EVALUATION OF FOUR DIFFERENT METHODS TO CALCULATE RELATIVE RESPONSE FACTORS AND ESTIMATED FUTURE YEAR OZONE DESIGN VALUES

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1. INTRODUCTION

Estimated design values for the future year (DVFs), as calculated from air quality modeling results, are used for a model attainment demonstration for the ozone (O_3) National Ambient Air Quality Standards (NAAQS). The DVF for O_3 is calculated by multiplying a baseline 5-year weighted design value by a model-derived Relative Response Factor (RRF). The U.S. EPA's guidance for a modeled attainment demonstration recommends calculating an RRF for a site using the 3x3 grid cell array surrounding the monitoring site (US EPA, 2018a). O_3 model performance in coastal areas is often poor due to the land/water interface in the air quality and meteorological models, especially for The Community Multiscale Air Quality (CMAQ) model (Dreessen et al., 2019; LMOS, 2019). This is particularly true in the New York City metropolitan area, where high population density, numerous emission sources, and complex land/sea circulations make it difficult to predict O_3. Therefore, at monitoring sites in these regions the RRF/DVF may not be reliable when including water cells (more than 50 percent of the grid cell area is water). The guidance allows for consideration of a modified 3x3 method (considering a removal of the unrepresentative cells) for those monitoring sites that may be affected by a specific local topographic or geographical feature such as a water body (US EPA, 2018a; US EPA, 2018b).

In this study, four different RRF/DVF calculation methods were evaluated for those monitoring sites in coastal areas. The CMAQ and Comprehensive Air quality Model with eXtensions (CAMx) modeling results were used for the evaluation using both the 2016/2023 version 1 modeling platform and the 2011/2017 Mid-Atlantic Regional Air Management Association, In. (MARAMA) beta modeling platform.

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2. MODELING SETUP AND METHODS

2.1 Modeling Setup

To perform 2011 (base year) and 2017 (future year) photochemical simulations, CMAQ version 5.0.2 and CAMx version 6.40 were used for the simulations over the Ozone Transport Commission (OTC) domain at 12-km horizontal resolution (12OTC1) with 35 vertical layers. CMAQ used the Carbon Bond-Version 5 (CB05), while CAMx used the Carbon Bond-Version 6 (CB6r2). We used the 2011 MARAMA beta platform based on the EPA's "ek" emission inventory with changes made by MARAMA (MARAMA, 2017). The modeling period was from mid-May to August. EPA's 2011 meteorology data were used for both model simulations.

For 2016 (base year) and 2023 (future year) simulations, we used most updated version of the 2016 v1("fi") platform, developed by the U.S EPA working in conjunction with the National Emissions Inventory Collaborative, with Eastern Regional Technical Advisory Committee (ERTAC) Electricity Generating Unit (EGU) emissions, available from http://views.cira.colostate.edu/wiki/wiki/10202 and ftp://newftp.epa.gov/air/emismod/2016/v1/postv1_updates/. CMAQ version 5.3.1 with CB06 mechanism and CAMx version 7.00 with CB6r4 mechanism were applied. Simulations were conducted for the expanded OTC domain at 12-km horizontal resolution (12OTC2) with 35 vertical layers for the 2016 O_3 season from April to October. Initial and boundary conditions were extracted from in-house CMAQ model runs with the 36-km CONUS domain (36US3) using the 2016 v1("fh") emissions platform. EPA's 2016 meteorology data were used for both model simulations.

2.2 RRF/DVF Calculation

The US EPA's guidance provides an approach to calculate the RRFs and DVFs using the 3x3 method (US EPA, 2018a). The RRF for a site is the ratio of the future-to-base year air quality modeling projections, based on changes in emissions and is used to project DVFs. The projected DVF is calculated as:

$$DVF = RRF \times DVB \quad (1)$$

where *DVF* is the estimated design value for the future year, *RRF* is relative response factor, and *DVB* is the base design value based on a 5 year weighted average of observed DVs (e.g., 2014-2018 for 2016 DVB).

