A PRELIMINARY EVALUATION OF MODELS-3 CMAQ

Using particulate matter data from the IMPROVE Network

Brian K. Eder, Michelle R. Mebust and Sharon K. LeDuc*

1. INTRODUCTION

The Clean Air Act and its Amendments require the United States Environmental Protection Agency (EPA) to establish National Ambient Air Quality Standards for Particulate Matter (PM) and to assess current and future air quality regulations designed to protect human health and welfare. Air quality models, such as EPA's Models-3 Community Multiscale Air Quality model (CMAQ) [*Byun and Ching*, 1999], provide one of the most reliable tools for performing such assessments. CMAQ simulates air concentrations and deposition of various pollutants including PM. These simulations, which can be conducted on a myriad of spatial and temporal scales, support both regulatory assessment as well as scientific studies by research institutions. Within CMAQ is an aerosol component, or module, designed to simulate the complex processes involving PM, which is commonly separated into $PM_{2.5}$ (particles with aerodynamic diameters ≤ 2.5 μm) and PM_{10} (aerodynamic diameters ≤ 10 μm).

In order to determine its value to the air quality regulatory communities, CMAQ needs to be evaluated using observational data. One such evaluation, which compared visibility parameters derived from CMAQ to visibility parameters obtained from National Weather Service observations, revealed that CMAQ was able to replicate general spatial and temporal patterns [*Eder et al.*, 2000]. The current evaluation compares PM simulated by CMAQ with PM data collected by the Interagency Monitoring of PROtected Visual Environments (IMPROVE) network.

---

* Brian K. Eder**, Michelle R. Mebust, Sharon K. LeDuc** NERL, U.S. Environmental Protection Agency, RTP NC, 27711,USA. ** On assignment from Air Resources Laboratory, National Oceanic and Atmospheric Administration, RTP, NC, 27711,USA

2. CMAQ

2.1. General description

CMAQ, which is an Eulerian model, simulates the atmospheric and land processes affecting the transport, transformation and deposition of air pollutants and their precursors [*Byun and Ching*, 1999]. CMAQ follows first principles and employs a "one atmosphere" philosophy that tackles the complex interactions among multiple atmospheric pollutants and between regional and urban scales. Pollutants considered within CMAQ include tropospheric ozone, PM, airborne toxics, and acidic and nutrient species. The model also calculates visibility parameters.

2.2. CMAQ aerosol component description

The aerosol component within CMAQ, described in *Binkowski* [1999], was derived from the Regional Particulate Model (RPM) [*Binkowski and Shankar*, 1995], itself an extension of the Regional Acid Deposition Model (RADM) [*Chang et al.*, 1990]. Particle size distributions are represented as the superposition of three lognormal modes. $PM_{2.5}$ particles (also called fine particles) are represented by two modes, the Aitken and accumulation modes, each having variable standard deviations. Aitken mode particles are those with diameters smaller than about 0.1μm. Accumulation mode particle diameters range between 0.1 and 2.5μm. Each mode receives primary emitted material, is subject to wet and dry deposition, and may form through condensation of gaseous precursors. The two modes interact through coagulation, and the Aitken mode may grow into the accumulation mode and partially merge with it. The fine particle species considered within the CMAQ aerosol component include sulfate, nitrate, ammonium, water, primary organic aerosols, secondary organic aerosols from anthropogenic and biogenic origin, elemental carbon, and primary aerosol material not otherwise specified. The coarse particle mode within CMAQ, representing particles having aerodynamic diameters between 2.5 and 10 μm, consists of wind-blown dust and other large particles of unspecified origin. Coarse mode particles in the model also undergo wet and dry deposition.

