Examples of criteria assessment using 4-D interpolation results for entire CB4 segment.

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Elgin S. Perry, Ph. D.
377 Resolutions Rd., Colonial Beach, Va. 22443
phone: 410-610-1473
email: eperry@chesapeake.net

One of the primary motivations behind development of the 4-D interpolation procedure is to create a tool for assessing short time duration Dissolved Oxygen Criteria such as the instantaneous minimum and the weekly mean. Development of the 4-D interpolator is at a stage where it is possible to begin testing methods for assessing these short-term criteria. In this document we present the results of testing assessment of the instantaneous minimum and the weekly mean criteria for the open water designated use in the entirety of segment CB4.

The scope of the interpolations for CB4 extended for the entire year of 2022. Each stochastic interpolation provides hourly predictions on a spatial domain defined by 886 1 km x 1 km surface cells defined by the current interpolator grid, and at depths at 1-meter increments down to the bottom as defined by the bathymetry at each surface cell. The result is 8760 hourly predictions for each of 3,809 spatial cells for a total of 33,366,840 spatio-temporal cells in each stochastic interpolation. One hundred of these interpolation simulations have been computed and stored, but the examples shown here use only ten of the one hundred.

It should be noted that concepts of testing the CFD and 10% rule presented here are the same as previously presented for a small number of cells in CB4. However, scaling these evaluations up to the level of a full segment has entailed some computational and data management challenges which have been overcome by our Tetra-tech partners.

These criteria assessment examples are computed for the period 6/1/2022-8/31/2022 in each of the 3,809 spatial cells of CB4 which reduces the scope to 2208 hours and a total of 8,410,272 spatio-temporal cells. While the summer assessment period ends on September 30, this illustration ends with August 31 to facilitate comparison to the Gooses Reef Vertical Array observations for the same period.

For this exercise, the open water is restricted to 1-5 meters of depth. In the future, the open water will be delimited by the pycnocline, but at present, this dynamic pycnocline feature remains under development.

Instantaneous Minimum Examples

The open water instantaneous minimum criterion is assessed by comparing the hourly predictions for the assessment period to the summer instantaneous minimum criterion of 3.2 mg/l. Each prediction in the interpolation domain defined by: latitude (1km), longitude (1km), depth(1m), and time(1hr), is compared to the summer instantaneous minimum criterion of 3.2 mg/l to determine pass/fail. The cell-by-cell pass/fail results are aggregated over the segment following the CFD methodology of the 2003 Criterion addendum (EPA 2003). Briefly, the fraction of violations across all spatial cells, latitude, longitude and depth, in the assessment period is computed for each hour. These hourly fractions of space are then ranked from largest to smallest and assigned fraction of time values by the formula (rank / N+1) where N is to total number of hours in the assessment period. For each simulation, these paired space and time values are plotted in cartesian coordinates and compared to a standard reference line (Figure 1.) The ten simulation curves illustrate uncertainty in the CFD assessment.

