Use of CMAQ Modeling System in Forecasting $PM_{2.5}$ Air Quality over New York State

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Objectives

• Apply and evaluate the usefulness of grid-based photochemical models such as CMAQ (Community Multi-scale Air Quality) Model in providing near-real-time air quality forecast for New York State.

• Evaluate the performance of CMAQ model for $PM_{2.5}$ predictions.

Approach

• Application of the air quality forecasting system developed by the National Weather Service (NWS), National Oceanic & Atmospheric Administration (NOAA) and the US Environmental Protection Agency (EPA).

• System consists of a meteorological model (ETA in 2004 and 2005, and WRF since June 2006) coupled with the PREMAQ emissions and meteorology processor, and the CMAQ photochemical model.

• Uses a horizontal grid resolution of 12 km.

• Emission inventories were updated annually as described by Mathur et al. (2004). On-road mobile source emissions were estimated using approximations to the MOBILE6 model (Pouliot et al., 2003).

• Each CMAQ simulation was performed for 48 hours starting at 12:00 Greenwich Mean Time (GMT), initialized using simulated concentration fields from the previous day. Time invariant boundary conditions were used.

• Feasibility of near real-time air quality forecasts was evaluated during June-September 2004 and January-March 2005 (Hogrefe et al., 2007). Air quality forecast modeling is ongoing on a daily basis from June 2005. All model inputs and outputs are archived for retrospective model evaluation.

• Air quality forecasts are posted at 2 PM daily on the website at ftp://ftp.dec.state.ny.us/dar/air_research/aqf/forecast/today/index.html

Data Analysis

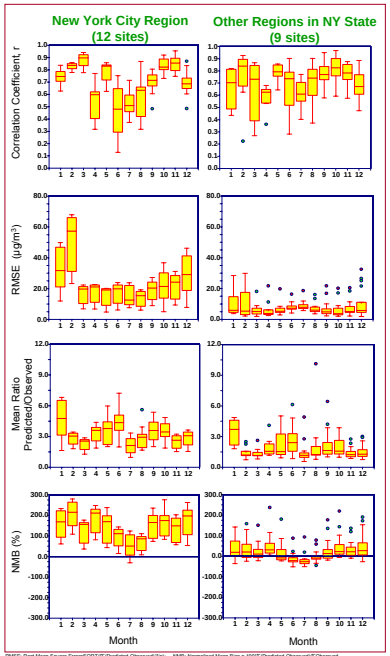
• Data analysis is conducted for simulations from June 2005 to December 2006 for $PM_{2.5}$ for New York State.

• CMAQ-predicted, 24-hr averaged, total $PM_{2.5}$ concentrations were compared with 24-hr averaged $PM_{2.5}$ measurements using Tapered Element Oscillating Microbalance (TEOM) reported in AIRNOW (http://www.epa.gov/airnow) **(Figure 1).**

• CMAQ-predicted, 24-hr averaged, $PM_{2.5}$ mass and species concentrations were compared with 24-hr measurements from sites within the Speciation Trends Network (STN) **(Figure 2)**. Organic carbon (OC) data from measurements was converted to organic matter (OM) by multiplying by 1.4, to enable comparisons with model output.

• Availability of continuous measurements at Bronx, NY (AIRS ID 360050110) enabled comparison of observed and predicted diurnal profiles of mass and $PM_{2.5}$ species **(Figure 3)**.

Figure 1 : Comparison Statistics for 24-hr Averaged $PM_{2.5}$ Concentrations Between TEOM Measurements and CMAQ Predictions



• Correlations during winter were 1.5 to 2.5 times higher than that in summer **(Figure 1)**.

• Model performance at sites within NY city region was poor compared to that at other sites in NY state, as illustrated by RMSE and NMB. Sites in NY city region showed median RMSE > 15 µg/m³, and median NMB > 50%, while other sites showed median RMSE typically 5 µg/m³ and median NMB within ±25%.

• Except NY City region, the model under-predicted $PM_{2.5}$ during summer, while over-predicting for other seasons.