2.3. CMAQ model simulation characteristics

The 2000 release of Models-3 CMAQ was used in this evaluation. The modeling domain covers the eastern U.S. (Figure 1.), with each grid cell covering 36 km by 36 km. The entire month of June 1995 was simulated. The domain's vertical profile contains 21 layers of varying thickness. The simulation used Version 2 of the Regional Acid Deposition Model chemical mechanism (RADM2), which includes 57 species and 158 reactions, 21 of which are photolytic. The meteorological fields were derived from MM5, the Fifth-Generation Pennsylvania State University/National Center for Atmospheric Research (NCAR) Mesoscale Model [*Grell et al.*, 1994]. Emissions were processed with the Models-3 Emission Processing and Projection System (MEPPS) [*Benjey et al.*, 1999].

3. IMPROVE speciated data

IMPROVE is a collaborative monitoring effort governed by a steering committee composed of representatives from Federal, regional and State organizations [*Pitchford and Scruggs*, 2000]. The network was designed to (1) establish current visibility and aerosol conditions, (2) identify the chemical species and emission sources responsible for visibility degradation, and (3) document long-term visibility trends at over 100 locations nationwide. The IMPROVE monitors collected two, 24-hour integrated samples (midnight to midnight, local time) per week in 1995. Additional information concerning IMPROVE can be obtained from a web site (vista.cira.colostate.edu/improve) maintained by Colorado State University.

Unfortunately, the majority of IMPROVE monitors are located in western states; as a result, only 18 sites fell within the model evaluation domain (Figure 1). All the sites are rural, except the urban WASH (Washington D.C.) site. Information concerning these sites can be found in Table 1.

Figure 1. IMPROVE stations within the CMAQ domain used in this evaluation.

Table 1. IMPROVE site information

Code	Location	Long (°W)	Lat (°N)	Elev. (m)
ACAD	Acadia NP, ME	68.308	44.415	129
OWA	Boundary Waters, MN	91.950	47.950	524
BRIG	Brigantine NWR, NJ	74.472	39.475	9
CHAS	Chassahowitzka NWR, FL	82.567	28.750	2
DOSO	Dolly Sods, WV	79.205	39.143	1158
GRGU	Great Gulf Wilderness, NH	71.217	44.300	439
GRSM	Great Smoky Mountains NP, TN	83.987	35.710	815
JEFF	Jefferson, VA	79.433	37.667	299
LYBR	Lye Brook Wilderness, VT	73.123	43.243	1010
MACA	Mammoth Cave NP, KY	86.075	37.277	248
MOOS	Moosehorn NWR, ME	67.283	45.117	76
OKEF	Okefenokee NWR, GA	82.117	30.765	49
ROMA	Cape Romain NWR, SC	79.583	33.033	3
SHEN	Shenandoah NP, VA	78.450	38.543	1098
SHRO	Shining Rock Wilderness, NC	83.283	35.650	1621
SIPS	Sipsey Wilderness, AL	87.382	34.358	279
UPBU	Upper Buffalo Wilderness, AR	93.245	35.880	723
WASH	Washington, D.C.	77.063	38.932	16

4. Evaluation

The scope of this evaluation was somewhat hindered by the IMPROVE network's twice-a-week sampling schedule, which when incorporated into the one-month simulation period, limited the number of comparisons. (144 possible observations (18 stations, 8 days: June 3, 7, 10, 14, 17, 21, 24 and 28)). Summary statistics for each of the 5 species included in the evaluation are found below. Scatterplots are found in Figure 2.

Table 2. Summary statistics for speciated aerosol data

Species	N	Source	Mean ($\mu g/m^3$)	CV*	r^2	Mean bias**	Min. ($\mu g/m^3$)	Max. ($\mu g/m^3$)
Sulfate	129	CMAQ	4.98	79.16	0.63	0.37	0.43	17.17
		IMPROVE	4.83	71.63			0.13	14.82
Nitrate	129	CMAQ	0.21	255.77	0.005	-0.20	0.00	3.95
		IMPROVE	0.31	64.28			0.00	1.10
$PM_{2.5}$	129	CMAQ	9.06	62.06	0.55	-0.21	0.60	26.09
		IMPROVE	12.96	55.39			0.00	33.17
PM_{10}	129	CMAQ	13.74	73.74	0.13	-0.26	1.00	55.64
		IMPROVE	19.40	50.26			0.00	51.48
Organic Carbon	112	CMAQ	1.53	44.23	0.25	-0.26	0.32	4.10
		IMPROVE	2.32	47.34			0.34	5.59

