APPLICATION OF CMAQ FOR REGIONAL HAZE SIP MODELING IN MANE-VU

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1. INTRODUCTION

In 1999 the U.S. Environmental Protection Agency (USEPA) issued final Regional Haze rule that requires states to develop and implement plans to reduce haze and to improve visibility in 156 mandatory Class I Federal areas (national parks and wilderness areas). Because haze condition is caused by air pollutants (particulate matters and precursors) from numerous emission sources over broad geographic areas, EPA had established five regional planning organizations to work coordinately to address visibility impairment issue from regional perspective. The RPO for Mid-Atlantic and Northeastern region is the Mid-Atlantic/Northeast Visibility Union (MANE-VU). Geographically it includes Connecticut, Delaware, the District of Columbia, Maine, Maryland, Massachusetts, New Hampshire, New Jersey, New York, Pennsylvania, Rhode Island, Vermont, and Northern Virginia. There are seven Class I areas within MANE-VU region, Acadia National Park, Moosehorn Wilderness Area, and Roosevelt Campobello International Park in ME; Brigantine Wilderness Area in NJ; Great Gulf Wilderness Area, and Presidential Range – Dry River Wilderness Area in NH; and Lye Brook Wilderness Area in VT. Across Eastern US man-made fine particle pollution leads substantial visibility impairment which reduces average visual range down to about one-third the visual range of typical natural condition (NESCAUM, 2001). Throughout the region Sulfate is identified as the dominant contributor to haze forming fine particulate matter (PM2.5) in the atmosphere, while organic carbon is found to be the 2nd most important contributor. Sulfate alone accounts for 40%~70% of total PM2.5 mass year round, and 70%~82% of estimated particle-induced light extinction at MANE-VU Class I areas. Hence, visibility impairment is most severe in the southern and western portions of MANE-VU region that are closest to large power plant sources of sulfur dioxide (SO_2) emissions located in the Ohio River and Tennessee Valleys (NESCAUM, 2002). In Eastern US summertime visibility is driven by the regional sulfate, while wintertime visibility depends on a combination of regional and local influences coupled with local meteorological conditions (inversions) that can lead to the concentrated build-up of emissions from local sources (NESCAUM, 2006). Such characters suggest the most effective emission management approach for MANE-VU to achieve visibility improvement is to rely on broad-based regional SO_2 control efforts combined with local source SO_2 and OC reduction, as well as reducing ambient NO_x level.

To meet visibility improvement objectives in Class I areas subject to Regional Haze rule, MANE-VU has adopted a weight of evidence approach relying on several independent methods including Community Multiscale Air Quality (CMAQ) modeling to assess contribution of haze-causing emission sources and regions and to demonstrate reasonable progress toward natural conditions for Regional Haze State Implementation Plans (SIPs). As a key role on addressing MANE-VU Regional Haze issues, the Northeast States for Coordinated Air Use Management (NESCAUM) has been working cooperatively with the Mid-Atlantic Regional Air Management Association (MARAMA) and the Ozone Transport Commission (OTC), as well as State Agencies and University partners (NJDEP/Rutgers, NYDEC, UMD, and VADEQ), using CMAQ system for annual simulations of 2002 base case year, 2009, and 2018 future year driven by the Fifth-Generation Pennsylvania State University /National Center for Atmospheric Research (NCAR) Mesoscale Model (MM5) generated meteorological fields and the Sparse Matrix Operaor Kernel Emissions (SMOKE) modeling system processed emission inputs. This paper will describe in detail the modeling methodology; demonstrate CMAQ performance on PM2.5 species and visibility; assess projected visibility improvement for future years; and discuss impacts of proposed control strategies.