The RRF is based on the average of the 10 highest predicted daily maximum 8 hour (MDA8) O_3 ≥60 parts per billion (ppb) of the base year where possible. If there are fewer than 5 days with MDA8 ≥60 ppb, an RRF is not calculated.

In this study, RRFs are calculated with four different methods. Grid cells used in the RRF calculation are described in the next section.

2.3 Four Methods for RRF calculations

The first method is the EPA's recommended 3x3 method (US EPA, 2018a). The second method is a modified 3x3 method that eliminates the grid cells that are classified as water cells and that do not contain the monitoring site (US EPA, 2018b). This method ("no water 1") includes a water cell in the RRF calculation even if the monitoring site is located in the water cell. The third method is a further modified 3x3 method that excludes all water cells even if the monitoring site is located in a water cell ("no water 2"). The fourth method is a 1x1 method that uses one grid cell where the monitoring site is located.

2.4 Sites Located in Water Cells

Water cells are those grid cells with areas >50% water, as defined by the Weather Research Forecasting Model (WRF). Figure 1 shows monitoring sites located in a water cell in the 12OTC1 domain. It shows only those sites where measured 2017 design values (DVs) are available and therefore used for comparisons of the four methods.

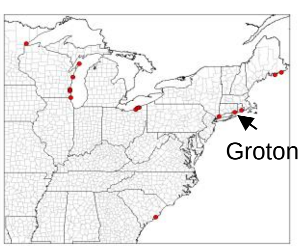


Fig. 1. Monitoring sites located in a water cell where 2017 measured DVs are available in the 12OTC1 domain for the 2011 platform.

3. RESULTS

3.1 Projected 2017 O_3 DVFs vs. measured 2017 DVs with 4 methods

Four different methods to calculate RRF/DVF were evaluated by comparing projected 2017 DVFs with the measured 2017 O_3 DVs. Figure 2 shows measured 2017 O_3 DVs and projected 2017 DVFs estimated with the 3x3 method using the CMAQ and CAMx modeling results focusing on the northeastern US. Measured 2017 DVs are higher than the projected 2017 DVs from both CMAQ and CAMx indicating both models underpredicted measured DVs in 2017 using the 2011/2017 MARAMA beta modeling platform. Overall, CMAQ and CAMx seem to project O_3 DVFs similarly using the 3x3 method.

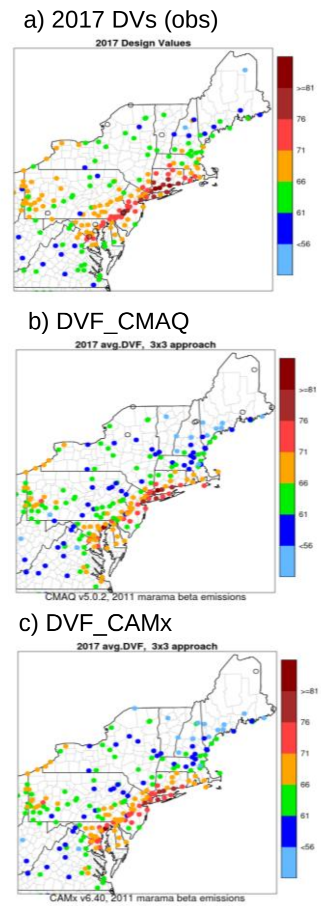


Fig. 2. (a) Measured 2017 (2015-2017) O_3 DVs (in ppb) based on observed O_3 in the northeastern US. (b) projected 2017 DVFs (in ppb) with 3x3 method based on the CMAQ v5.0.2 results in the northeastern US. (c) projected 2017 DVFs (in ppb) with 3x3 method based on the CAMx v6.40 results in the northeastern US. Open circles are sites where DVF was not calculated.

