Model Performance Review at Monitors with Complex Meteorology Land-Water Interfaces

Prepared by:

Alpine Geophysics, LLC

387 Pollard Mine Road

Burnsville, NC 28714

January 2016

EPA ozone attainment modeling guidance[1] states that "[t]he most important factor to consider when establishing grid cell size is model response to emissions controls. Analysis of ambient data, sensitivity modeling, and past modeling results can be used to evaluate the expected response to emissions controls at various horizontal resolutions for both ozone and PM2.5 and regional haze. If model response is expected to be different (and presumably more accurate) at higher resolution, then higher resolution modeling should be considered. If model response is expected to be similar at both high and low(er) resolution, then high resolution modeling may not be necessary. *The use of grid resolution finer than 12 km would generally be more appropriate for areas with a combination of complex meteorology, strong gradients in emissions sources, and/or land-water interfaces in or near the nonattainment area(s).*" (emphasis added)

In its recent modeling for the Cross State Air Pollution Rule (CSAPR), EPA simulated a national domain using a 12km grid resolution domain wide. While this makes running a national, regional simulation easier from a technical perspective, it ends up neglecting the important issue of the complex meteorology and/or land-water interfaces in or near the nonattainment or maintenance monitors of interest.

Photochemical modeling along coastlines is complex for two reasons. Firstly, the temperature gradients along land/water interfaces can lead to localized on-shore/off-shore flows; and secondly the photochemical model formulation spreads the emissions in a grid cell throughout the full grid volume of the cell.

Given the importance of certain monitors located in areas of complex meteorology, an analysis was undertaken to examine the performance of the model when compared against observations, and to examine how the model results are used in the attainment test calculation to determine estimated future attainment status.

Figures 1 and 2 present two unique areas in the eastern U.S. that are challenged by these complex meteorology land-water interfaces. For each monitor, we have reviewed the EPA published model performance evaluation (MPE) metrics for ozone and compared them to additional MPE metrics from the same modeling platform.

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[1] http://www3.epa.gov/scram001/guidance/guide/Draft_O3-PM-RH_Modeling_Guidance-2014.pdf

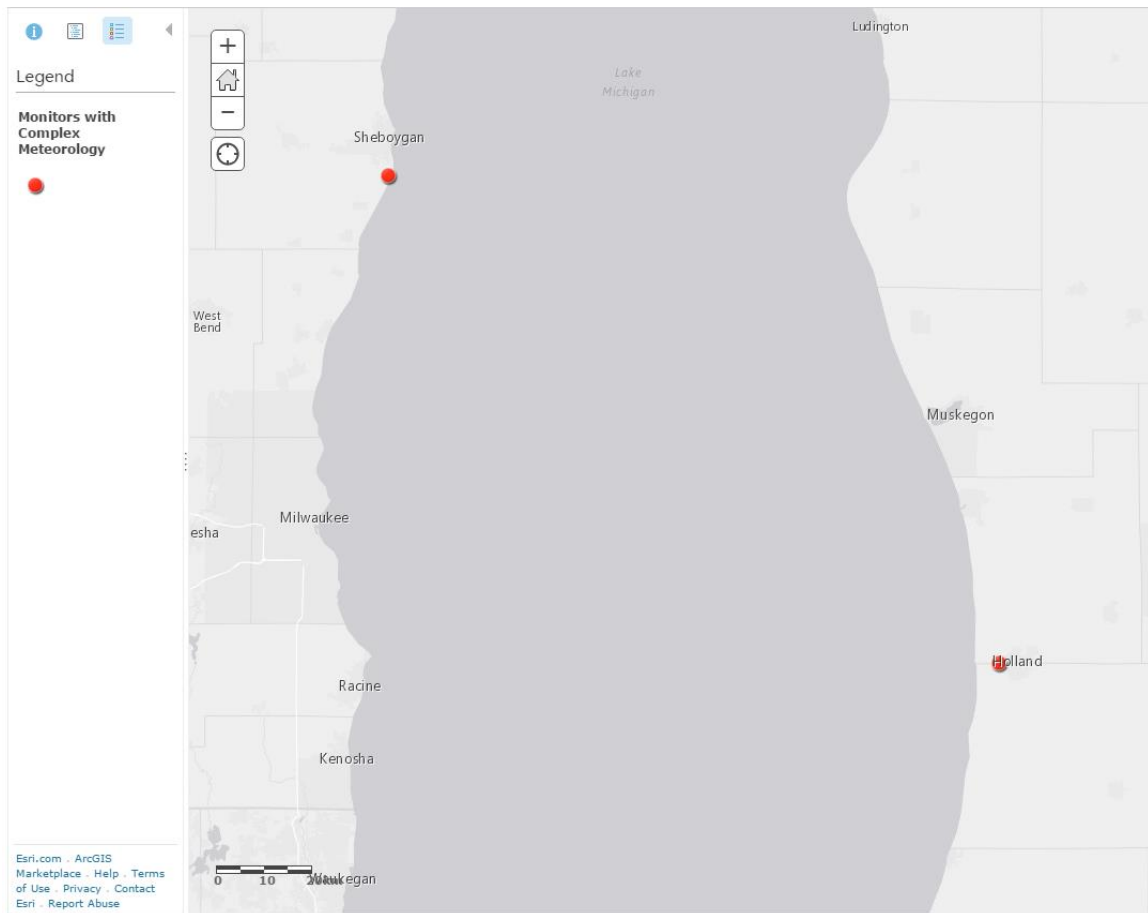**Figure 1.** Connecticut monitors located on land/water interface.