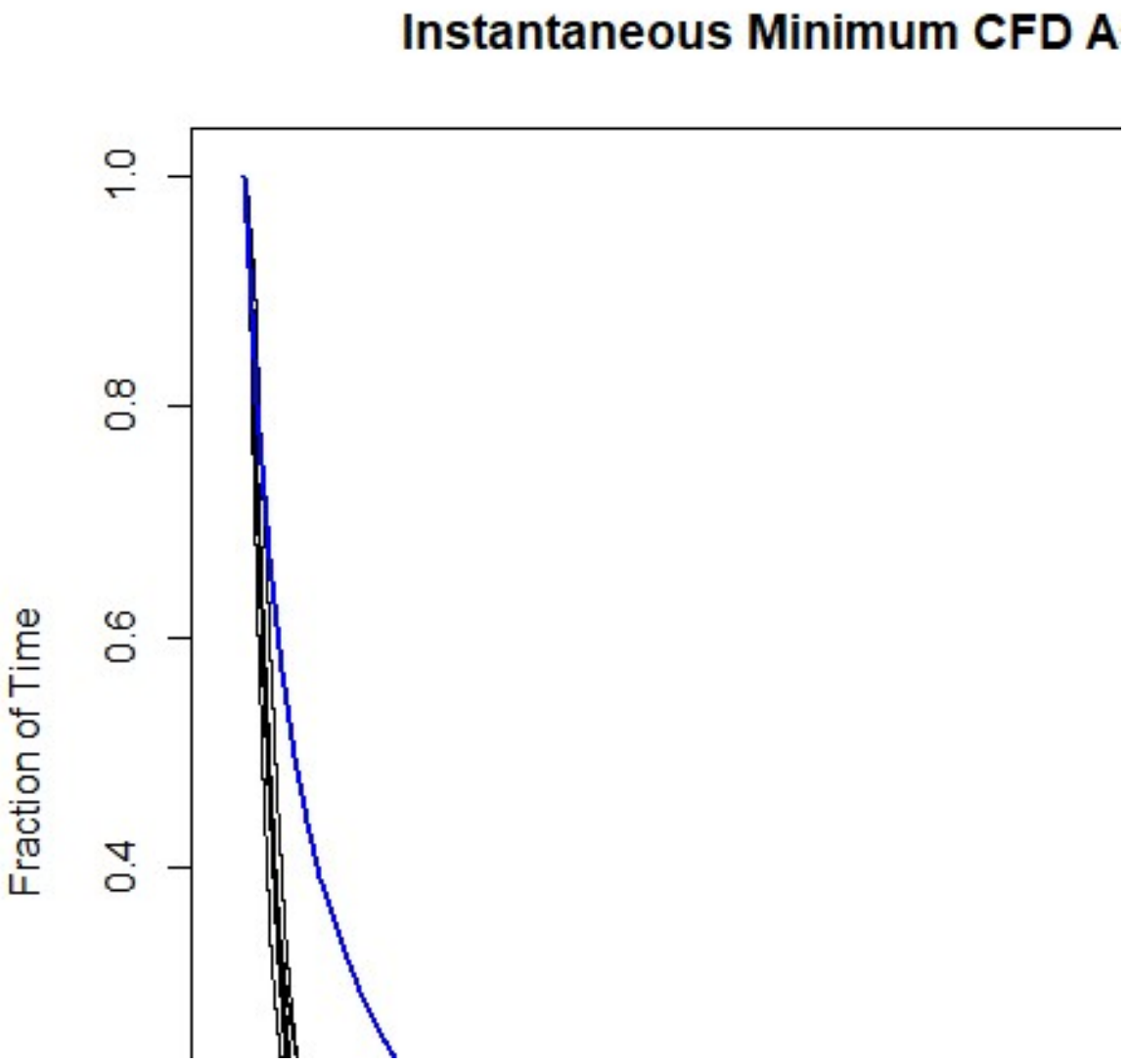


Figure 1. CFD assessment curves for the instantaneous minimum criterion in segment CB4 for the period 6/1/2022-8/31/2022.

In addition to the CFD assessment, it might be worth considering if the instantaneous minimum could be evaluated using a simple 10% rule. This is not the approach currently used for tidal criteria assessment in the Chesapeake Bay, but it has been considered in the past, and has the benefit of being simpler to understand. For this possible assessment, the fraction of violations over the 4-dimensional domain defined by time, latitude, longitude, and depth dimensions is computed for each simulation (Table 1.) A non-parametric density function (Figure 2.) was estimated for these fractions and is used to illustrate the uncertainty of the mean violation rate for segment CB4 and the probability of exceeding 0.10. For this example, the probability of exceeding 10% is estimated to be less than 0.0001.

Table 1. Fraction of Instantaneous Minimum Violations Over Space and Time for Each of Ten Simulations.

simulation	criteria violations	count	fraction violations
1	222070	8410272	0.026
2	245999	8410272	0.029
3	281274	8410272	0.033
4	274834	8410272	0.033
5	224135	8410272	0.027
6	189384	8410272	0.023
7	259074	8410272	0.031
8	240456	8410272	0.029
9	233703	8410272	0.028
10	215423	8410272	0.026