Figure 3 shows projected 2017 DVFs compared to measured 2017 DVs for each RRF calculation method for the monitoring sites located in a water cell only. For both models the 3x3 method projected DVFs are generally lower than the measured DVs. Using the 3x3 no water 1 method and the 1x1 method, differences in projected DVFs between the two models are larger, compared to the 3x3 method. The 3x3 no water 2 method results show that differences in projected DVFs between the two models are smaller compared to the previous two methods. The projected DVFs are closer to the measured DVs, compared to the other methods.

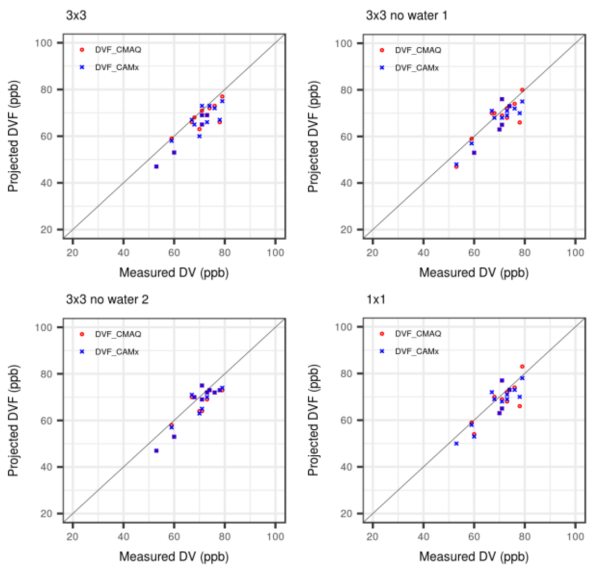


Fig. 3. projected 2017 DVFs vs. measured 2017 DVs for the four RRF calculation methods for sites located in a water cell only in the 12OTC1 domain.

3.2 O_3 Model performance of CMAQ and CAMx for the 2016 platform

A model performance evaluation for O_3 was conducted to demonstrate if the 2016 base year modeling results can simulate observed concentrations. Various statistical metrics are recommended to characterize model performance (USEPA, 2018a). Mean bias (MB) averages the difference between the model and observation paired in time and space. Mean bias of MDA8 O_3 was calculated when observed MDA8 O_3 is ≥ 60 ppb. Spatial plots of mean bias for the period from July to August at each monitoring site in the modeling domain are shown in Figure 4 for both (a) CMAQ and (b) CAMx as an example. CMAQ results show large overprediction of O_3 in coastal areas, especially for the sites located in a water cell. CAMx appears to be biased high over areas far from the coast.

In addition to the seasonal statistical model performance evaluation, time series plots of observed and modeled MDA8 O_3 were generated at selected monitoring sites. Figure 5 shows time series plots of observed and modeled MDA8 O_3 concentrations from both CMAQ and CAMx at (a) Groton, CT, identified as a water cell and (b) the Susan Wagner High School (New York City), identified as a land cell. This illustrates a model performance comparison between the water cell and land cell in the nonattainment area. Both models underpredicted O_3 in April and May at both monitoring sites. In July and August, CMAQ overprediction of O_3 is more pronounced at Groton, compared to CAMx. On the other hand, the CMAQ O_3 bias at the Susan Wagner High School site is lower, compared to the bias at the Groton site. Even though both models generally capture temporal variations of O_3 at both sites, CMAQ model performance tends to be poorer at sites in a water cell, such as Groton.

Overall, both CMAQ and CAMx O_3 model performance statistics are close to the ranges discussed in recent literature reviews (Simon et al., 2012; Emery et al., 2017).