* Coefficient of Variation ** Bias defined as (IMPROVE - CMAQ)/CMAQ

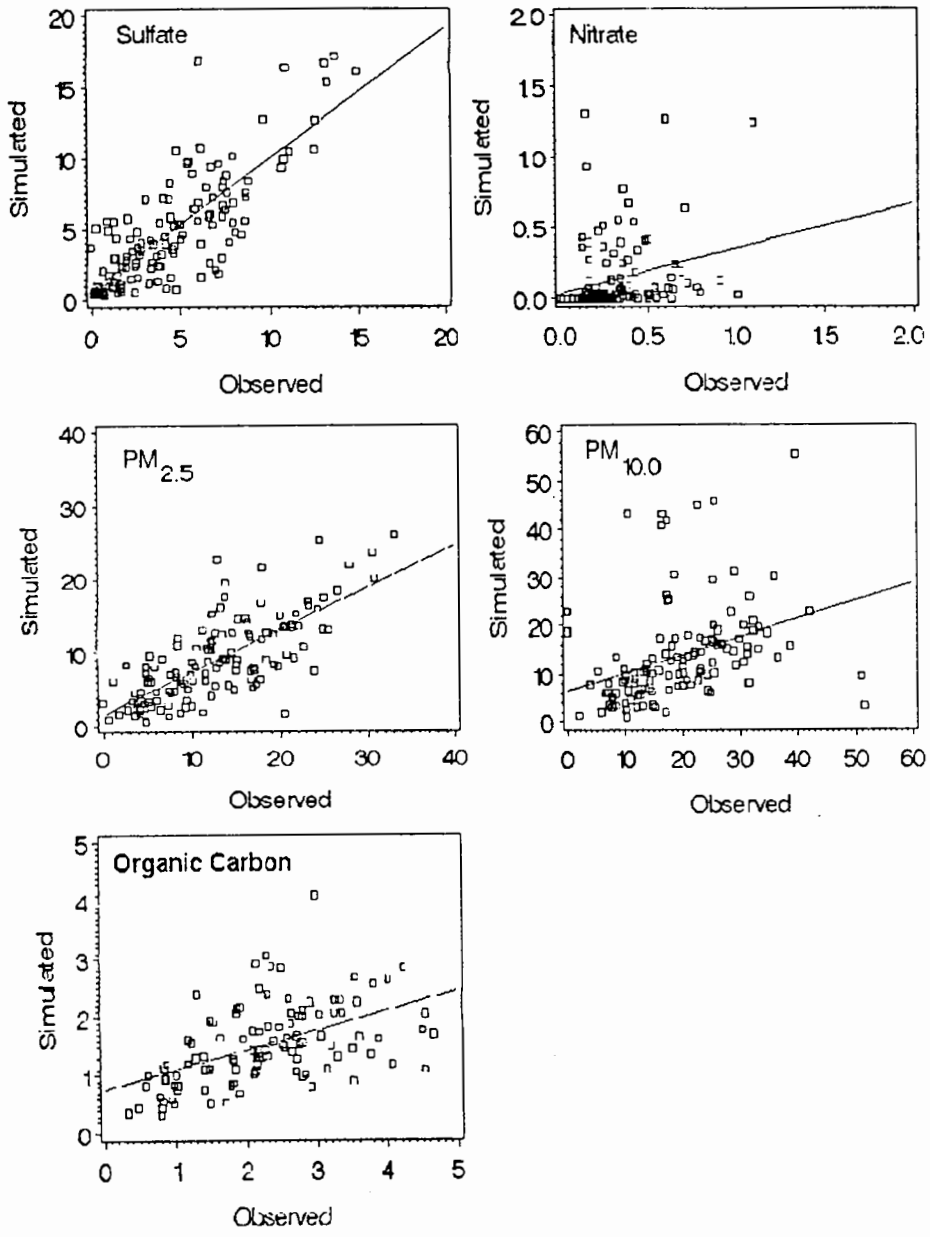

Figure 2. Scatterplots of observed (IMPROVE) versus simulated (CMAQ) for each species. Regression line is shown. Units are in $\mu g\ m^{-3}$

4.1. Sulfate

Examination of Figure 2 and Table 2 reveals a fairly good level of agreement between simulated and observed sulfate concentrations. The simulated mean (4.98μg/m^3), and coefficient of variation (79.16%) closely match those observed (4.83μg/m^3, 71.63%). The overall r^2 is 0.63 and the regression equation is CMAQ=0.60+0.91*IMPROVE. Given that the CMAQ aerosol module descends from models designed to address the acid rain problem, it is not surprising that CMAQ simulated sulfate concentrations agree well with observed sulfate measurements.

There is, however, a tendency for CMAQ to over predict concentrations (mean bias of 0.37). Examination of the bias across space and time (not shown) reveals that it is positive at 13 of the sites and on all but two days. An inflated positive bias (2.91) was observed at the DOSO (Dolly Sods/Otter Creek Wilderness in WV) site/grid cell. This inflated bias can be attributed to very small concentrations of sulfate observed at this location (in particular on two days, 24 June and 28 June).

4.2. Nitrate

Unlike sulfate, examination of Figure 2 and Table 2 reveals a very poor level of agreement between simulated and observed concentrations of nitrate. While the simulated mean (0.21 μg/m^3) was relatively close to the observed mean (0.31 μg/m^3), the coefficient of variation was not (255.77% versus 64.28%). This poor agreement is also reflected in the scatter plot, overall r^2 (0.005) and the regression equation of CMAQ=0.40+0.32*IMPROVE.