Count = 3809 spatial cells x 2208 hours = 8410272 interpolator cells

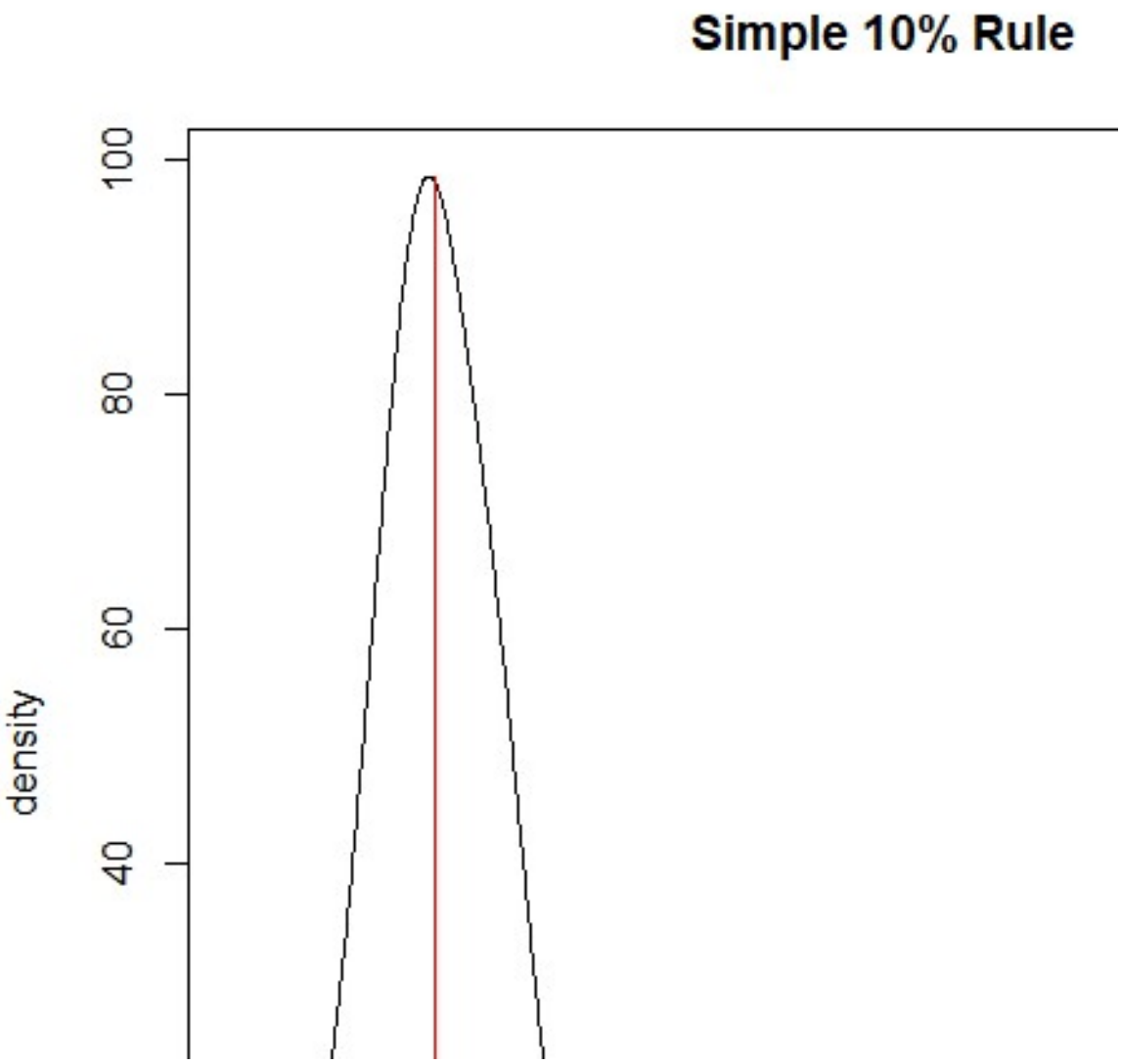


Figure 2. The Density function (black line) is estimated from 10 simulations of fraction of violations in segment CB4. The mean violation rate = 0.028 (red line). The blue line shows the 10% threshold and the probability of exceeding the 100% threshold is less than 0.0001.

Weekly Mean Examples

Weekly mean criteria have not been assessed to-date in the tidal Chesapeake Bay. Considering how they could be evaluated led us to an initial question of how to compute a weekly mean. Therefore, the weekly mean criterion assessment is illustrated by two methods in these examples. One method partitions the full assessment time period into sequential weeks and the other uses a moving window approach to define the population of weeks. Both methods are computed from the hourly predictions described above. The sequential weeks method defines weeks as independent groups of seven days beginning with the first day of the assessment period. For this assessment period, there are 13 sequential weeks and the remainder at the end of the period is excluded from the assessment (Table 2). The population of weeks for the moving window approach is defined by overlapping weeks starting a week on each day of the assessment period and continuing on to one week from the end (Figure 3, Table 2). There are 86 moving window weeks in the assessment period.

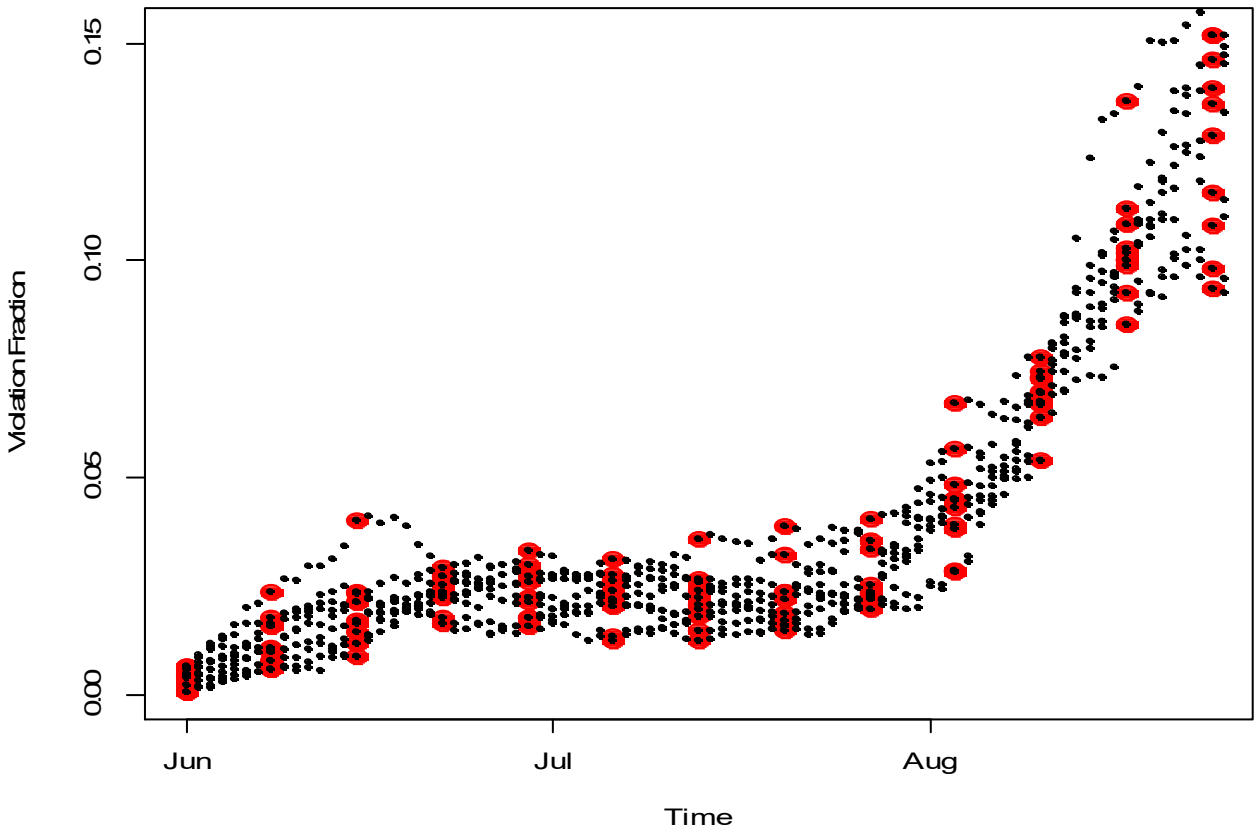


Figure 3. Sequential Weekly Means (red) and Moving Window Weekly Means (black) of fraction of violations as a function of time for 10 simulations in segment CB4 during the period 6/1/2022 – 8/31/2022.

Table 2. Illustration of Sequential Week Means vs. Moving Window Week Means using artificial data.