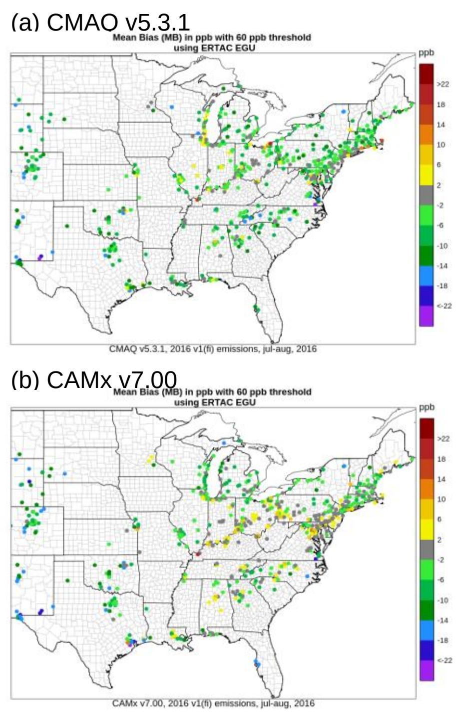
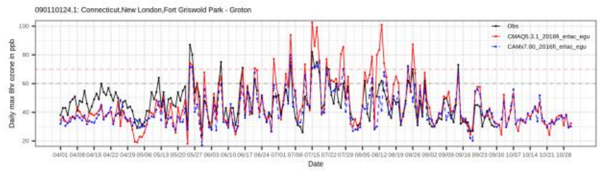


Fig. 4. MDA8 O_3 mean bias (modeled – observed) when observed MDA8 O_3 >= 60 ppb from July to August, 2016 for (a) CMAQ v5.3.1 and (b) CAMx v7.00.

(a) 090110124, Groton, Connecticut



(b) 360850067, Susan Wagner HS, New York

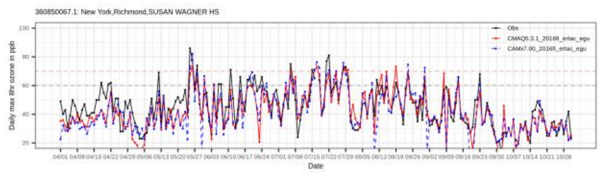


Fig. 5. Time series of MDA8 O_3 of at (a) Groton (site: 090110124, water cell) and (b) the Susan Wagner High School (site: 360850067, land cell).

Comparisons of average observed and modeled hourly O_3 for the top 10 modeled MDA8 O_3 days at Groton (water cell) are shown in Figure 6. Diurnal profiles based on the CMAQ modeled top 10 days are compared in Figure 6 (a), while diurnal profiles based on the CAMx modeled top 10 days are shown in Figure 6 (b). Average CMAQ modeled O_3 concentrations show high bias of about 30 ppb during afternoon hours, whereas the CAMx overpredictions were much smaller. In contrast, the average observed and CMAQ and CAMx modeled hourly O_3 concentrations at the Susan Wagner High School (land cell) are much more consistent with each other as shown in Figure 7. These results indicate that base model performance is poor and projected DVFs for O_3 at water cells may not be reliable.

(a) CMAQ top 10 (b) CAMx top 10

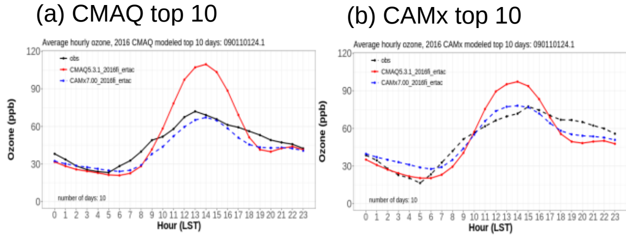


Fig. 6. Average hourly O_3 for modeled MDA8 O_3 top 10 days: (a) CMAQ top 10 days and (b) CAMx top 10 days (site: 090110124, Groton, water cell).

(a) CMAQ top 10 days (b) CAMx top 10 days

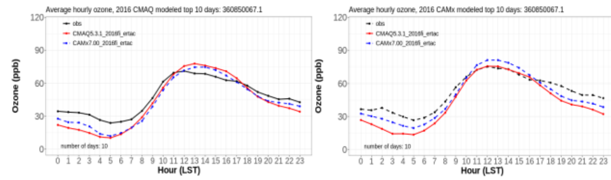


Fig. 7. Average hourly O_3 for modeled MDA8 O_3 top 10 days: (a) CMAQ top 10 days and (b) CAMx top 10 days (site: 360850067, Susan Wagner High School, land cell).