The model consistently underpredicts nitrate concentrations (mean bias = –0.20). Examination of this negative bias across time and space reveals that it is negative at all sites except two, GRSM (Great Smoky Mountains NP) and MACA (Mammoth Cave NP), and on half of the days. Subsequent investigation has determined that, in the CMAQ simulations used here, the ammonia emissions were too low. These ammonia under predictions no doubt contributed to the nitrate under prediction seen in the model output. Efforts are currently underway to determine more realistic ammonia emission levels, eventually allowing a more accurate model evaluation with respect to nitrate.

4.3. $PM_{2.5}$

A reasonable level of agreement can be seen between simulated and observed $PM_{2.5}$ concentrations (Figure 2., Table2.). The simulated mean (9.06 μg/m^3) and coefficient of variation (62.06%) reasonably match those observed (12.96 μg/m^3, 55.39%). as do the various percentiles. The overall r^2 is 0.55 and the regression equation is CMAQ=1.59+0.58*IMPROVE.

Because a large component of $PM_{2.5}$ is sulfate, the good agreement seen in the sulfate evaluation lends itself to reasonable $PM_{2.5}$ results. The model consistently under predicts $PM_{2.5}$ concentrations (mean bias = –0.21) across time (all 8 days) and space (16 of 18 sites).

4.4. PM_{10}

Examination of Figure 2 and Table 2 reveals a poor level of agreement between simulated and observed PM_{10} concentrations. Although the simulated mean (13.74 $\mu g/m^3$), and coefficient of variation (73.74%) are reasonably close to those observed (19.40 $\mu g/m^3$, 50.26%), the overall r^2 is only 0.13. The regression equation of CMAQ=6.52+0.37*IMPROVE and mean bias (–0.26) further reveal the model's tendency to underpredict PM concentrations. Examination of the bias reveals that it is negative at 16 of the sites and on all but one day (24 June). The only two sites with positive bias were SHEN (0.16) and WASH (1.29).