Day	Daily DO	Sequential Week Means	Moving Window Weeks							MWW Means
1	8.04									
2	6.96									
3	6.43									
4	5.82									
5	7.74									
6	8.27									
7	6.15	7.06	7.06							7.06
8	6.45			6.83						6.83
9	6.43				6.76					6.76
10	8.01					6.98				6.98
11	8.11						7.31			7.31
12	5.75							7.02		7.02
13	8.66								7.08	7.08
14	7.08	7.21	7.21							7.21
15	8.88			7.56						7.56
16	8.07				7.79					7.79
17	8.84					7.91				7.91
18	5.06						7.48			7.48
19	8.25							7.83		7.83
20	9.47								7.95	7.95
21	5.62	7.74	7.74							7.74
22	8.82			7.73						7.73
23	5.31				7.34					7.34
24	8.62					7.31				7.31
25	8.08						7.74			7.74
26	7.69							7.66		7.66
27	6.83								7.28	7.28
28	6.99	7.48	7.48							7.48
29	7.18			7.24						7.24
30	7.47	7.33			7.55					7.55

For both methods the weekly mean DO is computed for each spatial cell in each week. For each spatial cell the weekly mean DO is compared to the criterion and then violations are aggregated across space to estimate the spatial fraction of violations for each week. The weekly fractions of violations are then ranked and presented as the CFD for each simulation. The two methods of averaging produce similar results. Both show a high frequency of a small fraction of space out of compliance (Figures 4 and 5, upper left black lines on the right of the blue line) to a degree that violates the default reference curve. This shows there is a small amount of area of this segment that is almost always violating the weekly mean criteria during this example period.

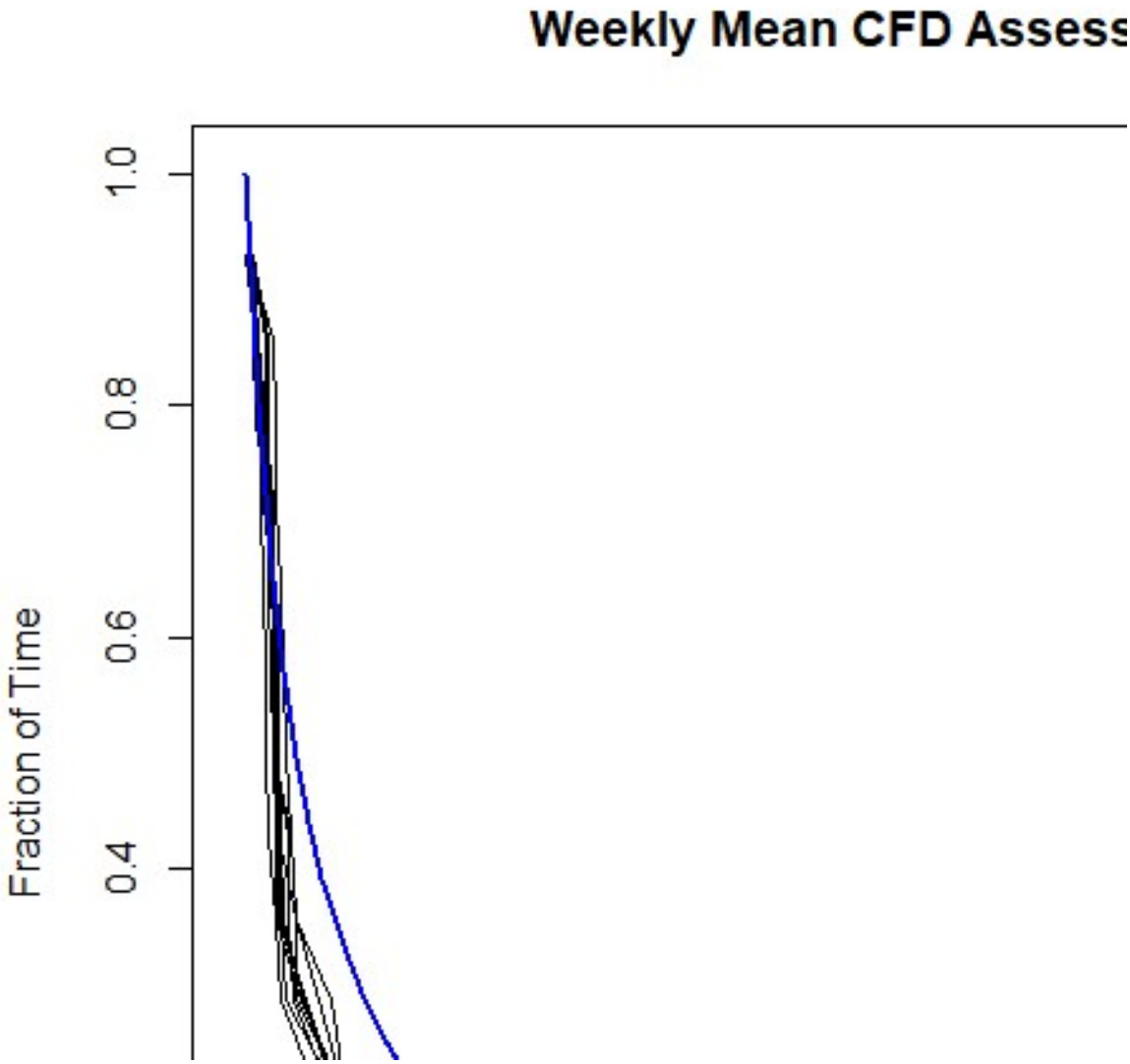


Figure 4. CFD assessment curves for the weekly mean criterion in segment CB4 for the period 6/1/2022-8/31/2022 using 13 sequential weeks.