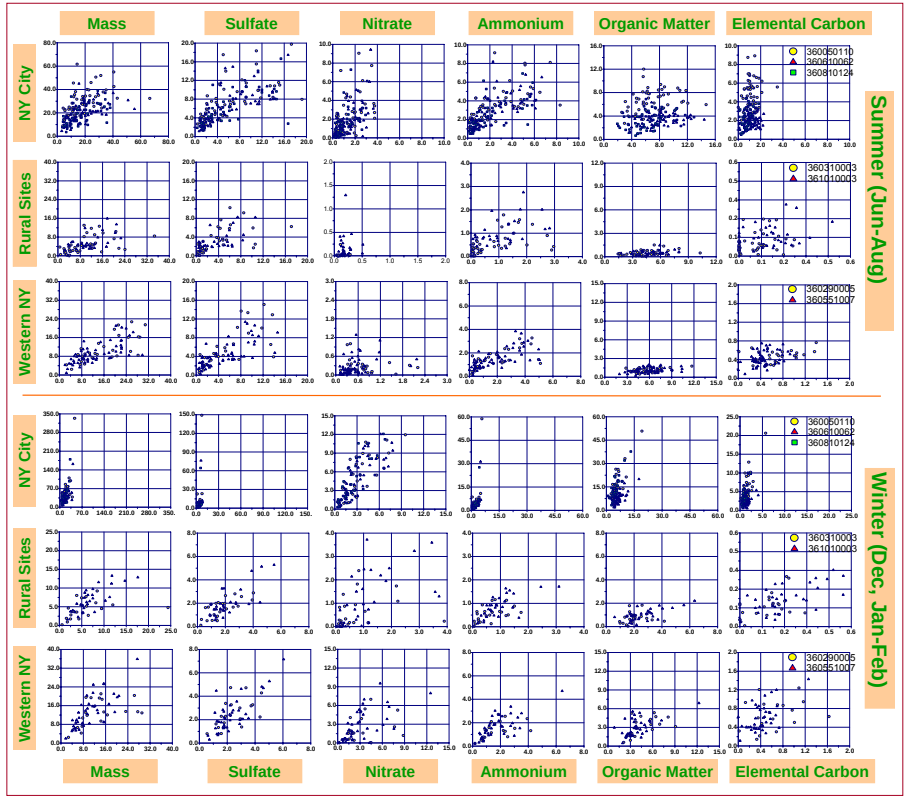


Figure 2: 24-hr $PM_{2.5}$ Mass and Species: STN (X-Axis) vs. CMAQ (Y-Axis)

(All concentrations are in µg/m³)

• Comparisons with 24-hr filter measurements showed that the model performance differed by region and $PM_{2.5}$ species **(Figure 2)**. Scatter plots are grouped into three regions: speciation monitors in NY city region ("NY City"), monitors at Whiteface Mountain and Pinnacle State Park ("Rural Sites"), and monitors in Western part of New York State at Buffalo and Rochester ("Western NY").

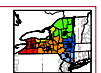
• Predictions of $PM_{2.5}$ concentrations in NY City region showed significant overestimations. This is mostly related to overestimation of primary emissions, as confirmed by the comparison of predicted versus observed EC during both summer and winter.

• Model under-predicted total $PM_{2.5}$ mass concentrations at Rural and Western NY sites, particularly at higher observed concentrations (>15 µg/m³) and mainly during summer.

• About 70% of sulfate predictions at all sites showed correlations greater than 0.60. Organic matter was under-predicted significantly at Rural and Western NY sites (NMB as low as -91%) during summer, probably due to underestimation of secondary organic aerosol concentrations.

• One specific event in winter (02/16/2006) showed abnormally high $PM_{2.5}$ (300 µg/m³) prediction in NY City. Further investigation suggests that the model- predicted planetary boundary layer (PBL) height for that region was unrealistically low, ranging from 35 to 55 m for that day. The strong inversion coupled with high emissions density resulted in large predicted $PM_{2.5}$ concentrations. This stresses two key factors: PBL (not a key parameter in weather prediction) is important in air quality forecasting of $PM_{2.5}$, and predicting such meteorological parameters need to be improved. It also stresses the need for error-checking options in the forecasting system.

