Models-3's Application in FAQS Project: Impact of Urban Definition's Change on Model Results

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We have applied MM5/SMOKE/CMAQ to an ozone episode in Georgia's metro areas. Model results are generally in good agreement with AIRS measurements. We have further investigated how urban definitions that are used in allocating emissions impact simulated chemical concentrations. Results show the importance of the accuracy of urban definitions in air quality modeling.

1. INTRODUCTION

Three metropolitan areas in Georgia other than Atlanta: Augusta, Columbus, and Macon, may also be experiencing poor air quality. Many endeavors (OTAG, SOS, SCISSAP) have been used to investigate the air pollution in Atlanta metro area, which has failed to attain air quality standards since 1979, and a better understanding of the problem has been obtained. However no studies addressed the three metro areas before 1999 and the information needed to improve air quality in these areas is seriously lacking. In 2000, Georgia EPD launched a study to assess urban and regional air pollution, to identify the sources of pollutants and pollutant precursors, and to recommend solutions to the poor air quality in the three metro areas. As the three cities lie along Georgia's "fall line"- the line dividing the Piedmont region from the coastal plain- this study is called the Fall line Air Quality Study (FAQS). FAQS includes enhanced monitoring, emission inventory development, air quality modeling and control strategy recommendation.

In the past, several modeling studies have been conducted in Georgia by using the CIT model (Mendoza-Dominguez 2000) or UAM (Chang 1997), however all of these studies focused on the Atlanta area.

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We defined a new set of grids for FAQS (Fig. 1) that focuses on the three cities as well as the Atlanta metro area. We selected the ozone episode of August 11-20, 2000 as the first FAQS modeling scenario based on comprehensive analysis of the first FAQS field study. We applied MM5/SMOKE/CMAQ (EPA, 1999) to this base case simulation in an attempt to validate the models and to improve the models' performance.

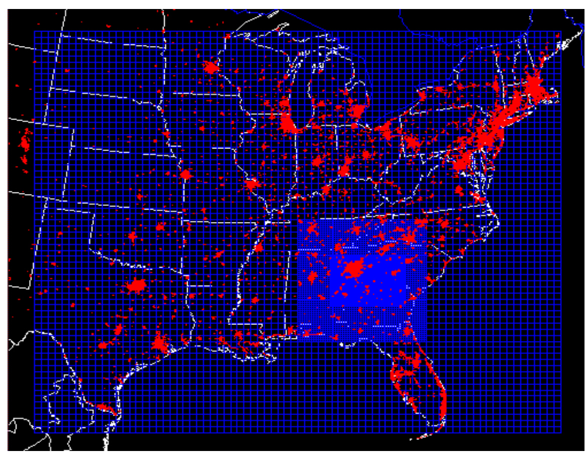

Fig. 1 FAQS modeling domain the three grids

In this abstract we report:(1) First application of MM5/SMOKE/CMAQ in the three metro areas with model performance evaluation; (2) Further Investigation of urban area definition's impact on the model results by three simulations with different spatial allocation of emissions; (3) Finally, the conclusions.

2. FIRST APPLICATION OF MODELS-3 IN GEORGIA'S THREE METRO AREAS

2.1 Model Setup and Parameters

The three grids in the FAQS domain (Fig.1) are FAQSD1, which has a 36-km resolution in the horizontal with 78x66 cells, FAQSD2, which has a 12-km resolution with 78x66 cells, and

FAQSD3, which has a 4-km resolution with 102x78 cells. All of the FAQS grids have a 22 layers vertical structure with 10 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 vertical structure with the top at 70mb. All of the grids are in 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 domains with the Southern Appalachian Mountains Initiative inventory for 1995 (Pechan, 2002) projected to 2000 by applying the projection factors obtained from EGAS 3.0 and EGAS 4.0. The spatial surrogates parameters were obtained from OTAG's area spatial surrogates datasets (MCNC website) and USGS's urban area and major highways GIS database (USGS website). SAPRC99 was used in SMOKE to split pollutant species. Mobile5b was used to generate the mobile emission factors for applying the VMT inventory. We applied BEIS3 with BELD3 database to generate the biogenic emissions. Since the spatial surrogates were lacking in some part area of FAQSD1, we only generated emissions fields in FAQSD2 and FAQSD3.

Default initial and boundary conditions from CMAQ were used for FAQSD2 and then the initial and boundary conditions for FAQSD3 were obtained from FAQSD2's concentration outputs.

We then applied CMAQ with SAPRC99 gas-phase mechanism to the August 11-20, 2000 ozone episode in FAQSD2 and FAQSD3.