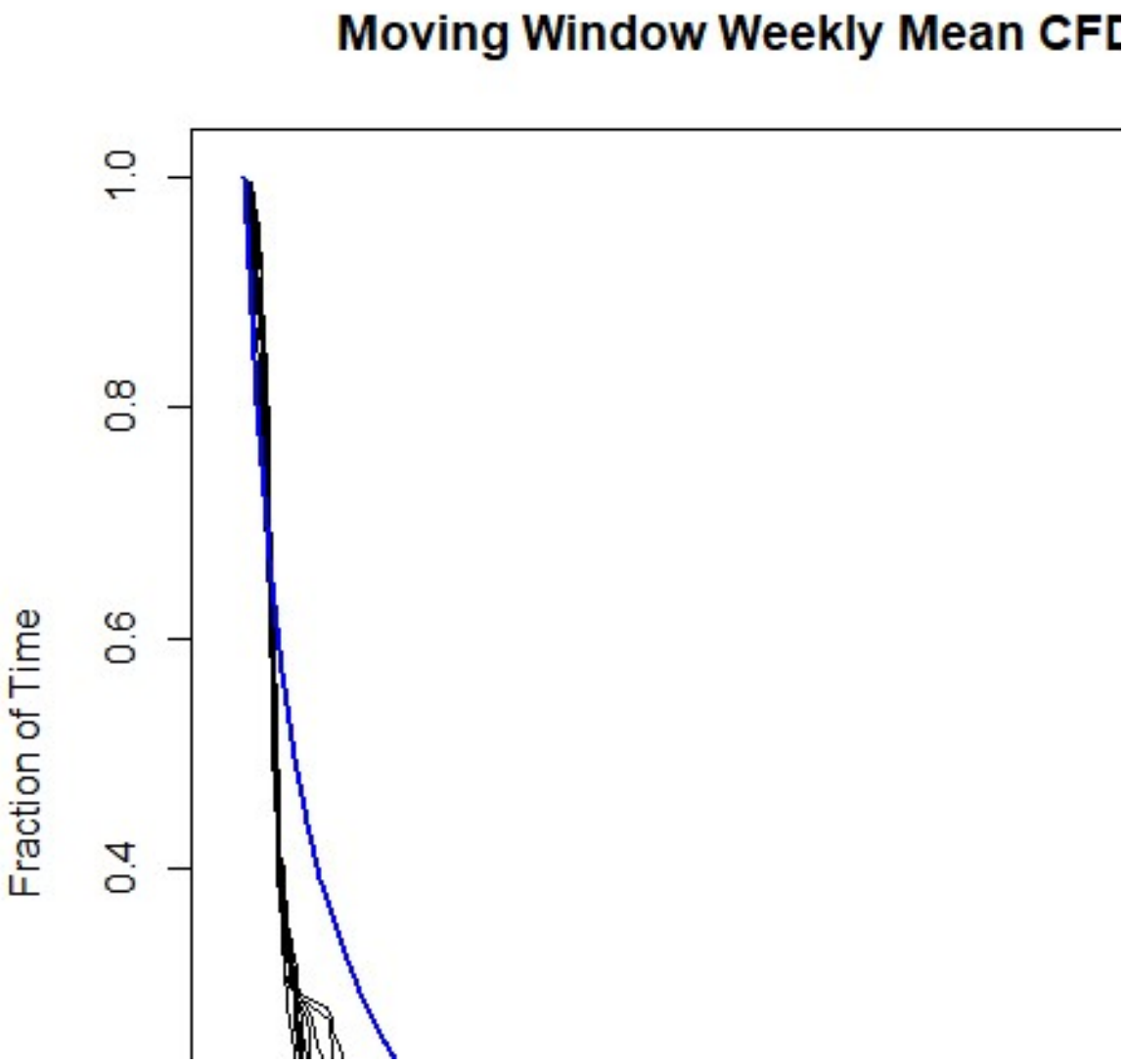


Figure 5. CFD assessment curves for the weekly mean criterion in segment CB4 for the period 6/1/2022-8/31/2022 using 86 moving window weeks.

For comparison, the weekly mean criterion is also assessed by the simple 10% rule based on the fraction of violations over the 4-dimensional domain for both sequential weeks (Table 3, Figure 6.) and moving window weeks (Table 4., Figure 7.) By both methods, the violation rate is well below the 10% threshold, and the violation rates are similar. The sequential weeks yields a mean violation rate of 0.040 and the moving window weeks method estimates violations at 0.039.

Table 3. Fraction of Sequential Weekly Mean Violations Over Space and Time for Each of Ten Simulations.

simulation	criteria violations	count	fraction violations
1	1826	49517	0.037
2	2063	49517	0.042
3	2372	49517	0.048
4	2222	49517	0.045
5	1886	49517	0.038
6	1491	49517	0.03
7	2242	49517	0.045
8	1980	49517	0.04
9	1970	49517	0.04
10	1775	49517	0.036