2. METHODS

MANE-VU has adopted the Inter-RPO domain description for its modeling runs. This 36-km domain covers the continental United States, southern Canada and northern Mexico. The dimensions of this domain are 149 and 129 grids for MM5 and 145 and 102 grids for CMAQ in the east-west and north-south directions, respectively. A 12-km inner domain was selected to better characterize air quality in MANE-VU and surrounding RPO regions. This domain covers the Northeast region including northeastern, central and southeastern US as well as Southeastern Canada. It extends from 66°W~94°W in longitude and 29°N~50°N in latitude with 175X175 grid cells for MM5 and 172X172 grid cells for CMAQ (Figure 1). Vertically there are 29 MM5 layers and 22 CMAQ layers from the ground surface up to ~50hPa (Figure 2). CMAQ domain has 10 layers below 850hPa (including 1 layer below 10m) to resolve boundary layer processes, 6 layers in between 850hPa and 500hPa, and 3 layers in between 500hPa and 300hPa. The domain has a finer vertical resolution within the troposphere so that it can capture complex atmospheric circulations between the east coast of the US and the northern Atlantic Ocean in the boundary layer, the free and upper troposphere, and potentially cross-tropopause transport. MANE-VU SIP modeling scenarios include annual simulation for 2002 base year on 36km domain, 2002 base year on 12km domain, 2009 future year on 12km domain (base case and control case), and 2018 future year on 12km domain control case. Future year 2009 and 2018 simulations both use 2002 12km meteorological field.

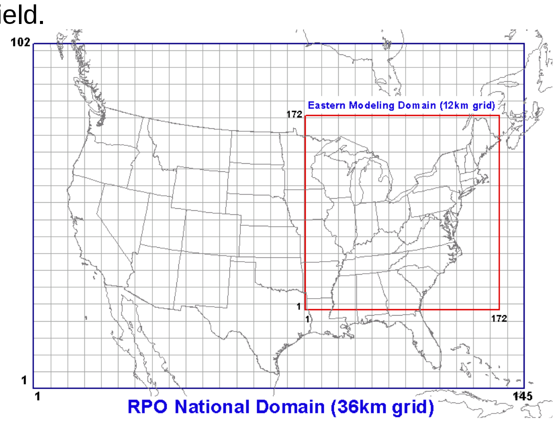

Figure 1. Modeling domains used in MANE-VU air quality modeling studies with CMAQ. Outer (blue) domain grid is 36 km and inner (red) domain is 12 km grid

Meteorological inputs for CMAQ are derived from MM5 meteorological fields generated by UMD. A modified Blackadar boundary layer scheme is used as well as physics options including explicit representations of cloud physics with simple ice microphysics (no mixed-phase processes) and the Kain-