Figure 2. Wisconsin and Michigan monitors located on land/water interface.

Figures 3, 4, and 5 are representations of these monitors and the EPA 12km grid cell spacing used in the CSAPR modeling, attainment demonstration, and significant contribution determination. As is noted, for each of the monitors identified (grey shaded cell), a portion of the grid cell is located over or adjacent to a water body. Studies indicate that air quality forecast models typically predict large summertime ozone abundances over water relative to land in the Great Lakes region[2] and that meteorology around the Long Island Sound is distinctly unique[3]; both warranting individualized attention and the fine grid resolution required to best account for these issues.

Additionally, the 3x3 neighborhood of grid cells used in determining the design values of the relative response factor (RRF) extends into the water bodies. This 3x3 is highlighted for each monitor in each figure. Under current guidance, the top ten modeled days within this 3x3 matrix are used in determining this RRF for each monitor. In this analysis we review the performance of the days selected for use in the RRF calculation for the grid cells determined to have been used in the attainment test.

Six monitors were initially identified for this review and are listed in Table 1 with EPA's performance metrics for days observed at or above 60 ppb as documented in the air quality TSD (AQTSD)[4]. EPA notes that the performance evaluation was conducted comparing observed concentration data with the modeled concentration data simulated in the grid cell in which the monitor was located. In reviewing this table, considering all days observed at or above 60 ppb, both the NMB and NME fall within the thresholds identified above. Based on this broad indicator of model performance (all days observed at or above 60 ppb) the model appears to be performing adequately.

In the AQTSD, EPA presents time series graphics comparing the model estimated and observed MDA8 ozone for May through September 2011, reproduced here as Figure 6. Note that while the model (red) does generally track the ozone observations (black) at each monitor, on many days the model overestimates the observed peaks.

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[2] http://www.atmos-chem-phys.net/15/5109/2015/acp-15-5109-2015.html
[3] http://www.ct.gov/deep/lib/deep/air/regulations/proposed_and_reports/section_2.pdf
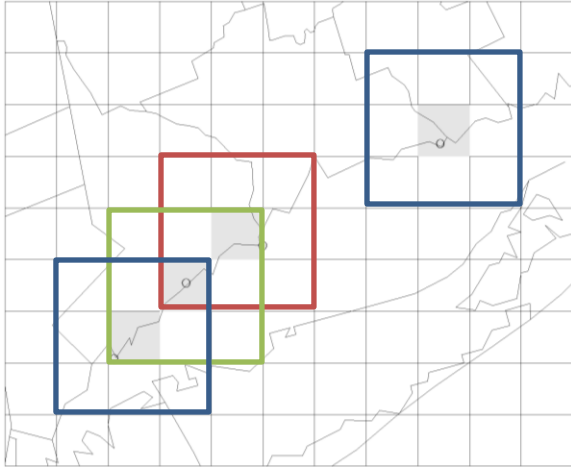[4] http://www3.epa.gov/crossstaterule/pdfs/AQModeling.pdf