Processes in the CMAQ aerosol module that involve PM_{10} need better representation. Efforts are underway to more accurately model wind-blown dust, as well as to include sea salt in aerosol dynamics.

4.5. Organic carbon

CMAQ simulates organic carbon with a modest level of agreement. The r^2 is 0.25 and the regression equation is CMAQ=0.76+0.34*IMPROVE. As with most of the other species, CMAQ generally underpredicts organic carbon concentrations (mean bias of –0.26). This bias is negative at 15 sites and across every simulation day; however, it is not as large as the bias seen for the other species, as 8 of the 18 sites and 5 of the 8 days are within 25%.

This modest level of agreement results partially from the crude physical representation (currently undergoing improvement) of organics within the CMAQ aerosol component. Further difficulties arise from incomplete knowledge regarding organic aerosol constituents, making it difficult not only to adequately model organic species, but to compare model results with observations.

5. Summary

This evaluation compared speciated aerosol data collected during the month of June 1995 against CMAQ simulations for five species: sulfate, nitrate, organic carbon, $PM_{2.5}$ and PM_{10}. With the exception of sulfate (36%), the model simulations generally produced negative biases (model predictions too low) of between –21 and –26%. This negative bias was generally consistent across the domain and throughout the simulation period. Agreement between model simulations and observations varied considerably across species, with r^2s of 0.63 (sulfate), 0.55 ($PM_{2.5}$), 0.25 (organic carbon), 0.13 (PM_{10}) and 0.005 (nitrate)

Several likely sources of error in the model simulation were identified and include inadequate emissions inventories and an incomplete understanding of aerosol dynamics, especially for PM_{10}. Inadequacies in evaluation data sets have also been identified. Fortunately, the EPA has recently implemented the National $PM_{2.5}$ Monitoring Network, consisting of mass monitoring (1100 sites), routine chemical speciation (300 sites) and

supersite characterization. These network measurements will eventually provide much more adequate data, thus allowing for a more thorough evaluation of CMAQ.

6. References

Benjey, W.G., J.M. Godowitch and G.L. Gibson, Emission subsystem, in *Science algorithms of the EPA Models-3 Community Multiscale Air Quality (CMAQ) modeling system*, edited by D.W. Byun and J.K.S. Ching, pp. 4-1 – 4-107, EPA-600/R-99/030, U.S. Environmental Protection Agency, U.S. Government Printing Office, Washington D.C., 1999.

Binkowski, F.S., The aerosol portion of Models-3 CMAQ, in *Science algorithms of the EPA Models-3 Community Multiscale Air Quality (CMAQ) modeling system*, edited by D.W. Byun and J.K.S. Ching, pp 10-1 –10-23, EPA-600/R-99/030, U.S. Environmental Protection Agency, U.S. Government Printing Office, Washington D.C., 1999

Binkowski, F.S. and U. Shankar, The regional particulate matter model, 1. Model description and preliminary results, *Journal of Geophysical Research, 100*, 26,191–26,209, 1995.

Byun, D.W. and J.K.S. Ching, *Science algorithms of the EPA Models-3 Community Multiscale Air Quality (CMAQ) modeling system*, EPA-600/R-99/030, U.S. Environmental Protection Agency, U.S. Government Printing Office, Washington D.C., 1999.

Chang, J.S., F.S. Binkowski, N.L. Seaman, D.W. Byun, J.N. McHenry, P.J. Samson, W.R. Stockwell, C.J. Walcek, S. Madronich, P.B. Middleton, J.E. Pleim and H.L. Landsford, The regional acid deposition model and engineering model, NAPAP SOS/T Report 4, in *National Acid Precipitation Assessment Program, Acidic Deposition: State of science and technology, Volume I*, Washington D.C., 1990

Eder, B.K., M.R. Mebust, F.S. Binkowski and S.J. Roselle, A preliminary evaluation of Models-3 CMAQ using visibility parameters, International Symposium on the Measurement of Toxic and Related Air Pollutants, September 12–14, 2000, Research Triangle Park, NC.