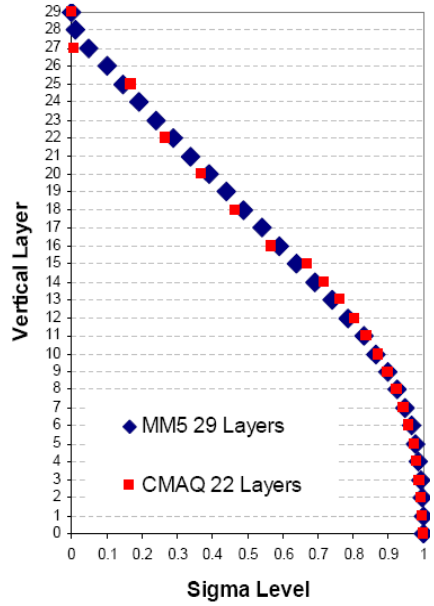

Figure 2. Vertical structure of modeling domain

Fritsch cumulus parameterization. MM5 results have been evaluated using ENVIRON's METSTAT program with observations from CASTNET and TDL networks. Model results of surface wind speed, wind direction, temperature, and humidity are paired with measurements by hour and by location and then compared statistically. Overall acceptable small bias, high index of agreement and strong correlation between MM5 perditions and CASTNET and TDL data are observed. Since MM5 uses TDL data for nudging, the model predictions are in better agreement with TDL data than with CASTNET data. MM5 performs better in Midwest and Northeast than Southeastern US (He et al., 2006). MANE-VU has made its best effort to apply most update emission inventory. To date MANE-VU SIP modeling base year 2002 emission includes MANE-VU 2002 Inventory Version 3, CEM data, MWRPO Inventory Base K, VISTAS Inventory Base G, Canada 2002 Inventory for point source and 2000 Inventory for all other sources, and Mexico 1999 Inventory. Biogenic emissions are calculated using BEIS3 with BELD3 data. Mobile source emissions are processed using MOBILE6. All emissions processing for the 2002 base case 36 km and 12 km simulations were performed by NYDEC using SMOKE2.1 compiled on a Red Hat 9.0 Linux operating system with the Portland group Fortran compiler version 5.1. The emissions processing was performed on a month-by-month and RPO-by-RPO basis. Future year 2009 emission is processed by NYDEC and VADEQ including OTB/OTW/CAIR strategies and beyond. Future year 2018 emission is processed by NESCAUM following NYDEC's 2009 emission approach. Emission scenarios include OTB/OTW/CAIR strategies plus several regional haze control strategies (e.g. BART, low sulfur fuel in region, ICI Boiler control programs). NYDEC has completed annual 2002 CMAQ modeling on the 36km domain to provide dynamic boundary condition for all simulations performed on the 12km domain. Three-hourly boundary conditions for the outer domain were derived from an annual model run performed by researchers at Harvard University using the GEOS-CHEM global chemistry transport model (Park et al., 2004). MANE-VU SIP modeling on 12km domain uses CMAQ V4.5 with IOAPI V3.0 and NETCDF V3.5 libraries. The CMAQ model is configured with the Carbon Bond IV mechanism (Gery et al., 1989) using the EBI solver for gas phase chemistry rather than the SAPRC-99 mechanism due to better computing efficiency with no significant model performance differences for Ozone and PM as compared to observations.

3. RESULTS

CMAQ performance for PM2.5 species and visibility is examined based on CMAQ 2002 annual simulation on the 12km resolution domain. Measurements from IMPROVE and STN networks are used to pair with model predictions by location and by time and by specie for evaluation. Only Sulfate results are shown here as example. Figure 3 (a) presents the domain wide paired comparison of PM2.5 Sulfate daily average concentration between CMAQ prediction and two sets of observations (STN & IMPROVE). It shows that predicted PM2.5 Sulfate and measured Sulfate are in a good 1:1 linear relationship with r^2 varying from 0.6 to 0.7. CMAQ also agree well with measured PM2.5 total mass because of good agreement of the dominant Sulfate specie. Other PM2.5 species Nitrate, OC, EC, and Fine Soil are also evaluated. MANE-VU CMAQ performance on PM2.5 species is consistent with other RPOs' SIP modeling results. CMAQ prediction is found to has stronger correlations on north region of the domain than do the south region. Correlation coefficients within MANE-VU region are highest (~0.9 in average) compared to other RPO regions. Correlation coefficients are also higher in summer time than annual values. This indicates that CMAQ performs better for summer than for other seasons. Statistical analysis is conducted on MANE-VU CMAQ prediction following Boylan's suggestion (2005) on model PM performance goal and criteria. Mean Fractional Error (MFE) and Mean Fractional Bias (MFB) of Sulfate are shown in Figure 3 (b) and 3 (C), respectively. CMAQ performs well on both parameters standard.