2.2 Model Performance

We applied two methods examine the surface meteorological fields especially of the wind speed and wind direction at 10 meters height, and air temperature and humidity at 2 meters height. It is difficult to evaluate the model performance if FDDA is used in the meteorological simulation and no observational data left for comparison. However, any comparison with observations, even if they have been used in FDDA can still ensure that the air quality modeling inputs of meteorological parameters are in agreement with the reality. We compared the FAQSD1 surface meteorological fields at 3-hour intervals, cell-by-cell, with gridded observed meteorological fields interpolated from 3-hourly NCEP ETA surface analysis data and corrected by NWS surface observational data. The statistical performance measures used here are the mean bias error (MBE) and the root mean square error (RMSE) between simulations and observations. The calculated MBEs and RMSEs are 1.28°F and 4.05°F respectively for the surface temperature, -0.66 g/kg and 1.93g/kg for the surface mixing ratio, -0.18 m/s and 1.47 m/s for the surface wind speed and -1.01° and 39.42° for the surface wind direction. We then compared the hourly meteorological variables in the corresponding grid cell in FAQSD2 with the hourly surface observational data at NWS stations. All the 21 NWS stations located in FAQSD2 and reported during the episode are used in the comparison. The calculated correlation coefficients of simulations and measurements at all stations are 0.816 for surface air temperature (Fig.2), 0.642 for surface relative humidity, 0.002 for surface wind speed and 0.631 for surface wind direction respectively.

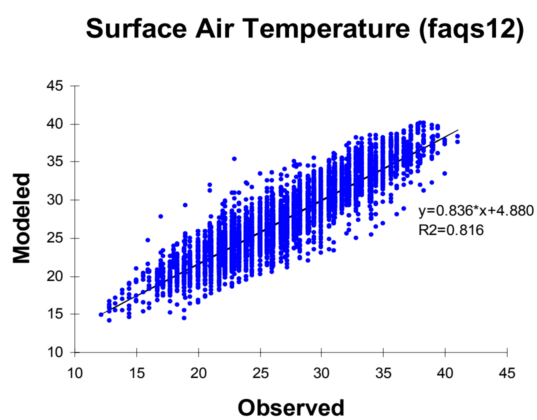

Fig. 2 Surface air temperature comparison at the NWS stations in FAQSD2

We compared the hourly CMAQ ozone simulation values in corresponding FAQS cells with the hourly measurements at AIRS ozone monitoring sites. We used ozone data during the episode for all 21 AIRS ozone sites in both Georgia and FAQSD2, 18 of them located in FAQSD3. The calculated MBEs and RMSEs are 2.24 ppb and 28.14 ppb for FAQSD2 and 4.35 ppb and 29.27 ppb for FAQSD3 respectively.

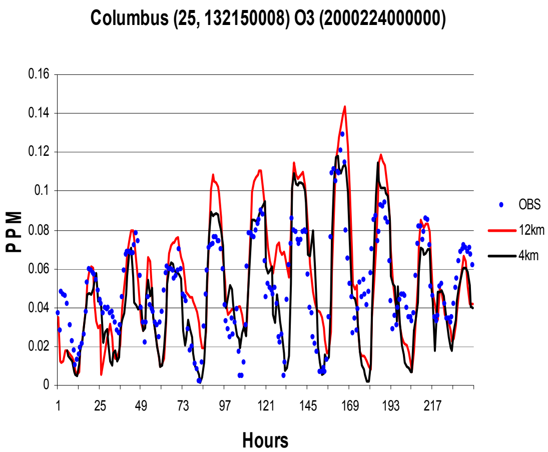

Fig.3 Ozone simulations and measurements in time series at site number 25 at Columbus

Figure 3 shows a good agreement between the time series of ozone simulations and measurements at site number 25. At this site, the MBEs and RMSEs are respectively 3.40 ppb and 22.03 ppb for FAQSD2 and 3.27 ppb and 18.40 ppb for FAQSD3. At this site, results of the finer resolution grid are slightly better.

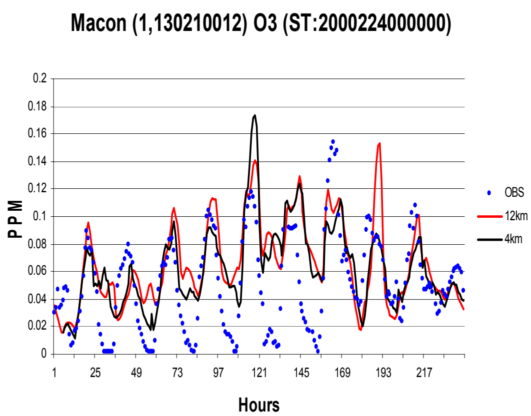

Fig.4 Ozone simulations and measurements in time series at the site number 1 at Macon

At a few sites, there is disagreement between the simulations and observations: the simulated ozone values are much higher than the measurements especially at night (Fig. 4). Most probably, the NOx emissions in those grid cells have been underestimated.

Note that the simulated ozone values for FAQSD3 are not in better agreement with the observations than the FAQSD2 results are although FAQSD3 has a much finer spatial resolution.

3. INVESTIGATION OF THE IMPACT OF URBAN DEFINITION'S CHANGE ON THE MODEL RESULTS

3.1 Methodology

The three cities and Atlanta are located in a fast developing region: the land use in this region changed significantly during the past decade. The accuracy of the spatial allocation of emissions could impact much on the air quality simulation results in this area.

