Application of the Segmented "Band-RRF" approach for 8-hour Ozone NAAQS Attainment Demonstration

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Introduction/Background:

The U.S EPA modeling guidance (2007) recommends using the Relative Response Factors (RRF) to project current Design Values (DV) into the future for the NAAQS attainment demonstration of ozone (O_3) and $PM_{2.5}$. However, it is known that higher O_3 mixing ratios are, in general, more responsive to emission controls of limiting precursors than lower mixing ratios are. The current form of the RRF concept does not allow for this enhanced response to emissions controls at the high end of the simulated/measured O_3 distribution and uses a single RRF value to represent a broad range of O_3 values in the baseline and future years.

We have developed segmented RRF approach termed "Band-RRF" that takes into account the varied model responses for different ranges of O_3 mixing ratios. The Band-RRF approach was previously demonstrated for the now-revoked 1-hour O_3 NAAQS in the San Joaquin Valley (SJV) (Kulkarni et. al., 2014). Here, we present the application of the band-RRF concept to the 8-hour O_3 NAAQS. We will also discuss the applicability of the Band-RRF concept to the 24-hour and annual $PM_{2.5}$ NAAQS.

Meteorological and Photochemical Modeling:

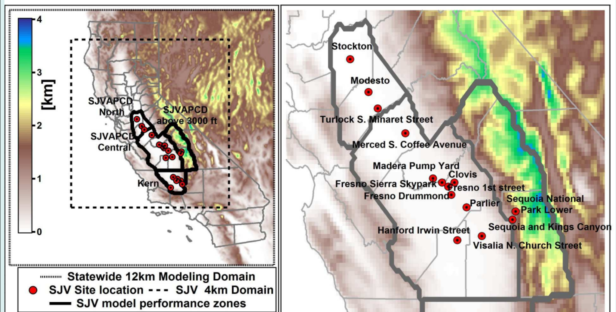

Figure 1: The ozone monitoring stations in the San Joaquin Valley (SJV). The outer box of the left panel is the California statewide 12 km modeling domain. The shaded and black line contours denote the gradients in topography (km) and the boundaries of sub regions used in model performance analysis. Simulations for this study were conducted using the 4 km inner modeling domain that covers the entire Central Valley of California. The insert on the right shows the zoomed in view of the site locations.

1. Meteorology Model: WRFv3.3.1
2. Air Quality Model: CMAQv4.7.1 with SAPRC99 chemical mechanism and the AERO5 aerosol module
3. Modeling Period: 2007 O_3 Season (May – September)
4. Biogenic emission inventory: 2007 inventory calculated by MEGAN with California-specific emission factors
5. Boundary conditions for the 12 km domain: MOZART global model output
6. Two sets of anthropogenic emission inventory: Day-specific 2007 and 2019 inventory for model performance evaluation, calculating relative response factors (RRFs) and future DVs
7. CMAQ simulations: Modeling of 2007 and 2019 using the day specific inventory for calculating future DVs

CMAQ Model Performance Statistics for 8-hour O_3

Table 1: Daily maximum 8-hour O_3 (> 60 ppb) performance statistics by modeling sub-regions and entire SJV region for May-September 2007 (See figure 1 for definition of sub-regions)

Parameter	SJVAPCD North	SJVAPCD Central	SJVAPCD above 3000 ft.	Kern	Entire SJV
Number of data points	67	641	221	590	1519
Mean obs (ppb)	67.6	71.2	79.6	74.2	73.4
Mean model (ppb)	77.9	74.3	73.5	73.8	74.2
Mean Bias (ppb)	10.3	3.1	-6.1	-0.4	0.7
Mean Error (ppb)	12.5	7.6	9	7.6	8
Normalized Mean Bias (%)	15.3	4.4	-7.6	-0.5	1
Normalized Mean Error (%)	18.6	10.7	11.3	10.2	10.9
Index of Agreement	0.46	0.69	0.62	0.73	0.68

Note: The statistical metrics used in this table are defined in Simon, H., Baker, K. R., and Phillips, S.: Compilation and interpretation of photochemical model performance statistics published between 2006 and 2012, Atmospheric Environment, 61, 124-139, 2012.