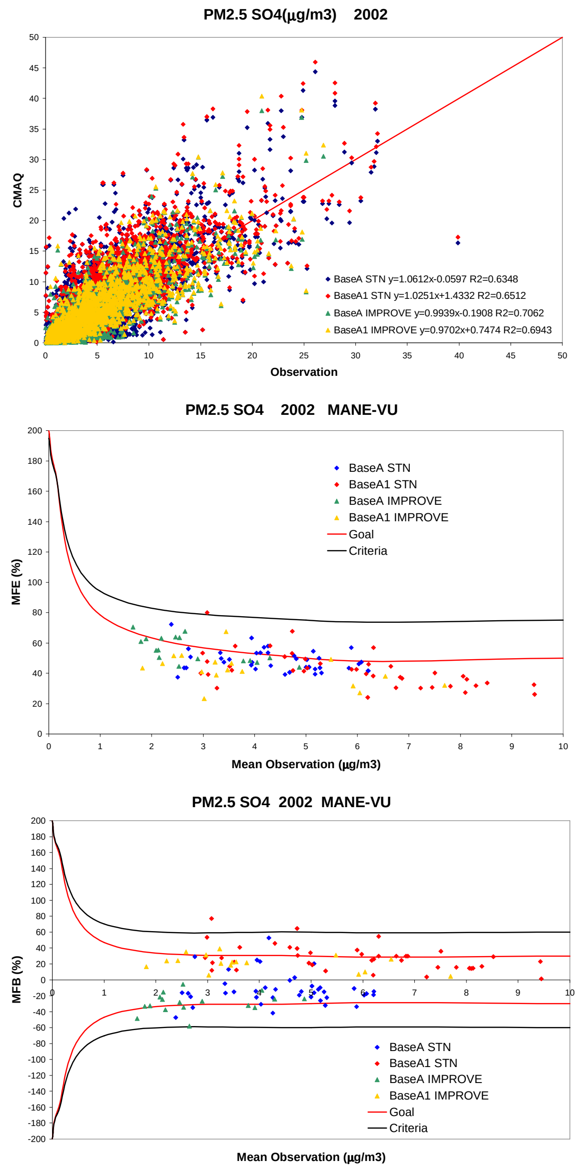

Figure 3. Paired comparison of Sulfate between CMAQ prediction and IMPROVE measurement. (a TOP) Domain wide daily average; (b MIDDLE) Mean Fractional Error; (c BOTTOM) Mean Fractional Bias

Figure 4 shows the paired comparison of domain wide daily aerosol extinction coefficient for 2002 between prediction and measurement with 1:1 line and ±20% lines. The modeled Bext shows a near 1:1 linear relationship (slope of 0.74 and r^2 of 0.53) with IMPROVE observed Bext. Mean bias is -6.31 Mm^{-1}, which is less than 1% compared to mean Bext of either observation (76.54 Mm-1) or prediction (70.22 Mm-1). MFE of 35% and MFB of -13% both meet the standard goal. CMAQ prediction of the aerosol extinction coefficient agrees well with IMPROVE observation because CMAQ performs well on sulfate, which dominates aerosol extinction.

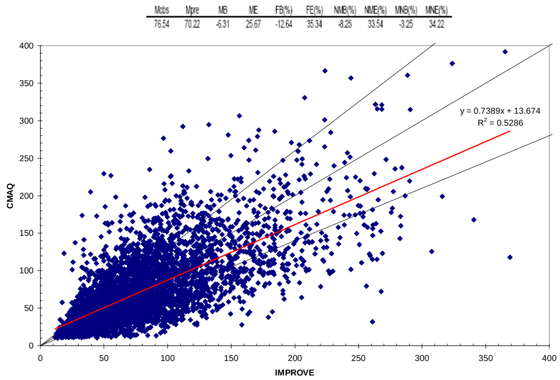

Figure 4. Paired comparison of extinction coefficient between CMAQ prediction and IMPROVE measurement

The results from annual simulations of the 2002 base case, 2009 and 2018 future case scenarios provide insight into the current and expected ambient levels of fine particles and haze causing constituents. Figure 5 shows the dominant PM2.5 specie Sulfate reduction of 2018 to 2002. The model results predict the greatest percentage sulfate reduction (~45%) to occur in West Virginia and its immediate surrounds, with minor reductions calculated for areas west of the Mississippi River and moderate declines (~20%) in the more northeastern section of MANE-VU.