We developed three different spatial surrogate data sets and applied each one of them to the emissions allocation in SMOKE. We collected EPA spatial surrogate datasets (EPA website) that is based on 1990 census urban definitions but revised by EPA (described as D1990). We developed a new spatial surrogate dataset which based on D1990 but integrated with 2000 census data (Tiger/Line website) of urban definitions, roads, population and housing (D2000). We collected the OTAG spatial surrogate datasets and developed the third datasets by integrating the USGS urban area definitions and major highways GIS database (DUSGS, which has been used in the first simulation). Figure 5 shows the difference between these three datasets in urban area definitions in Georgia's metro areas. A new set of temporal profiles (EPA website) was used in the SMOKE modeling.

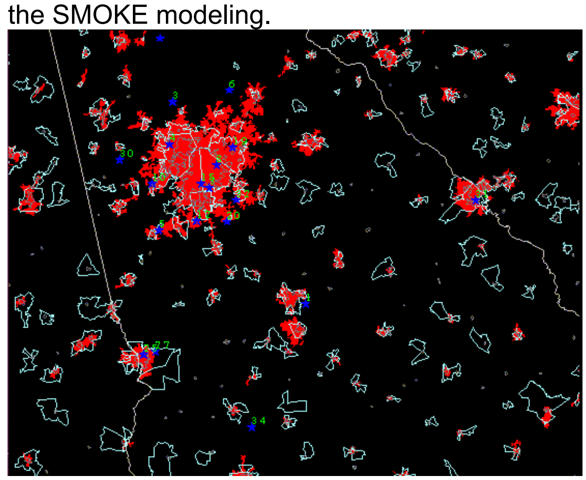

Fig.5 Urban definitions of D2000 in red shadow, D1990 in light blue line and DUSGS in gray line, and ozone monitoring sites as blue star

We then applied CMAQ to the same ozone episode in FAQSD2 (the grid with 12-km resolution) with these three different emissions but with the same meteorological fields and other conditions. For efficiency, we redesigned the FAQS grids vertical structure as 13 layers with 7 layers in the lowest kilometer.

3.2 Analysis of Results

We applied the same measures used above for the verification of CMAQ results. The same ozone measurements at the 21 AIRS sites were used in the comparison. The MBEs and RMSEs between simulations and measurements at all sites within FAQSD2 are respectively 1.80ppb and 23.97ppb for the case of D2000, 1.14ppb and 23.99 ppb for the case of D1990 and 1.27 ppb and 23.93 ppb for the case of DUSGS. These statistical results show no improvement by applying the more accurate urban definitions to air quality modeling in the Georgia metro areas.

Further analysis showed that the reason for no improvement in ozone simulations is that there is very little difference in urban/rural definitions of the FAQSD2 cells the observation sites located among the three data sets. Almost all of the FAQSD2 cells the AIRS sites in Georgia located kept the similar urban/rural definitions in the three different data sets, except only one, Site-number 4 which is located northwest of the Atlanta metro area. Obvious improvements in ozone simulations at night at this site are shown in Fig. 6: The results of D2000 and of D1990 are much better than of DUSGS and the results of D2000 are a little better than of D1990.

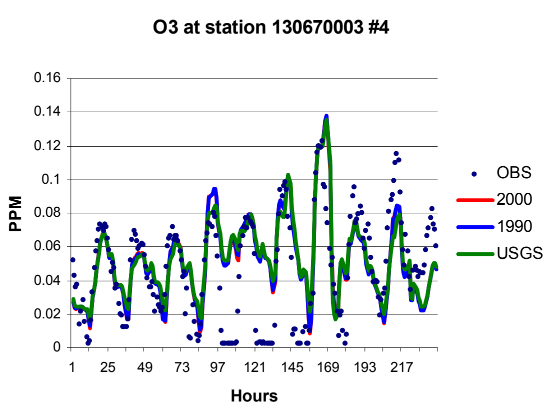

Fig.6 Ozone simulations of three cases with measurements in time series at site number 4

4. CONCLUSIONS

We applied Models-3 to an ozone episode in Georgia metro areas and obtained good agreement between the simulations and observations.

We also pointed out the disagreements in results. The lack of improvement in simulation with finer spatial resolution may be due to the inaccurate spatial surrogates used in emissions allocation. The underestimation of NOx emission may be introduced by insufficient spatial resolution and/or inaccurate spatial allocation of surrogates even if the total emission has been estimated accurately.

We tried to explain the disagreements by applying three different spatial surrogate data sets to air quality modeling in FAQSD2 (the grid with 12-km resolution). We believe that using more accurate urban definitions in air quality modeling will result in better model results. Unfortunately, we were not able to prove this with the 12-km resolution grid and the limited number of data sites that are available. We expect that when we use 4-km grid resolution the difference between the spatial surrogate data sets will become more obvious. An extended conclusion is that when the future year's air quality is predicted the change in land use should be considered in the spatial allocation of emissions.

Future work will examine spatial resolution and other factors as possible cause for the disagreements.

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