Figure 3. Connecticut monitor 12km grid cells and representative 3x3 neighborhood.
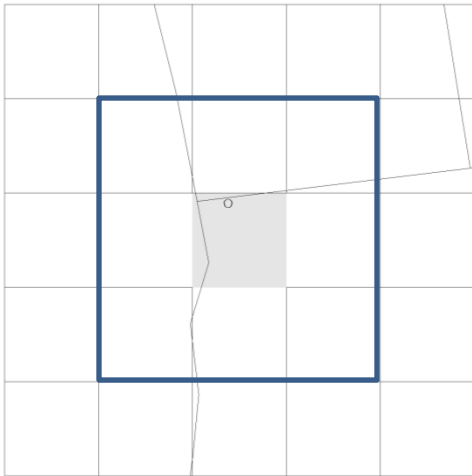

Figure 4. Michigan monitor 12km grid cells and representative 3x3 neighborhood.
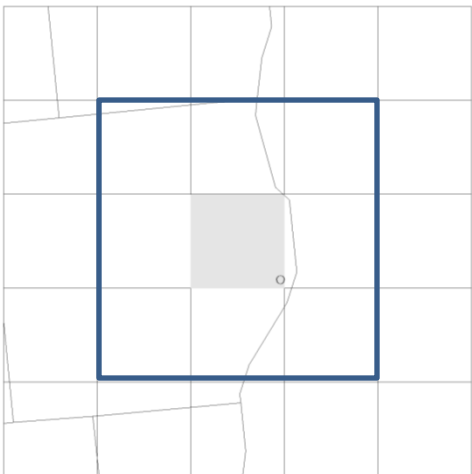

Figure 5. Wisconsin monitor 12km grid cells and representative 3x3 neighborhood.

Table 1. EPA May-September 2011 Ozone Model Performance Statistics for Days with Observations >= 60 ppb

Monitor	State	County	Number of Obs >= 60 ppb	Obs Mean (ppb)	Model Mean (ppb)	Mean Bias (ppb)	Mean Error (ppb)	Normalized Mean Bias (NMB)	Normalized Mean Error (NME)	Fractional Bias	Fractional Error
90010017	Connecticut	Fairfield	28	69.65	71.63	1.98	11.88	2.84	17.06	0.3	17.1
90013007	Connecticut	Fairfield	26	72.95	74.31	1.35	9.47	1.86	12.98	1.2	12.3
90019003	Connecticut	Fairfield	29	71.95	75.00	3.05	8.82	4.23	12.25	3.5	11.2
90093002	Connecticut	New Haven	25	74.28	77.87	3.60	9.20	4.84	12.39	4.5	11.8
260050003	Michigan	Allegan	33	69.33	69.84	0.51	8.39	0.73	12.10	-0.2	11.8
551170006	Wisconsin	Sheboygan	26	72.94	65.79	-7.15	11.11	-9.80	15.23	-10.3	15.7

