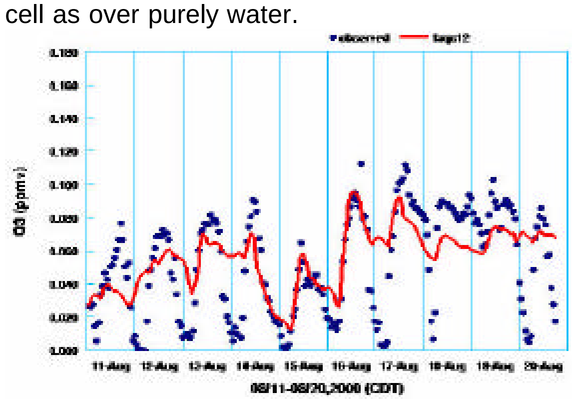

Fig.5 Time Series Plot of Simulated and Observed Surface Ozone Concentrations at AIRS station 121130014 in Santa Rosa County, FL, A Minimum Kzz of $10^{-4}m^2/s$ and a 9-point averaging method were used in CMAQ.

A 9-point averaging method was used in CMAQ to re-calculate the Kzz for the grid cells over the mixed landuse with water. After re-running CMAQ, the aberrantly high surface ozone spikes dissapeared(Fig. 5). After these modifications, the simulated ozone concentrations matched very well with the observed concentrations during the day time.

3.2 Emissions Under- or Overestimation

Since OH has little impact on nighttime chemistry (Sillman, 2002), CO and isoprene can be treated as conservative species during the night time. Considering of the stable conditions during this episode, vertical diffusivity is the major process reducing CO and isoprene concentrations during night time. CO emissions are significant from 7pm through 12pm, while isoprene emissions are small during night. CO was underestimated by CMAQ independent of Kzz minimum (Tab.1), which suggests that the CO emissions inventory was systematically underestimated. It can also seen (Table1) that isoprene concentrations are overestimated during the 7pm through 12pm period, which suggests that isoprene emissions are probably overestimated. The higher bias of isoprene concentrations at the locations on other rural comparing to other landuse strongly suggests an overestimation of isoprene in rural areas (Table 2).

Table 1 NMB during the period of 7pm through 12pm

MinKzz	1.0	0.3	0.1	0.03	0.0001
CO	-43.44	-30.97	-20.75	-16.59	-15.25
ISOP	180.03	282.56	365.61	389.12	392.67

Table 2 NMB of isoprene at different locations

MinKzz	1.0	0.3	0.1	0.03	0.0001
Urban	54.83	90.92	177.94	156.76	170.44
Forest	48.16	77.11	170.95	110.88	112.53
OtherR	143.05	202.37	326.10	280.11	287.23

3.3 Optimal Kzz Cutoff

Since the possible overestimation of isoprene emissions and the underestimation of CO emissions, it is difficult to determine an optimal Kzz cutoff. However one can find that the changes of overall NMB along the changing of Kzz cutoff are different between the species including ozone and NO (Table 3), the most chemistry active species at nighttime. Considering the over- and underestimation of some species emissions, it appears that an optimal Kzz cutoff might lie between 1.0 and 0.1 m^2/s for this episode.

Table 3 Overall NMB of different species (no cutoff)

MinKzz	1.0	0.3	0.1	0.03	0.0001
O_3	31.81	21.34	15.28	13.23	12.74
NO	-59.02	-18.50	32.56	62.54	75.30
NO_x	-11.50	16.38	42.93	56.83	62.50
TNMOC	36.33	67.63	95.88	109.08	113.33
CO	-46.18	-36.23	-26.63	-21.57	-19.39
ISOP	71.07	108.87	145.21	162.03	168.53

4. CONCLUSIONS

We applied MM5/SMOKE/CMAQ to FAQS episode of August 11^{th}-20^{th}, 2000, and tested by resetting the Kzz minimum in CMAQ.

Artificially high surface ozone values were found resulting from the OSU land surface model applied in MM5. A method of using 9-point averaging was proposed to fix this problem. A consistent bias between simulated and observed CO suggests that there is an underestimate in CO emissions. On the contrary, isoprene might be overestimated in rural locations. Analysis suggests also that an optimal Kzz cutoff may lie between 0.1 and 1.0 m^2/s.

5. ACKNOWLEDGEMENTS

We would like to thank Georgia Environmental Protection Division for the financial support.

6. REFERENCES

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