Count = 3809 spatial cells x 13 sequential weeks = 49517 cells

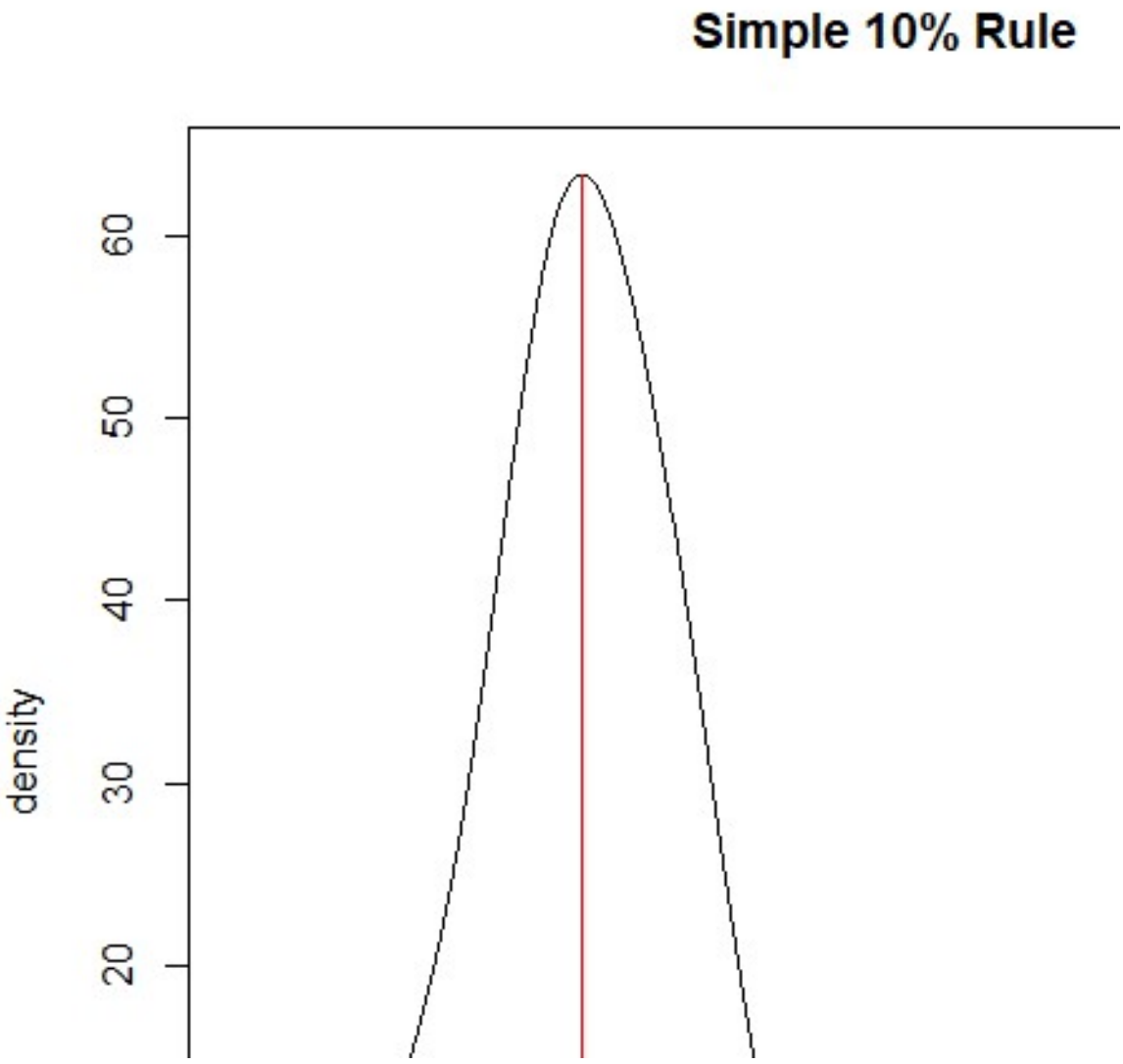


Figure 6. The Density function (black line) is estimated using 10 simulations of fraction of violations of the weekly mean criterion using sequential weeks in segment CB4. The mean violation rate = 0.040 (red line). The blue line shows the 10% threshold and the probability of exceeding the 100% threshold is less than 0.0001.

Table 4. Fraction of Moving Window Weekly Mean Violations Over Space and Time for Each of Ten Simulations.

simulation	criteria violations	count	fraction violations
1	11974	327574	0.037
2	13112	327574	0.04
3	15446	327574	0.047
4	14692	327574	0.045
5	12450	327574	0.038
6	9953	327574	0.03
7	14252	327574	0.044
8	12350	327574	0.038
9	12778	327574	0.039
10	11339	327574	0.035

