

Regional Model Estimates of Acidic and Mercury Depositions over Refined Spatial Scales in Northeastern U.S. and the Contribution from New York Power Production Point Sources

Summary Report

October 2016

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Summary Report

Prepared for:

New York State Energy Research and Development Authority

Albany, NY

Gregory Lampman Senior Project Manager

Summary Prepared by:

University at Albany, SUNY

Emily Wolfe, M.A. Spanish Linguistics

Report prepared by:

SEDEFIAN Consulting

Malta, NY

Leon Sedefian, Principal Investigator

and

New York State Department of Environmental Conservation

Albany, NY

Mike Ku, Kevin Civerolo, Winston Hao, Eric Zalewsky Project Managers

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Acronyms and Abbreviations

CMAQ	Community Multiscale Air Quality
EGU	Electric Generating Units
Hg	Mercury
NEI	National Emissions Inventory
NH3	Ammonia
NOx	Nitrogen Oxides
NYS	New York State
SMOKE	Sparse Matrix Operator Kernel Emissions
SO2	Sulfur Dioxide
TS	Total Sulfur
WRF	Weather Research and Forecasting
WTE	Waste to Energy

1 Purpose and Objectives

The objective of this study was to address two of the limitations found in previous regional modeling assessments by refining previously used coarser 12km grid to a 4km grid resolution in a novel application of the Community Multiscale Air Quality (CMAQ) modeling system over an annual timescale. These CMAQ simulations of acidic and mercury deposition over the Northeast U.S. and, more specifically, over New York State (NYS) determined the ability of the model to better simulate expected patterns of important input data such as precipitation as well as the resultant deposition. Secondly, and intrinsically connected with the refined grid modeling, was the practical issue of determining the extent to which NYS's major power sector sources influence the overall deposition impacts from all simulated natural and anthropogenic emissions. While modeled data comparisons addressed the first question, the more important second question required the incorporation of the most recent available emissions inventory and the detailed review of the NYS major source data. The purpose was to use the refined grid data and the associated emissions and meteorological data to more accurately predict acidic and mercury deposition. The results presented met the expectations of the study.

2 Pertinent Previous Modeling Results

Before incorporating the most recent data and modeling methods in the current study, investigators conducted a review of previous studies specific to CMAQ applications for deposition estimates to better understand any drawbacks of the current modeling approaches. Previous studies of acidic and mercury deposition presented and discussed in the report include model comparisons to observed wet deposition throughout the U.S. leading to improvements in the modeling methods over the last two decades. These studies indicated the tendency of CMAQ to both over and underestimate observed levels associated with limits in proper precipitation estimates. Therefore, the investigators found these studies lacked definitive findings to present day, specifically with regard to mercury (Hg) deposition. However, the physical and chemical processes in the CMAQ model have improved over the years, as well as the data used to simulate the effects of factors such as the underlying land use. The model has become a state-of-the-science approach in many current federal and State regulatory applications.

3 Models and Methodologies

At the time of this study, the latest version of the Environmental Protection Agency's (EPA) CMAQ regional modeling system was implemented to predict annual acidic and mercury deposition over a 4km grid over the Northeastern U.S., centered on NYS. Several other updates to the CMAQ system were developed as part of the current study. The refined 4km grid scale used in the study has not been previously implemented in any regulatory applications, making the present study unique in its methodology. However, due to lack of previous use for calculating long-term averages of deposition on a refined grid, the model has also not been tested regarding its ability to provide accurate projections.

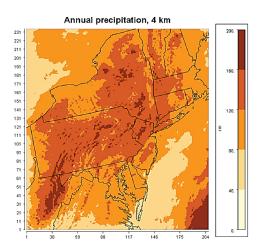
The CMAQ modeling system consists of two input components; 1) meteorological data simulated by the Weather Research Forecasting (WRF) model of atmospheric parameters such as wind flow conditions, and 2) an emission model, Sparse Matrix Operator Kernel Emissions (SMOKE), for simulating natural and man-made emissions over the refined grid. CMAQ used these inputs to simulate chemical transformation of the precursor pollutants and their subsequent dispersion in the atmosphere and deposition over land. Simulated deposition in CMAQ for both the wet component, associated with precipitation conditions, and dry deposition as pollutants come in contact with and adhere to the underlying surface. Simulations are carried out for every hour of meteorological data and summed over the timescale of interest. Thus, the annual deposition results represent accumulated values over the full year, while the winter and summer results presented in the study are total deposition only over these corresponding periods.