Grell, G.A., J. Dudhia and D.R. Stauffer, A description of the fifth-generation Penn State/NCAR mesoscale model (MM5), NCAR Technical Note, NCAR/TN-398+STR, 1994

Pitchford, M.L. and M. Scruggs, IMPROVE network – Current and future configurations, in: *Spatial and seasonal patterns and temporal variability of haze and its constituents in the United States*, W.C. Malm, principal author, pp. 1-1 – 1-18, Cooperative Institute for Research in the Atmosphere, Colorado State University, ISSN 0737–352–47, 2000

Disclaimer. This document has been reviewed and approved by the U.S. Environmental Protection Agency for publication. Mention of trade names or commercial products does not constitute endorsement or recommendation for use.

NERL-RTP-AMD-01-116

TECHNICAL REPORT DATA

1. REPORT NO.	2.	3.1
EPA/600/A-01/076		

4. TITLE AND SUBTITLE	5.REPORT DATE
A Preliminary Evaluation of Models-3 CMAQ using particulate matter data from the IMPROVE network	6.PERFORMING ORGANIZATION CODE
7. AUTHOR(S) Brian K. Eder, Michelle R. Mebust, and Sharon K. LeDuc	8.PERFORMING ORGANIZATION REPORT NO.
9. PERFORMING ORGANIZATION NAME AND ADDRESS Same as Block 12	10.PROGRAM ELEMENT NO. 11. CONTRACT/GRANT NO.
12. SPONSORING AGENCY NAME AND ADDRESS U.S. Environmental Protection Agency Office of Research and Development National Exposure Research Laboratory Research Triangle Park, NC 27711	13.TYPE OF REPORT AND PERIOD COVERED Preprint, FY-01 14. SPONSORING AGENCY CODE EPA/600/9
15. SUPPLEMENTARY NOTES	

16. ABSTRACT

The Clean Air Act and its Amendments require the United States Environmental Protection Agency (EPA) to establish National Ambient Air Quality Standards for Particulate Matter (PM) and to assess current and future air quality regulations designed to protect human health and welfare. Air quality models, such as EPA's Models-3 Community Multiscale Air Quality model (CMAQ) [*Byun and Ching*, 1999], provide one of the most reliable tools for performing such assessments. CMAQ simulates air concentrations and deposition of various pollutants including PM. These simulations, which can be conducted on a myriad of spatial and temporal scales, support both regulatory assessment as well as scientific studies by research institutions. Within CMAQ is an aerosol component, or module, designed to simulate the complex processes involving PM, which is commonly separated into $PM_{2.5}$ (particles with aerodynamic diameters ≤ 2.5 μm) and PM_{10} (aerodynamic diameters ≤ 10 μm). In order to determine its value to the air quality regulatory communities, CMAQ needs to be evaluated using observational data. One such evaluation, which compared visibility parameters derived from CMAQ to visibility parameters obtained from National Weather Service observations, revealed that CMAQ was able to replicate general spatial and temporal patterns [*Eder et al.*, 2000]. The current evaluation compares PM simulated by CMAQ with PM data collected by the Interagency Monitoring of PROtected Visual Environments (IMPROVE) network.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b.IDENTIFIERS/ OPEN ENDED TERMS	c.COSATI

18. DISTRIBUTION STATEMENT	19. SECURITY CLASS *(This Report)*	21.NO. OF PAGES
RELEASE TO PUBLIC	UNCLASSIFIED	8
	20. SECURITY CLASS *(This Page)* UNCLASSIFIED	22. PRICE