Post-processing of CMAQ-predicted $PM_{2.5}$ Concentrations

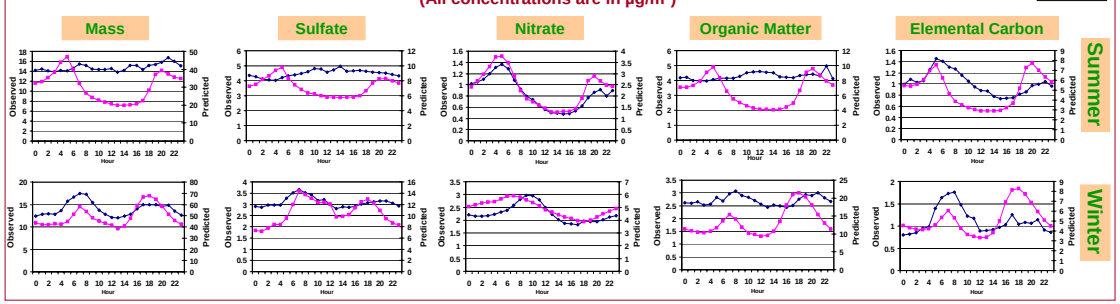


• A preliminary approach has been developed to adjust CMAQ-predicted $PM_{2.5}$ concentrations after completion of CMAQ simulations (i.e., post-process CMAQ outputs based on historical model-performance). Both unadjusted and adjusted forecasts are posted on the website and should be considered as the range within which the "true" value will likely fall.

• The correction approach consists of a combination of regression and bias-based adjustments, and varies by season and the air quality forecast region within NY (see inset map). For NY City region (region 2 in map), since the results indicate overestimated emissions, the CMAQ predictions are adjusted by multiplicative factors (0.90 for OM, 0.25 for EC, 0.23 for unspeciated $PM_{2.5}$ [A25]) before applying bias/regression corrections. The website includes a link to a "README" file that describes the adjustment procedure currently in effect.

Figure 3: Observed and Predicted Diurnal Average Concentrations for $PM_{2.5}$ Mass and Species at Bronx, NY

(All concentrations are in µg/m³)



Evaluation of Predicted Diurnal Profile

• For all species, the absolute value of model predictions was higher.

• The CMAQ predictions tracked observed diurnal profiles more closely during winter than summer **(Figure 3)**.

• The predicted profile showed a dual peak (~5-7 AM and 5-8 PM), and a depression during mid-day hours for both seasons. During summer, the measured profiles showed no specific pattern, except for nitrate and EC. This suggests that the inconsistent profiles seen during summer could probably be related to the temporal profiles used to allocate emissions for each hour of the day, in addition to vertical mixing processes in urban region closer to land-sea interface.

Conclusions and Future Work

• Model performance was acceptable at most locations within NY State, except at NY City region, as illustrated by root mean square error (RMSE) and normalized mean bias (NMB). The model over-predicts $PM_{2.5}$ concentrations for the New York City region, irrespective of the season (median RMSE >15 µg/m³, and median NMB >50%). The overestimation is typically related to overestimation of primary emissions, and partly due to shallow planetary boundary layer predictions at certain periods during winter.

• Organic matter was significantly under-predicted (NMB as low as -91%) during summer at rural regions within NY State, likely due to an underestimation of secondary organic aerosol (SOA) concentrations. This suggests the need for improvement in SOA mechanisms.

• Comparison of predicted and observed diurnal profiles shows inconsistencies during summer. This could be due to a combination of factors including incorrect temporal allocation of emissions and vertical mixing processes in urban regions.

• Future work will include emissions modeling within NYSDEC, to enable better understanding of discrepancies observed in diurnal profiles.

• A continuation of current effort focuses on improving the adjustments to model-predicted $PM_{2.5}$ concentrations to provide more realistic forecasts. Results suggest that there is an urgent need for improving the modeling system ability in estimating $PM_{2.5}$ levels and thus the forecasting capability over New York State.

References

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Acknowledgements and Disclaimer

This work was performed by the NYSDEC in cooperation with EPA and NOAA. The results presented here have not been reviewed by EPA and NOAA. The views expressed in this paper are those of the authors and do not necessarily reflect the views or policies of NYSDEC. The near real-time air quality forecasts presented here are currently in research-mode only, and do not constitute official NYSDEC air quality forecasts.