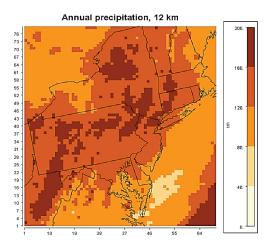
3.1 Testing of the refinements and updates to CMAQ

Prior to the application of CMAQ to predict annual acidic and mercury deposition over the 4km grid using the full emissions inventory, the investigators first looked at the ability of the CMAQ/WRF system to resolve precipitation data, as it is an essential parameter for wet deposition. Through an iterative process of comparing the simulated conditions to observations, a number of adjustments were made to the WRF simulations to better resolve observed patterns. In addition, the results over the 4km grid were compared to the corresponding 12km grid to guide the final choice of modeling approaches.

Figure 1 depicts an illustration of the differences noted in the quality of data resolution from the 4km vs. 12km grids. The graph on the left represents the resultant precipitation simulation over the 4km grid while the graph on the right is for the 12km grid. The 4km grid provides more details at the finer scales, although the general patterns are similar between the two grids. The refinements are associated with two aspects of the simulations. First, through the iterative comparisons to some of the observed patterns over the smaller scales, WRF simulations were correspondingly adjusted, and second, the 4km grid WRF simulations make fuller use of the variations in the available observed data from the modeling domain and smooth the model predictions less than the 12km simulations. Thus, the precipitation patterns generated by WRF over the 4km grid allows the simulation of variability on a scale smaller than previous assessment. The same refinement is also performed for other input data such as emissions and land use.

Figure 1. CMAQ/WRF simulated precipitation on the 4km (left) and 12km (right) grids





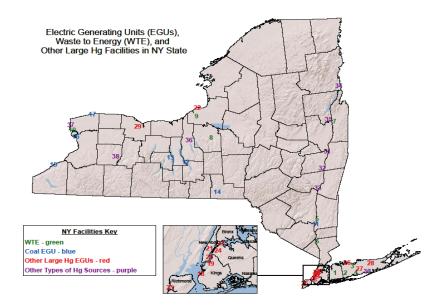
4 Development of the Emissions Inventory of Sources tracked in CMAQ Modeling.

The CMAQ simulations used the latest available national level data from EPA's 2011 National Emissions Inventory (NEI), which contains the necessary facility emissions and stack information. These data prepared for CMAQ input by the SMOKE emissions processor generated the necessary modeling data over the 4km grid. Prior to this study, data use for deposition estimates relied upon the 2005 NEI or an updated version for only certain source categories. Most importantly, this study sought to identify the NYS major source contributions to statewide acidic and mercury deposition from all source categories modeled. Some of these source categories, such as Electric Generating Units (EGUs) and Waste to Energy (WTE) facilities were previously identified as important due to large emissions.

Thus, investigators identified and extracted these specific facilities from the NYS sector of the 2011 NEI and conducted a detailed data review to ensure that the most reliable emission rates and stack parameters were used in the modeling. This is particularly important to the study as EGUs, especially those burning coal, are required by federal and NYS to reduce emissions of nitrogen oxides (NOx), sulfur dioxide (SO2) and Hg due to their relatively high emissions. In the review of the potential set of large NYS sources, it was determined to include certain "other" category sources, such as cement plants and metal-processing facilities, in the category of large mercury emitters, but not for acidic deposition purposes. Therefore, the sets of important NYS major point sources for acidic vs. mercury deposition were not the same, but had many sources in common, especially the coal-burning EGUs. In essence, due to known limitations in any inventory information, the team behind the report carried out a meta-analysis of reported NYS point source data in the 2011 NEI. The review considered more recent information available to DEC staff, such as industry reported data on facility specific basis resulting from required testing of these facilities.