3.3 Preliminary 2023 O_3 DVFs estimated using 4 methods

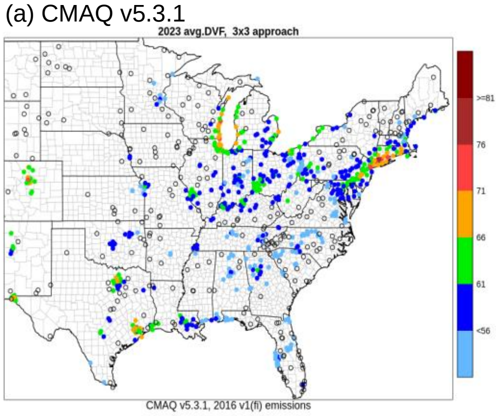
Four different RRF calculation methods using the 2016 platform were compared to see if no water methods improve the model-based DVF predictions by comparing two model results.

The modeled attainment test for the 2015 O_3 NAAQs in 2023 is required for the moderate nonattainment areas such as the New York-Northern New Jersey-Long Island, NY-NJ-CT area (83 FR 10376, March 9, 2018; 83 FR 25776, June 4, 2018). The site-specific RRFs were calculated and multiplied by the corresponding site-specific DVBs to obtain projected 2023 DVFs. Spatial plots of the DVFs calculated using the 3x3 method are shown in Figure 8 (a) and (b), for the CMAQ model and the CAMx model result, respectively. Overall, the results from both models are comparable to each other although it looks like CMAQ has quite a few more open circles than CAMx in the Southeast. Several sites around the NY-NJ-CT nonattainment area and the Lake Michigan area show exceedances of the 2015 O_3 NAAQS of 0.070 parts per million (ppm) (or 70 ppb).

Figure 9 shows the comparisons of projected 2023 O_3 DVFs between the models using the 4 different RRF calculation methods. There are 5 nonattainment areas in the northeastern US including one moderate nonattainment area (i.e., the New York-Northern New Jersey-Long Island, NY-NJ-CT area) and four marginal nonattainment areas (i.e., Greater Connecticut, CT, Philadelphia-Wilmington-Atlantic City, PA-NJ-MD-DE, Baltimore, MD, and Washington, DC-MD-VA) (https://www.epa.gov/green-book). The DVFs at the 73 monitoring sites within the five O_3 nonattainment areas in the northeastern US were compared between CMAQ and CAMx. As shown in Figure 9, the DVFs between the two models show better agreement for the 3x3 no water 2 and

1x1 methods, compared to the 3x3 and 3x3 no water 1 methods.

(a) CMAQ v5.3.1



(b) CAMx v7.00

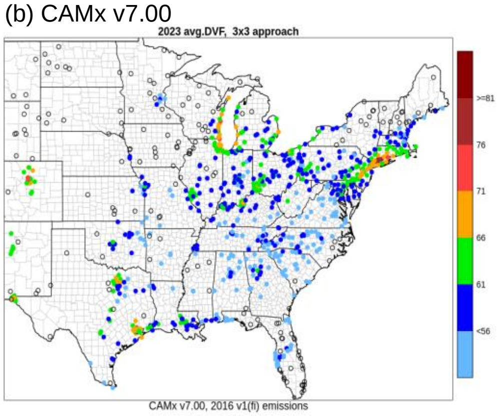


Fig. 8. Preliminary 2023 DVFs (in ppb) with 3x3 method using (a) CMAQ v5.3.1 and (b) CAMx v7.00.