Count = 3809 spatial cells x 86 sequential weeks = 327574 cells

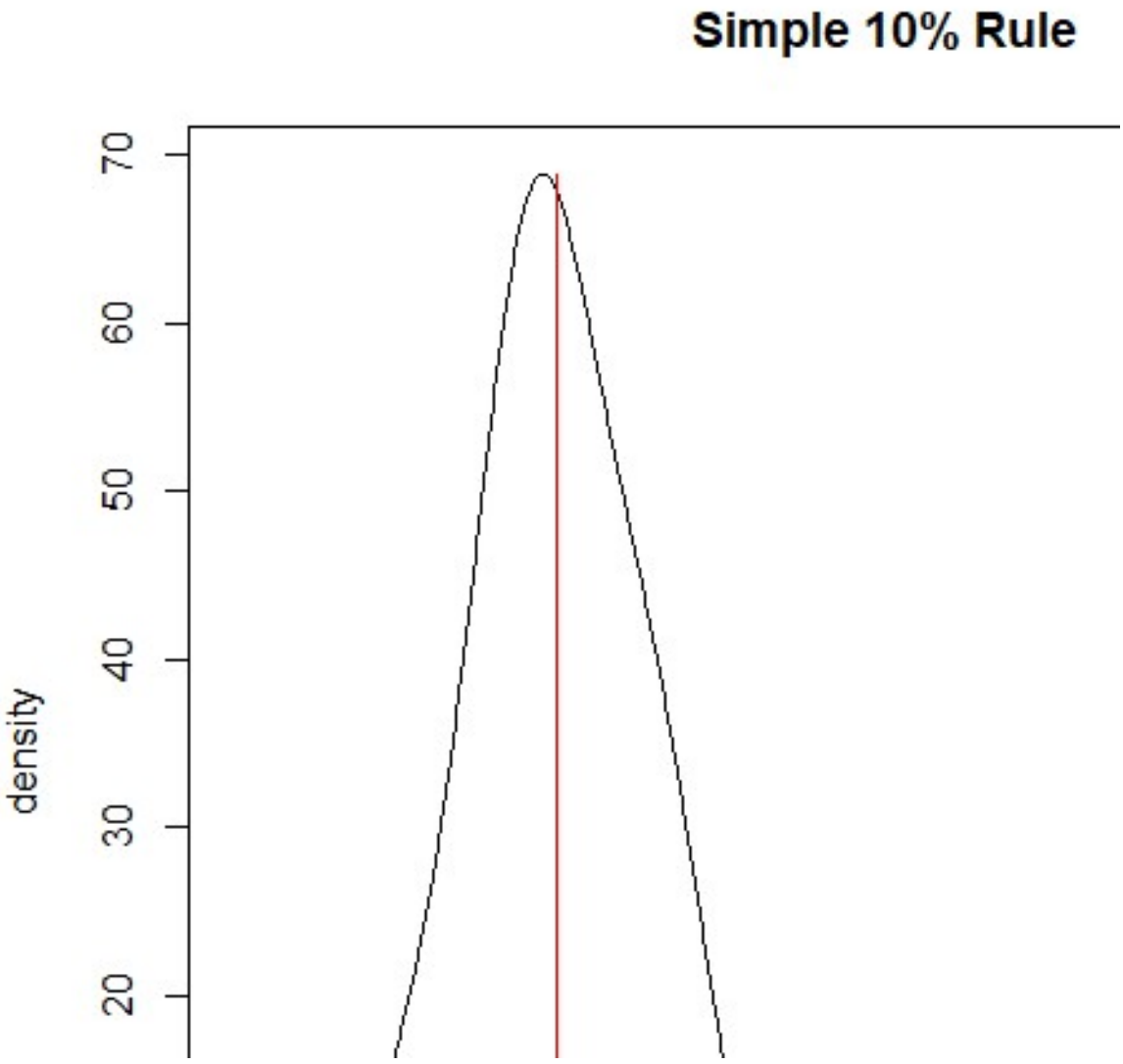
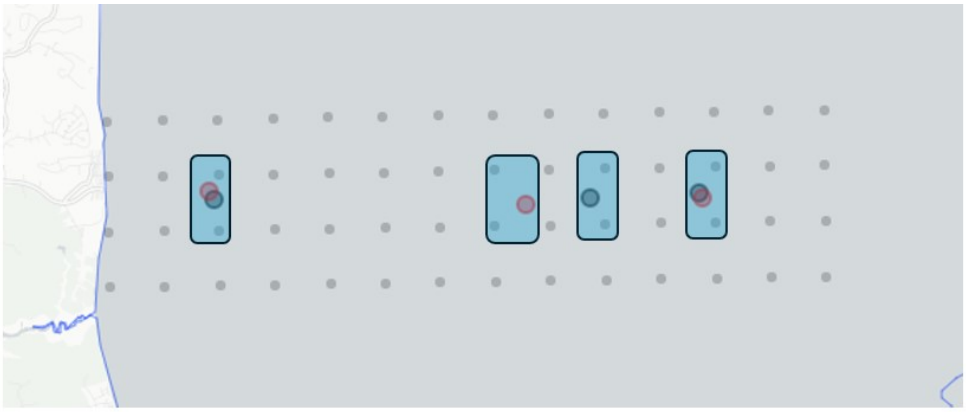


Figure 7. The Density function (black line) is estimated using 10 simulations of fraction of violations of the weekly mean criterion using moving window weeks in segment CB4. The mean violation rate = 0.039 (red line). The blue line shows the 10% threshold and the probability of exceeding the 10% threshold is less than 0.0001.

Comparison to Gooses Bottom Reef Vertical Array Data

To get a comparison to observed data, the instantaneous minimum violation rate for the open water depths of the East and West Gooses Reef vertical arrays are compared to neighboring cells of the 4-D interpolator that are just to the north and south of the array locations. (Figure 8.) This is the data that was collected by NOAA in 2022 (https://sensors.ioos.us/#metadata/114122/station/data and https://sensors.ioos.us/#metadata/114123/station/data). Tidal water quality criteria assessment in the Chesapeake Bay is on the segment and designated use scale. This comparison to monitoring data is only at a very small spatial scale in order to understand and evaluate the interpolation results, not to provide a method for conducting an assessment.



Station	UIDSTR	Depths
CB4.3W	3700004269000, 3700004268000	1, 3, 5, 7, 9
west-gooses	i=2, j=3	
CB4.3C	3750004269000, 3750004268000 *(bottom depth closest to CB4.3C)*	1, 3, 5, 7, 9, 11, 13, 15, 17, 19, 21, 23, 25
XEF3551	3770004269000, 3770004268000	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12
CB4.3E	3790004269000, 3790004268000	1, 3, 5, 7, 9, 11, 13, 15, 17, 19, 21, 23, 24
east-gooses		

Figure 8. The interpolator grid superimposed with fixed stations (red) and East and West Gooses Reef Vertical Array Locations.