Emissions of NOx, an important acidic deposition precursor, are the result of combustion of different fuels, not just coal-burning, and could be large even for the cleaner fuels such as gas. Thus, this study includes all NYS EGUs for acidic deposition estimates. Based on previous studies, the investigators concluded that NYS point sources of importance for CMAQ tracking of mercury impacts were a subset of the ones used for acidic deposition. Figure 2 shows the final set of 38 NYS large point sources tracked in the CMAQ modeling with the legend identifying their types. Of these 38 sources, 26 had large mercury emissions, with the largest contributors in the "other" source category.

Figure 2. Locations of the set of large point sources in NYS tracked in CMAQ



The review of the emissions and stack parameter data for the large NYS sources resulted in a reduction of about one-quarter of the mercury emissions for these sources in the 2011 NEI, but no real change in the precursor emissions for acidic deposition. This is not surprising since emissions of SO2 and NOx are monitored and reported by industry for these large point sources and no similar industry-wide monitoring exists for mercury. The review also found a need to revise about one-third of the stack parameters for the large NYS sources, although a majority of these changes were of minor nature for the purposes of deposition estimates. A significant effort was also spent on finding reported information on the relative percentages of the three forms of mercury: elemental, oxidized gas, and particulates, in order to best categorize the emissions of these species from the various source types. This was important since the three species behave very differently with regard to their deposition potential for both wet and dry components. Thus, while the majority of the emissions were found to be of the elemental form, its deposition was expected to be much less than for the oxidized form due to insolubility and much lower dry deposition velocity.

The report also provides an instructive summary of relative emissions of the pollutants from pertinent source categories in the 2011 NEI. It was found that for Hg, the NYS point sources of importance for CMAQ tracking make up essentially all of the NYS point source sector emissions (nearly 93 percent). Regarding acidic deposition, however, the CMAQ sources tracked constituted 50 to 70 percent of all of NYS point source emissions for the precursors SO2 and NOx. Furthermore, the total of all NYS source emissions (including small stationary and mobile sources) for all these pollutants are less than 10 percent of the emissions for the rest of the states in the modeling area. It was also noted that the emissions of another acidic deposition precursor, namely ammonia (NH3), were essentially due to agricultural sources, with less certainty in the quality of NH3 emissions in general. Relative to the rest of the U.S., past data from the EPA indicated that coal-burning EGUs dominated the Hg and SO2 emissions.

4.1 Future scenario using the EPA 2018 emissions inventory and the effects on the New York power sector subset of sources.

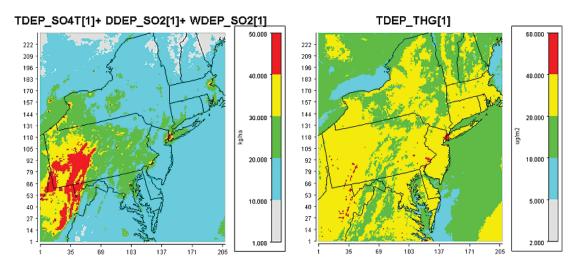
In addition to the CMAQ modeling performed with the 2011 NEI to determine the contribution from the NYS major point sources, projected emissions in a "future" scenario were also modeled for acidic deposition only. Data was available from EPA for a projected NEI in the year 2018, assuming that many of the coal burning EGUs throughout the eastern half of the U.S. would either shut down or greatly reduce operations. This assumption is based on impending federal regulations to control acidic deposition pollutants. The emissions for this future inventory suggested a large reduction in the SO2 and NOx emissions, but no change in NH3 emissions. Estimates show that in 2018 only one-fifth of the 2011 emissions for the NYS major sources will remain, while one-third of the total emissions of all states in the domain is due for reductions in SO2 emissions. NOx will experience a 70 percent reduction in the study's NYS major sources, though only a 14 percent reduction overall for domain wide emissions from other states. This lower NOx reduction results from the dominant of the mobile source category in the total emissions.