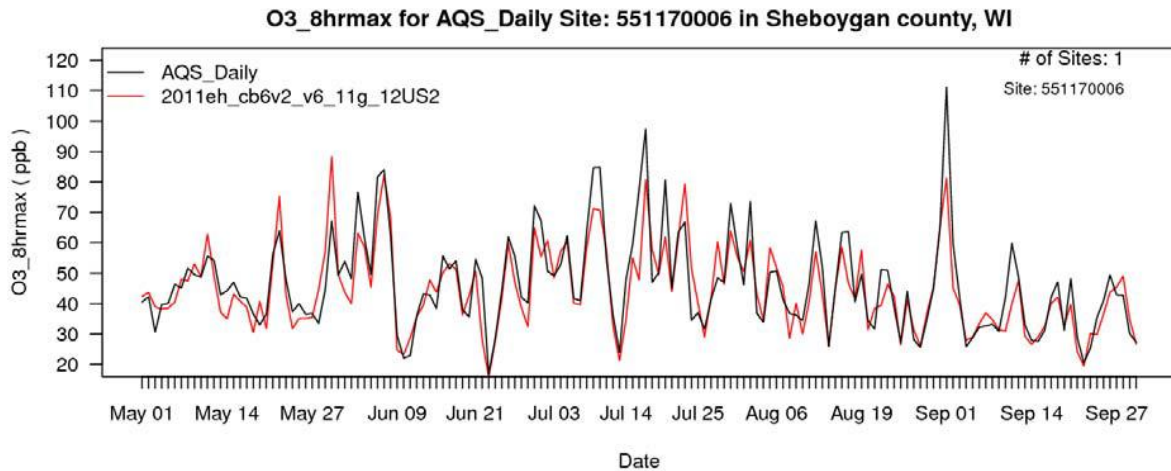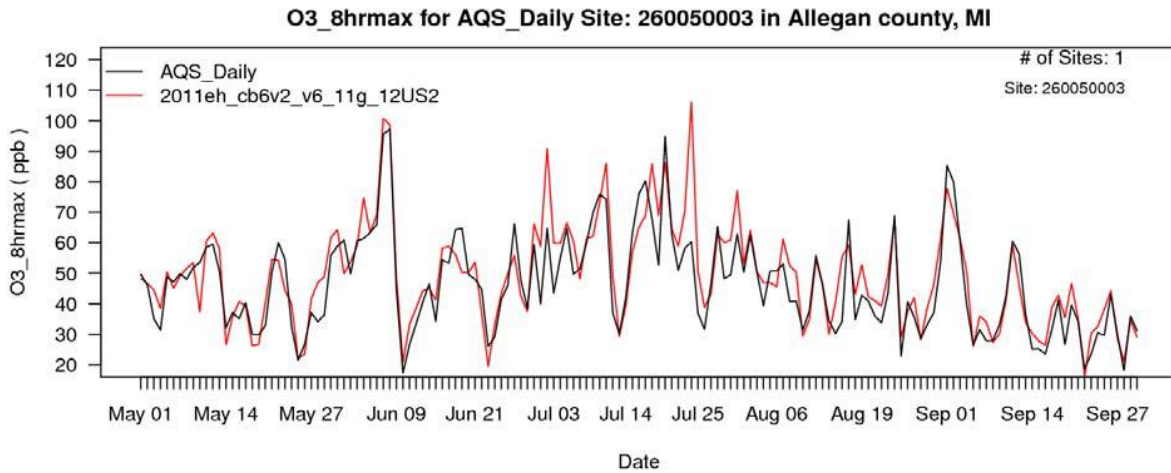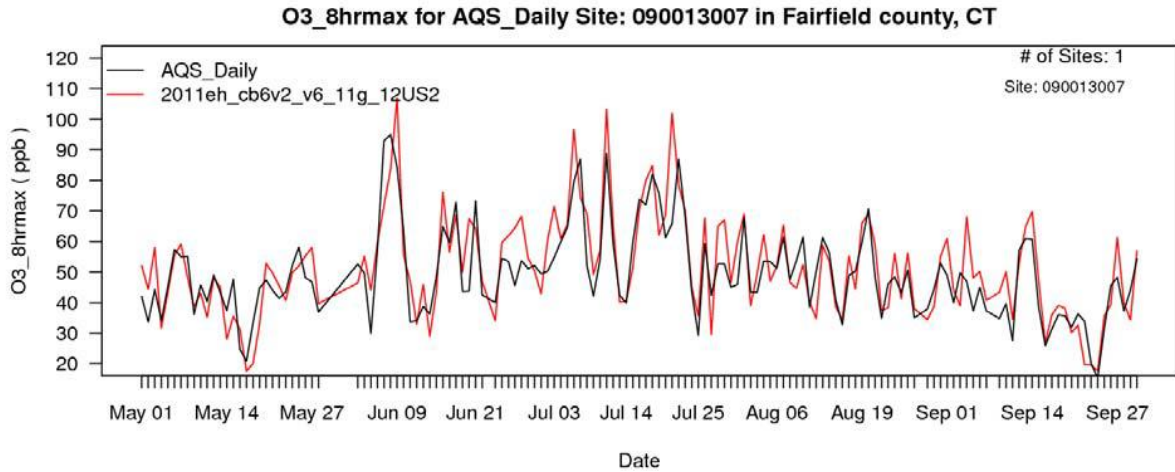Table source: 2011 ozone MPE Statistics, EPA-HQ-OAR-2015-0500-0013

Figure 6. Time series of observed (black) and predicted (red) MDA8 ozone for May through September 2011 at sites 090013007 in Fairfield Co., Connecticut (top), 26005003 in Allegan Co., Michigan (middle), and 551170006 in Sheboygan Co., Wisconsin (bottom).

It is also important to understand how the model is performing on the days that are being used in the attainment demonstration. As suggested in the draft EPA modeling guidance, and used in the CSAPR proposed rule, only the top 10 days with the highest modeled concentration in the vicinity of the monitoring site are considered.