8-hour O_3 Band-RRF Methodology Details:

The 8-hour O_3 DV is the average of the annual 4th highest daily maximum 8-hour O_3 mixing ratios over three consecutive calendar years (U.S. EPA, 2008). The 2007 8-hour O_3 DVs (based on the 2005-2007 measurement period) are shown in the 2nd column of Table 2 for representative sites in the SJV region. (See Figure 1 for site locations).

We now describe the procedure of applying the Band-RRF concept to the 8-hour O_3 standard using the example of the Arvin monitoring site. The time series (Figure 2) of the observed (solid black circles) and simulated "nearby" (i.e., in a grid cell within a 15 km radius of the monitor) daily maximum 8-hour O_3 values (black solid line) at Arvin shows good agreement.

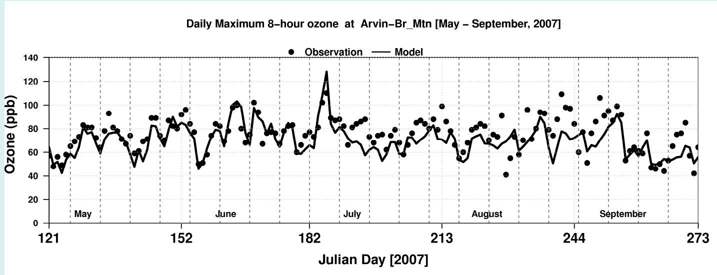

Figure 2: Time-series of observed (black circles), simulated (black line) daily maximum 8-hour O_3 for the simulation period (May-September 2007)

The calculation of future year 8-hr O_3 DV's using the Band-RRF approach involves the following steps as described in Kulkarni et al. (2014)

Calculation of Band-RRFs:

This builds upon the existing RRF approach. The reference-year simulated concentrations above a predetermined threshold (60 ppb for this work) were binned into regular 5 ppb bands from 60-100 ppb. All values above 100 ppb were segregated into a single band. Within each band, an RRF was calculated. The Figure 3 shows the Band-RRF values (y-axis) for each band (x-axis). The decrease in Band-RRF values with increasing band number confirms that the model is more responsive to emissions control at higher values. For the comparison, the "single" RRF for this site is shown as a dashed line parallel to the x-axis.

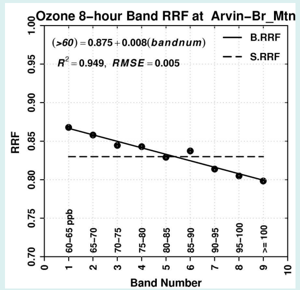

Figure 3: An illustration of the band-RRF procedure for Arvin site using the scatter plot of binned Band-RRF for 8-hour O_3 from 60 to 100 ppb (in 5 ppb increments) vs. the number of bands.

Representing the RRFs for missing bands of 8-hour O_3 mixing ratios:

To represent the missing bands, we performed a linear regression of available RRFs starting from the 60 ppb bin and only when at least three bands with simulated 8-hour O_3 mixing ratio $\geq$ 70 ppb were available (solid black line). We chose this criterion to prevent the lower less-responsive bands from dominating the fit.

Based on an analysis for all the representative SJV monitoring sites (not shown here) that are included in the SIP, we selected the 60 ppb threshold (with at least three bands that have simulated O_3 mixing ratio $\geq$ 70 ppb) for the Band-RRF regression. This choice increases the number of bands available for the regression and provides more stability. It also ensures that low values will not dominate the regression. In addition, including only the reference year data that fall within ±20% of the measured values in the RRF calculations further constrains the Band-RRF regression fit.

We have used the RRFs on the regression line for all bins instead of the actual Band-RRF points when available since the regression fit represents the average site specific RRF for that particular mixing ratio range. This approach also reduces the uncertainty caused by a band with very few data points (that are used in the RRF calculation for that particular band) and prevents it from having a disproportional impact on the future DV calculations.

Calculation of Future Year Design Value (DV):

To account for potential reshuffling of the annual 4th highest 8-hour O_3 mixing ratio, larger number of days (10 days per year with a total of 30 days during three years) were projected to the future and subsequently used in the future year DV calculation. The top 10 daily maximum 8-hour O_3 mixing ratios from each of the three years (i.e., 2005-2007) were projected to the future using the corresponding Band-RRFs, re-sorted, and the 4th highest 8-hour O_3 value was calculated at each monitor. The future DV is then calculated as the three-year average of the annual 4th highest O_3 mixing ratios at each monitor (4th column of Table 2). These DVs are in general lower than the corresponding single-RRF DVs (3rd column of Table 2). For instance, at the Arvin monitoring site, the Band-RRF-based future DV of 85.58 ppb is ~3 ppb lower than the corresponding single-RRF DV of 88.8 ppb.