5 Resultant CMAQ Deposition

CMAQ produces hourly wet and dry deposition data, which can be aggregated to annual accumulated deposition levels over the whole modeling area. The modeling for each of the species as well as their sum provides total deposition and allows the determination of the attribution of certain factors such as seasons. Wet deposition results from falling precipitation scavenging the pollutants while dry deposition occurs when these pollutants interact with the Earth's surface. The report details the modeling of the overall emissions from the 2011 NEI and the contribution of NYS large point sources, which provided a large set of results. Of importance to note is an initial assessment for mercury that found that total wet deposition due to all NYS sources, plus the impact due to emissions from other states in the modeling domain fell way short of the observed levels at monitoring locations within the domain. This was a direct result of omitting Hg emissions from sources outside of the CMAQ modeling domain. These emissions were not readily available in the EPA 2011 NEI. This was rectified by assembling these additional mercury source emissions for input to CMAQ as influx into the domain. The resultant wet Hg deposition matched observations well, which confirmed the dominance of these out of domain emissions on deposition in NYS and in surrounding areas. Previous studies have also shown the general dominance of far distant sources on mercury deposition in the northeast. The initial CMAQ result pointed out the minimal effect of all NYS sources on total mercury deposition in and around the State. Thus, subsequent modeling included all of the Hg emissions in and out of the domain, as it was for pollutants associated with acidic deposition.

Figure 3 presents an example of the CMAQ calculated annual deposition for acidic and mercury deposition over the modeling area. These are for annual total sulfur, which is the sum of sulfate plus SO₂, and total mercury including all of its three species. These results indicate that the overall highest impacts occur in southwestern Pennsylvania while impacts in NYS are in the middle range of the deposition scales. There is also a "washed out" sense to at least the acidic deposition over NYS, with higher values in the western part of the State.

Figure 3. Deposition of total sulfur (left) and total mercury (right) due to the 2011 NEI



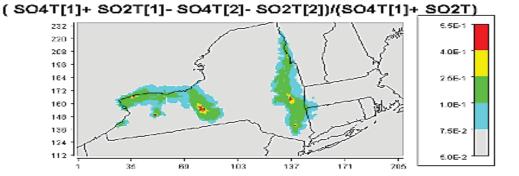
The study also concluded that of the three forms of Hg modeled: elemental, oxidized gaseous, and the particulate form, the oxidized form contributed the most to the total Hg deposition. This occurs even in light of the larger overall emissions of the elemental form of Hg since this form has relatively low wet and dry deposition potential. Furthermore, the overall Hg deposition mostly stems from areas of coalburning EGUs, WTEs and other large emitters from outside the State and the modeling area, with the contribution from NYS sources deemed small, as indicated previously.

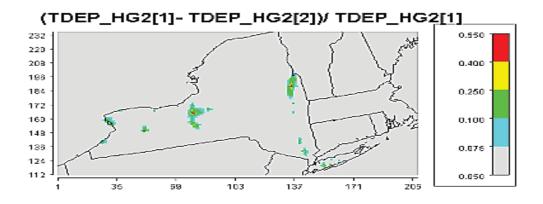
The study presents the deposition of acidic species sulfates and nitrates and the relative contributions from wet and dry components. For example, the wet component controls sulfate deposition, while total sulfur and nitrate have an important, if not dominant, dry deposition component. The CMAQ model also properly simulates the expected larger summertime sulfate deposition in the Catskill Mountains against those in the Adirondacks due to the larger rainfall in the former area.

As for the contribution of the set of selected large NYS point sources to the overall 2011 NEI impacts, the study found that these NYS sources are contributing minimally to all forms of deposition, except for total sulfur. The latter is because total sulfur includes the influence of SO2 deposition driven by the dry deposition component at the localized level around the large NYS facilities. Figure 4 shows example plots for annual total sulfur and mercury attributed to the set of large NYS sources. These plots show the differences between CMAQ modeling with the full 2011 NEI and another CMAQ modeling when the NYS "tracked" sources are removed from the 2011 NEI. The difference between these two CMAQ results are then normalized by the 2011 NEI results and represent relative differences in terms of the fraction of the overall deposition due to the NYS tracked sources.