To review this important issue, we generated the performance metrics for these three example monitors using the days selected in the MATS attainment test, and for days selected for the MATS attainment test with the associated grid cell concentration actually used in the RRF calculation (max concentration in the 3x3 grid).

Our analysis is an attempt to determine how the individual days selected for the attainment test are performing compared to all the other days observed at or above 60 ppb and whether the days selected are within the thresholds of the model performance. We further investigate whether the air quality model has performed well enough at 12km for these monitors to be considered adequate for future year attainment demonstrations and control strategy / significance determinations in the proposed rule.

The days selected and the associated observed and modeled concentration values are presented in Table 3. The performance statistics for these monitors on these days are presented in Table 4.

As is seen in Table 3, the MDA8 concentration value used to represent each monitor-day in the performance evaluations ("3x3 Center") is always lower and generally significantly lower than the maximum grid cell ("3x3 Max") used in the RRF calculation. This difference is calculated in the column titled "Delta ppb" and ranges from a low of 3.17 ppb (at Fairfield on July 6, 2011) to 29.84 ppb (at Sheboygan on July 30). The impact of this change results in poorer performance on these days at these monitors and in RRFs weighted to concentrations calculated over the water bodies and not to the grid cells and land-based grids more representative of the monitor's conditions.

Table 4 presents the Performance metrics have been calculated for the 10 RRF days using both the 3x3 center concentration and the 3x3 maximum concentration values. It can clearly be seen in this table that the monitor-sited, 3x3 center concentrations have much lower bias and error values than the over-water 3x3 maximum concentrations. And while it is recognized that the base year grid cell and future year grid cell will be paired (as used in the relative sense), the resulting RRF could show more or less responsiveness in emissions changes relative to the ozone concentrations at each associated monitor.

Figure 7 is a graphical representation of the number of times a particular grid cell's concentration was selected for the RRF calculation. As can be seen in this graphic, with blue highlighted areas to represent water boundaries, while the EPA performance evaluation and metrics are based on the ability of the model to simulate observed concentrations in the center cell where the monitor is located, in each example presented, the highest concentrations are dominantly selected from over-water cells.

Table 3. 10 Days Selected for MATS RRF Calculation at Example Monitors

| Monitor | Mon | Day | Year | MDA8 Ozone Conc. (ppb) | | | Delta ppb |
				Obs.	3x3 Center	3x3 Max	(Max - Center)
90013007	6	9	2011	84	106.79	122.21	15.42
	7	21	2011	65	102.08	114.90	12.82
	6	8	2011	95	83.44	112.78	29.34
	7	11	2011	88	103.31	106.48	3.17
	7	22	2011	87	78.48	102.61	24.13
	7	6	2011	79	96.69	100.40	3.71
	7	18	2011	82	84.76	98.08	13.33
	7	17	2011	72	79.96	90.80	10.84
	8	1	2011	67	69.00	86.68	17.68
	7	23	2011	68	70.08	86.13	16.05
260050003	7	24	2011	60	106.09	131.52	25.43
	7	2	2011	64	90.88	119.11	28.23
	6	7	2011	95	100.81	110.39	9.58
	6	8	2011	97	98.62	107.17	8.55
	7	11	2011	74	85.91	103.07	17.16
	7	31	2011	62	76.93	99.48	22.55
	7	20	2011	94	86.33	97.63	11.30
	7	18	2011	67	85.88	93.39	7.51
	9	1	2011	85	77.84	93.01	15.17
	7	10	2011	75	73.27	87.95	14.68
551170006	7	17	2011	97	80.72	99.20	18.48
	9	1	2011	111	81.21	96.49	15.28
	5	30	2011	67	88.29	94.14	5.85
	7	30	2011	72	63.78	93.62	29.84
	6	7	2011	84	82.28	91.59	9.31
	7	10	2011	84	70.68	91.37	20.69
	7	20	2011	80	61.92	87.31	25.39
	7	23	2011	66	79.26	87.00	7.74
	5	22	2011	63	75.21	86.86	11.65
	7	5	2011	62	60.29	83.63	23.34

Table 4. 2011 Ozone Model Performance Statistics for 10 Days Selected for MATS RRF Calculations