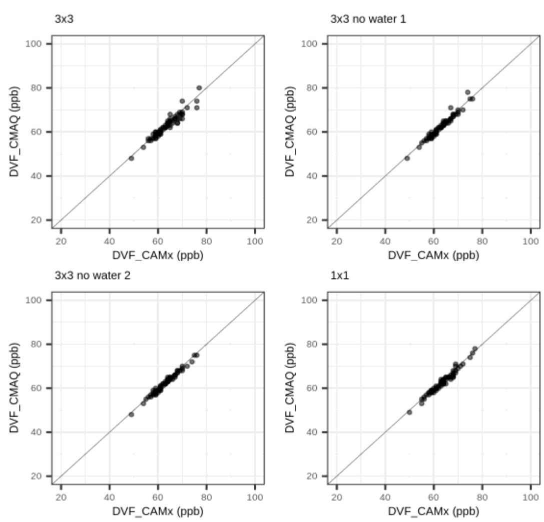


Fig. 9. Preliminary 2023 DVFs (CMAQ vs. CAMx) for the four RRF calculation methods for sites located in the O_3 nonattainment areas in the northeastern US.

Preliminary projected 2023 DVF values with each method based on both models for selected sites are shown in Table 1. The projected 2023 DVFs based on different methods show a wider range for CMAQ, compared to CAMx. For CAMx, 2023 DVFs show similar results among the 4 methods for most sites shown in this study, except for the site 090010017 (Greenwich, water cell), which shows relatively larger difference between the methods.

Table 1. Preliminary projected 2023 DVFs (in ppb) for selected sites.

Site ID	Cell	2014-2018 DVB	3x3	3x3 no water 1	3x3 no water 2	1x1
2023 DVF (CMAQ v5.3.1)						
90019003	land	82.7	80.6	75.5	75.5	76.4
90013007	land	82	74.6	75.1	75.1	74.5
360850067	land	76	74.2	70.3	70.3	70.3
90099002	land	79.7	71.8	70.8	70.8	71
90010017	water	79.3	71.7	78.8	72.2	78.8
90110124	water	74.3	67.9	71.3	66.7	71.3
550590019	water	78	72.7	73.3	72.2	73.7
551010020	water	76	70.9	71.9	69	72.7
390850003	water	73.7	68.4	69.8	66.4	69.8
2023 DVF (CAMX v7.00)						
90019003	land	82.7	77.5	76.3	76.3	76.3
90013007	land	82	75.9	75.5	75.5	75.2
360850067	land	76	70	69.8	69.8	69.5
90099002	land	79.7	72.1	72.3	72.3	72.2
90010017	water	79.3	76	74.7	73.8	77.3
90110124	water	74.3	67.3	67.7	66.9	69.2
550590019	water	78	72.1	71.8	71.7	72.3
551010020	water	76	69.8	70.3	70.1	70.8
390850003	water	73.7	67.4	67.2	66.1	68.2

4. CONCLUSIONS

Projections of DVFs at the sites located in a water cell are likely not reliable due to poor model performance, especially for the CMAQ modeling system. In this study, four different RRF calculation methods were evaluated using both 2011 and 2016 modeling platforms for those sites located in a water cell. Projected 2017 O_3 DVFs using the 2011 platform underpredicted measured DVs for 2017 in some sites in the northeastern US. DVFs with the 3x3 no water 2 method shows better agreement between the two models, as well as measured DVs for the sites located in a water cell.

The 2016 model results demonstrate that the CMAQ results show higher overprediction of O_3 in coastal areas compared to CAMx, especially at the sites located in a water cell. CAMx appears to be biased high over areas far from the coast. In the nonattainment areas in the northeastern US, the 3x3 no water 2 method and 1x1 method seem to show better agreement on average between the two model-projected 2023 DVFs.

In our model simulations, inclusion of grid cells classified as water results in a relatively large difference, compared to measured DVs, as well as between CMAQ and CAMx projected DVs. In the nonattainment areas in the northeastern US, using different RRF calculation methods may result in different modeled attainment test outcomes, especially for CMAQ. The exclusion of water cells shows better agreement between the two model-projected DVFs. Further study in other nonattainment areas and different model years is needed to see if exclusion of water cells gives better projections of DVFs.

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