The figure indicates less of an influence by the NYS large sources at the lower end of the scale (such as all the gray areas where the influence is less than .075 or 7.5 percent), while the more colorful areas are where these sources have a relatively larger impact (i.e., over 0.25 or 25 percent). However, the larger impacted areas are mainly confined around the coal-burning EGUs and some of the cement plants, specifically for mercury. It is important to remember that these are differences in deposition with and without the NYS sources while the overall influence of these sources on the total inventory results is small. It is also important to recognize that a review of the current state (mid-2016) of the coal-burning EGUs vs. the projected deposition based on 2011 emissions indicates that essentially all have either curtailed or eliminated coal-burning. In addition, some of the other facilities (e.g., LaFarge cement plant) are undergoing modernization. Therefore, the reductions in total sulfur deposition as well as mercury are considered as already accomplished.

Figure 4. Relative difference in annual total sulfur deposition (top) and mercury deposition (bottom) due to the NYS large point sources.





An important consideration from the standpoint of policymaking decisions, as well as possible technical improvements to CMAQ modeling is the question of how well do the simulated results in this study compare to observations. The report provides a detailed comparison of CMAQ calculated acidic species and total mercury wet deposition to corresponding observations at monitoring locations in the modeling domain. No similar data exists for dry deposition and, as such, the model performance was limited to the wet component. The results are presented for each of the four seasons and the annual levels in graphical form and from a statistical analysis with the finding that CMAQ has a tendency to underestimate the annual levels for all acidic species and total mercury. This, in turn, is due to underestimation during the summer and spring months, driven essentially by a corresponding underestimation of precipitation by CMAQ for the same seasons. Even with these underestimations, the model is within 30 percent of observation, with mercury surprisingly showing the lowest (less than 10 percent) deviation from observations. From the standpoint of the modeling community, these findings for the current study's application of CMAQ at the 4km grid scale are remarkably good.

Finally, a noteworthy result is the reduction in acidic deposition projected by CMAQ to occur due to the expected federal regulatory reductions in emissions of SO2 and NOx, as reflected in the 2018 inventory. The only pollutant without a projected reduction is ammonia due to its association with agricultural sources, which are not affected by the EPA regulations forming the basis of the 2018 emissions inventory. Comparison of the 2018 inventory results to the 2011 deposition for the other acidic species indicates a significant projected reduction of about half for the sulfur component and about a quarter for nitrate deposition throughout the modeling domain.

5.1 What is the significance of the predicted deposition in NYS and the influence of out of state sources on NYS deposition levels?

The presentation and discussion of the results of the study during a workshop held by the authors covered both technical aspects and policy issues. The results bring attention not only to the contribution of the NYS sources on deposition levels, but also potential large reductions still possible for acidic and mercury deposition from future emissions. The conclusive evidence of this study leads us to understand the need for actionable solutions for reductions in deposition which come from outside of NYS. This study also illustrates how federal and NYS regulations have considerably reduced deposition levels recorded in the past two decades, especially for wet deposition of sulfate and nitrate. Recent data analyzed indicates a reduction of well over 50 percent in these acidic components since the imposition of the NYS and federal regulations. However, the potential exists for other states to initiate emissions reductions similar to NYS if deposition levels are to decrease further in a considerable

manner. While the CMAQ results demonstrated a small impact from NYS and adjacent state emissions on Hg deposition, mercury is nonetheless a global pollutant that remains in the atmosphere for months to years. Therefore, if more can be done to reduce this pollutant, such as the current implementation of federal regulations on coal burning EGUs, it should continue.

One practical and timely use of the current results could be as input to ongoing work with watershed models, which are important tools for the management of sensitive ecosystems in NYS and elsewhere. Such models are capable and can establish "critical loads" to protect against the impacts of acid deposition. The refined sulfur and nitrogen deposition results from this study could provide a key input to the watershed models and should lead to refined estimates of critical load exceedances. Related to the concept of critical loads is the ongoing total maximum daily loading (TMDL) assessment of acidified surface waters in the Adirondack Forest Preserve. These waters have been impacted by decades of acid deposition, and they require monitoring and evaluation by the DEC. Watershed models are also used in the TMDL process, which could improve with the refined acid deposition projections from this study.

Going forward, policymakers should look to initiating dialogue between the states and the federal government on further potential acidic and mercury deposition reductions.

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New York State Energy Research and Development Authority

17 Columbia Circle Albany, NY 12203-6399 toll free: 866-NYSERDA local: 518-862-1090 fax: 518-862-1091

info@nyserda.ny.gov nyserda.ny.gov



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