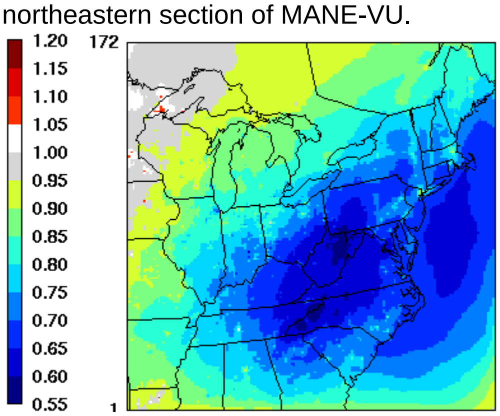

Figure 5. Average Sulfate reduction of 2018 to 2002

For regional haze purposes, site specific relative reduction factors were generated for the 20% best and worst days following USEPA Guidance. Relative reduction factors at 20% worst days for all haze relevant PM constituents at seven Class 1 sites are presented in Table 1. For each site and specie, the modeled change relative to the base year 2002 is shown. Therefore, negative values imply a modeled decrease while a positive value represents an increase. The values for 2009 and 2018 are additive. The sum of 2009 and 2018 values corresponds to the overall change from the base year to 2018. For example, Lye Brook shows a 28% decrease in Sulfate concentrations from 2002 to 2009, followed by another 10% decline (relative to 2002) between 2009 and 2018, yielding a total reduction of 38% between 2002 and 2018. For fine soil, levels increase 17% by 2009, then decline by 4% by 2018. The net change between 2002 and 2018 indicates an overall rise in fine soil concentrations of 13 percent. The model shows no evidence of nitrate replacement at these sites between the period of 2002 and 2018, despite the substantial reductions in predicted ambient sulfate levels.

Table 1. Relative Reduction factors at 20% worst days by site and specie

	YEAR	Sulfate	Nitrate	Organic Carbon	Elemental Carbon	Fine Soil	Coarse
Acadia	2009	-31%	0%	-7%	-19%	5%	6%
	2018	-7%	-5%	-6%	-17%	-1%	8%
Brigantine	2009	-29%	-1%	-8%	-23%	13%	11%
	2018	-10%	-11%	-9%	-20%	-2%	6%
Great Gulf	2009	-24%	-3%	-5%	-15%	16%	15%
	2018	-9%	-2%	-8%	-16%	-4%	7%
Lye Brook	2009	-28%	4%	0%	-16%	17%	10%
	2018	-10%	-3%	-8%	-19%	-4%	5%
Moosehorn	2009	-27%	-2%	-3%	-13%	9%	6%
	2018	-6%	-4%	-5%	-14%	-1%	6%
Dolly Sods	2009	-33%	-15%	4%	-10%	29%	34%
	2018	-16%	-11%	-11%	-22%	0%	11%
Shenandoah	2009	-29%	-24%	2%	-13%	23%	15%
	2018	-14%	-17%	-16%	-29%	-2%	8%

The results for modeled sulfate in Figure 6 show the application of the reduction factors from Table 1 to the baseline measured ammonium sulfate on the 20% worst days. The blue bar indicates the five-year average sulfate levels on the worst days for each site. Using the reduction factors for 2009 yields sulfate concentrations shown at the red bar, while applying the 2018 factor predicts mass values given by the green bar. These bars clearly indicate that more substantial reductions in sulfate levels are expected to occur by 2009 with smaller reduction in the latter modeled timeframe. CMAQ results presented in Figure 7 (a) and (b) show the modeled progress combining all six species' reduction factors. Based on the modeling, all sites except one are shown to meet their uniform progress goal by 2018. Brigantine Wilderness Area in New Jersey is projected to fall about a half deciview shy of the uniform rate under existing emission reduction plans.