Band-RRF 8-hour O_3 Future DVs

Table 2: 2007 and 2019 O_3 DVs for representative monitoring sites in the San Joaquin Valley of California. Listed here are the top 10 2007 DV sites for 8-hour O_3.

Monitoring Station	DV (ppb) Ambient (2005-2007)[a]	DV (ppb) Single (2007-2019)[b]	DV (ppb) Band (2007-2019)[b]
Arvin	107	88.8	85.5
Sequoia – King's Canyon	103	86.2	84.7
Edison	99	83.2	81.0
Fresno 1st street	98	81.6	78.3
Bakersfield	97	81.3	79.0
Fresno Sierra Skypark	95	79.1	76.1
Sequoia National Park	95	81.0	81.6
Visalia N. Church Street	95	80.4	78.7
Clovis	93	77.1	75.0
Parlier	93	76.7	74.3
Oildale	91	74.5	73.1

[a]The three year period included in the ambient design value calculations.
[b]The base year 2007 and future year 2019 used for air quality model simulations used in this study.

Extending Band-RRF to $PM_{2.5}$

Figure 4 illustrates that the high $PM_{2.5}$ concentrations respond more to emissions controls in a similar manner as ozone. The four panels in Figure 4 show daily 2019/2007 $PM_{2.5}$ ratios as functions of 2007 simulated $PM_{2.5}$ concentrations for four representative locations in the SJV. The simulated $PM_{2.5}$ data used in Figure 4 are described in Chen et al. (2014). One can follow the same procedural steps that were described for the 8-hour O_3 NAAQS to calculate the quarter- and component-specific RRFs for the $PM_{2.5}$ species.

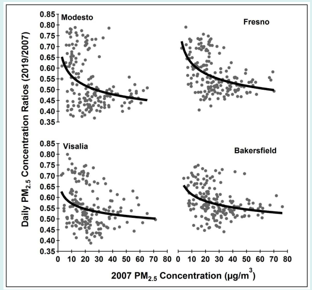

Figure 4: The daily concentration ratios (2019/2007) for total $PM_{2.5}$. The solid line represents the power form of the regression.

Implications:

Results of photochemical models are used in regulatory applications in a relative sense using Relative Response Factors (RRFs) which represent effects of emissions reductions over a wide range of ozone (O_3) values. It is possible to extend the concept of RRFs to account for the fact that higher O_3 mixing ratios (both 1-hour and 8-hour) respond more to emissions controls of limiting precursors than do lower O_3 mixing ratios. We demonstrate this extended concept, termed Band-RRF, for the 1-hour and 8-hour O_3 National Ambient Air Quality Standard (NAAQS or standard) in the San Joaquin Valley of California. This extension can also be made applicable to the 24-hour and annual $PM_{2.5}$ standards.

References:

- Chen, J., Lu, J., Avise, J., DaMassa, J., Kleeman, M.J., and Kaduwela, A.P. 2014. Seasonal Modeling of $PM_{2.5}$ in California's San Joaquin Valley. *Atmos. Environ.*, 92, 182-190. doi:/10.1016/j.atmosenv.2014.04.030
- Kulkarni, S., Kaduwela, A.P., Avise, J.C., DaMassa, J.A., and Chau, D. 2014. An extended approach to calculate the ozone relative response factors used in the attainment demonstration for the National Ambient Air Quality Standards *J. Air & Waste Management Association*, **64**(10), 1204-1213. doi:10.1080/10962247.2014.936984.
- U.S. Environmental Protection Agency. 2007. Guidance on the use of models and other analyses for demonstrating attainment of air quality goals for ozone, $PM_{2.5}$, and regional haze. EPA-454/B07-002. http://www.epa.gov/scram001/guidance/guide/final-03-pm-rh-guidance.pdf
- U.S. Environmental Protection Agency. 2008. Guideline on the data handling conventions for the 8-hour ozone NAAQS. EPA-454/R-98-017. http://www.epa.gov/ttn/caaa/t1/memoranda/guidefin.pdf

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