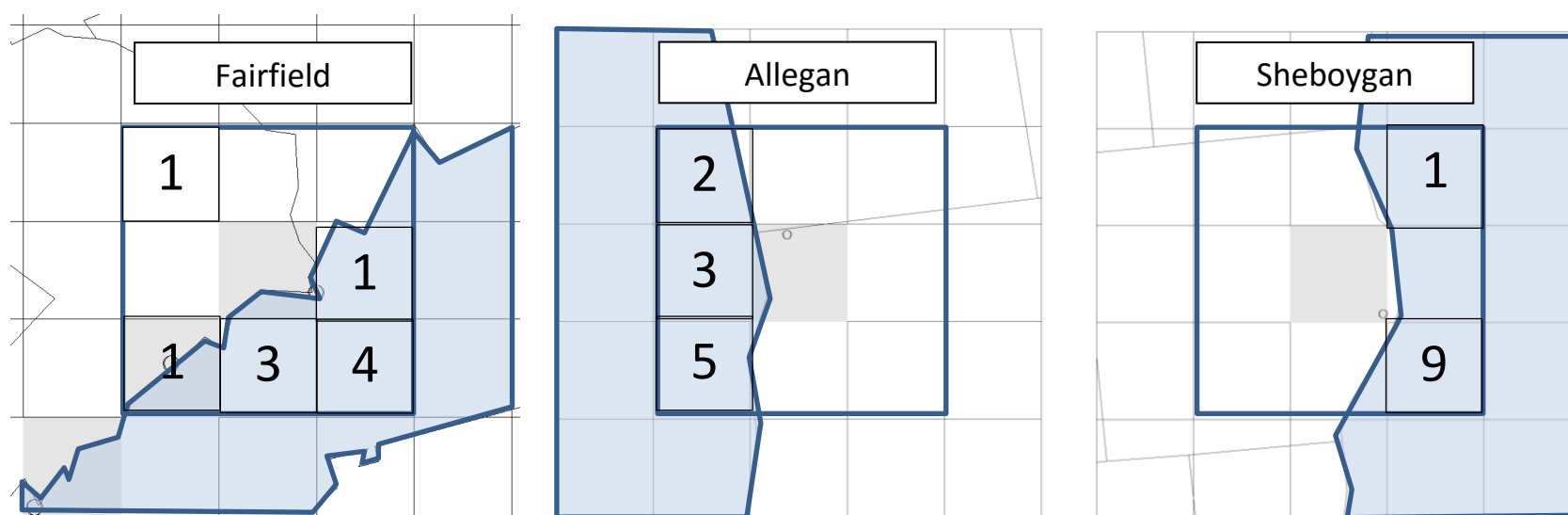| Monitor	State	County	Simulation	Obs Mean (ppb)	Model Mean (ppb)	Mean Bias (ppb)	Mean Error (ppb)	Normalized Mean Bias (NMB)	Normalized Mean Error (NME)	Fractional Bias	Fractional Error
90013007	Connecticut	Fairfield	3x3 center	78.70	87.46	8.76	12.77	11.13	16.23	10.1	16.6
			3x3 maximum	78.70	102.11	23.41	23.41	29.74	29.74	25.9	30.9
260050003	Michigan	Allegan	3x3 center	77.30	88.26	10.96	14.27	14.17	18.46	13.9	21.4
			3x3 maximum	77.30	104.27	26.97	26.97	34.89	34.89	30.1	40.2
551170006	Wisconsin	Sheboygan	3x3 center	78.60	74.37	-4.23	13.59	-5.39	17.29	-4.6	17.0
			3x3 maximum	78.60	91.12	12.52	15.42	15.93	19.62	16.3	21.7

Figure 7. Number of times grid cell concentration was selected for RRF calculation for example monitors; Fairfield, Allegan, Sheboygan (L to R). Water boundaries highlighted in blue.

Based on these results and on EPA's own guidance related to finer grid cell size selection for areas demonstrating a combination of complex meteorology, strong gradients in emissions sources, and/or land-water interfaces in or near the nonattainment area(s), we find that the 3x3 maximum ozone concentrations selected at these land/water boundary locations are insufficiently accurate, in both bias and error, to be considered as representative of the daily concentrations observed at each monitor and for the ten days selected for the RRF calculation.

Furthermore, we note that this poor performance will have a direct impact on the future year attainment demonstration and significant contribution calculations that use these values as their basis.