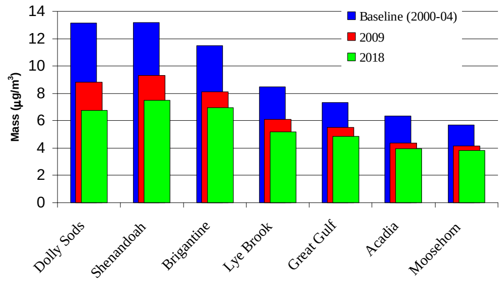

Figure 6. Sulfate mass predicted reduction for 20% worst days

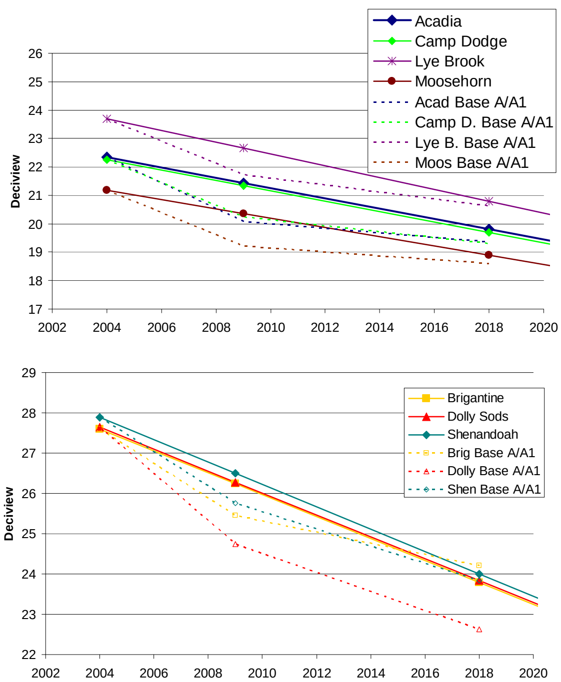

Figure 7. CMAQ Integrated SIP Modeling Platform simulation results for 2002, 2009 and 2018 relative to Uniform Progress Goals calculated according to current USEPA Guidance for (a TOP) Northeast Class I sites in MANE-VU and (b BOTTOM) Mid-Atlantic Class I sites in or near MANE-VU.

4. SUMMARY

MANE-VU has made significant technical effort to fulfill the requirements of the Regional Haze Rule by focusing on developing multiple analysis tools for assessing contributions to fine particle pollution and demonstrating reasonable progress reducing visibility impairment at Class I areas in the eastern United States. MANE-VU has adopted CMAQ modeling system to simulate base year 2002, and future year 2009 and 2018 with validated MM5 meteorological field and most update emission inventory. For the base year 2002 CMAQ accurately characterized sulfate, PM2.5, aerosol extinction coefficient and the Haze Index. It showed reasonable performance for PM2.5 Nitrate, OC, and EC. MANE-VU CMAQ performance on PM2.5 species is in consistent with other RPO's Regional Haze modeling results. The model performed better for summertime than for wintertime, and better in the MANE-VU region than in others regions. CMAQ predictions demonstrated that under current emission control plans all MANE-VU Class I areas would meet uniform progress goal by 2009 with significant margin, while all areas except Brigantine, NJ would meet uniform progress goal by 2018. Additional control strategy would have to be explored for MANE-VU to achieve visibility goal at Brigantine by 2018 and beyond. Beside primary CMAQ modeling analysis, NESCAUM also integrated other modeling techniques (such as REMSAD Sulfate Tagging, CALPUFF) as weight of evidence approach to help better identifying sulfate contribution by state and by source category. This would also overcome large uncertainties that might otherwise undermine confidence in the results obtained using any one modeling or analysis technique in isolation.

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REFERENCE

Boylan, J., and K. Baker. Photochemical Model Performance and Consistency. National RPO Modleing Meeting, Denver, CO. May 26, 2004.

Gery M.W., G.Z. Whitten, J.P. Killus, and M.C. Dodge. A photochemical kinetics mechanism for urban and regional scale computer modeling. J. Geophys. Res. 94, 12,925-12956, 1989.

He, S., E. Savelli, J.H. Woo, J. Graham, and G. Kleiman. Chemical Transport Model Results for Sulfate Source Attribution Studies in the Northeast US, Contributions to Regional Haze in the Northeast and Mid-Atlantic United States, Appendix C, Northeast States for Coordinated Air Use Management, Boston, MA May, 2006.

NESCAUM, Regional Haze and Visibility Impairment in the Northeast and Mid-Atlantic United States, Northeast States for Coordinated Air Use Management, Boston, MA, January, 2001.

NESCAUM, Updated Visibility Statistics for the MANE-VU Region Technical Memorandum #1, Northeast States for Coordinated Air Use Management, Boston, MA February, 2002.

NESCAUM, Contributions to Regional Haze in the Northeast and Mid-Atlantic United States, Northeast States for Coordinated Air Use Management, Boston, MA May, 2006.

Park, R. J., D. J. Jacob, B. D. Field, R. M. Yantosca, and M. Chin, Natural and transboundary pollution influences on sulfate-nitrate-ammonium aerosols in the Unite States: implications for policy , J. Geophys. Res., D15204, 10.1029/2003JD004473, 2004.