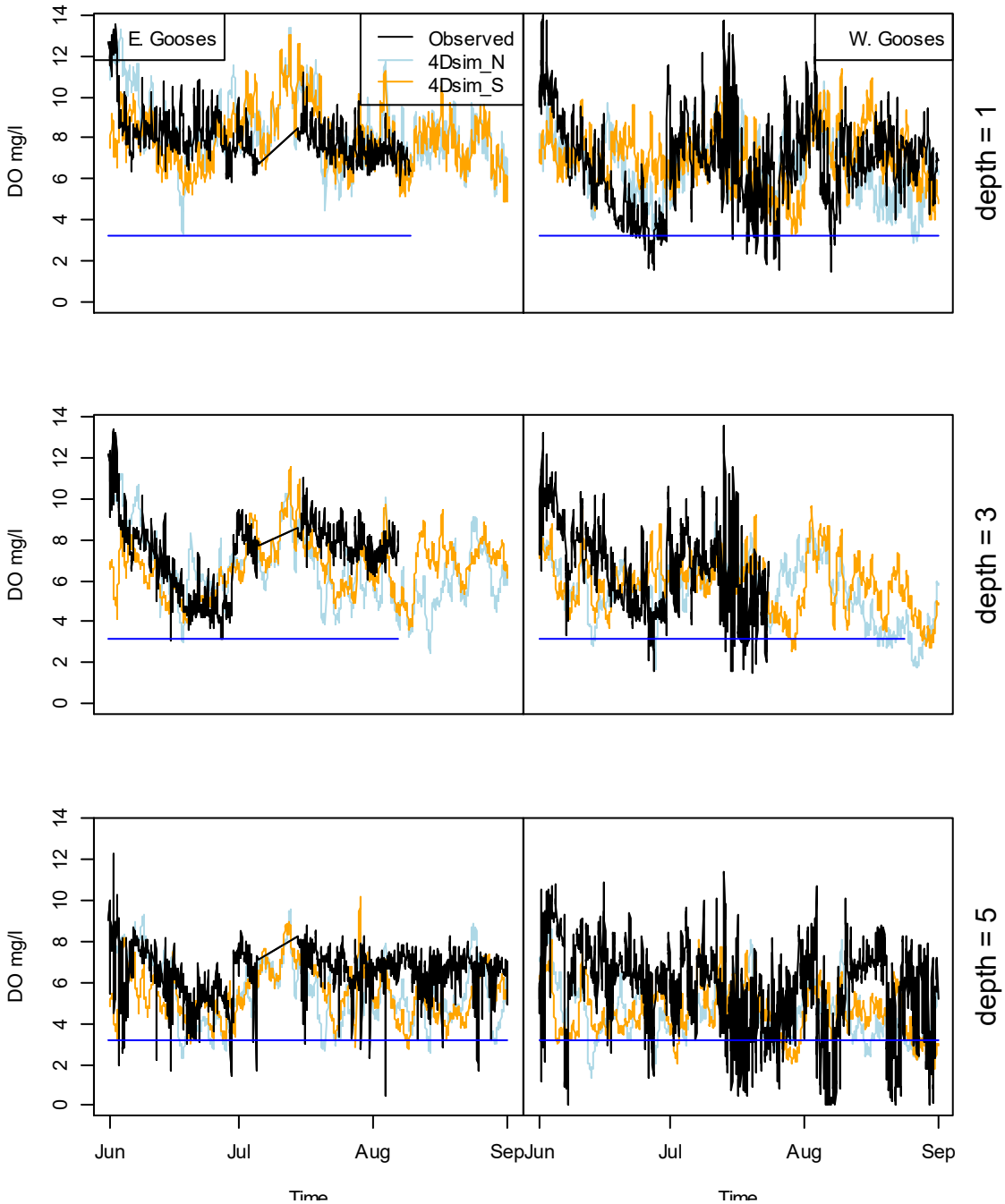


Figure 9. Comparison of simulated 4-D data (blue and orange) to observed data (black) for the Gooses Reef vertical array sites. The horizontal blue line shows the instantaneous minimum criterion. Simulated data just to the north of the observed site is in blue and to the south is in orange. Three depths (1,3,5) for the assessment period (6/1/2022 – 8/31/2022) are shown.

A comparison of the observed time series (Figure 9) for the East and West Gooses sites to nearby 4D interpolator grid cells shows that simulated data reflect the mean trends and the temporal autocorrelation of the observed data quite well.

Table 5. Fraction of violations for East Gooses Vertical Array for depths 1-5 for period 2022-06-01 to 2022-08-31.

Location	Violations	Count	Fraction
East Gooses Vertical Array	42	4747	0.0088
West Gooses Vertical Array	442	5624	0.0786

The observed data for West Gooses site is showing a higher violation rate than the East Gooses Site (Table 5.).

The mean violation rates for each interpolator grid cell near the observations is computed over the assessment period and shown below (Table 6.) for each of 10 simulations. The predictions of the interpolator reflect the lower violation rate seen also from the observed data near the East Gooses Reef site as compared to West. The range of predictions over the 10 simulations covers the observed violation rate presented in Table 6. For the East Gooses site, all of the simulations are well below the 10% threshold. For the West Gooses site, 6 out of 20 simulations exceed the 10% threshold.

Table 6. Open Water Interpolator Predictions from 10 Simulations Near Gooses Reef Vertical Array.

Simulation	West Goose grid cell 1	West Goose grid cell 2	East Goose grid cell 1	East Goose grid cell 2
1	0.0457	0.076	0.0025	0.0146
2	0.0507	0.0517	0.0208	0.0027
3	0.1293	0.0818	0.001	0.0014
4	0.1121	0.1431	0.0272	0.0092
5	0.0418	0.0766	0.0106	0.0088
6	0.0971	0.154	0.0093	0.0151
7	0.1555	0.076	0.0065	0.0036
8	0.0617	0.1064	0.0168	0.0032
9	0.0683	0.0542	0.0176	0.0012
10	0.0644	0.0991	5e-04	0.0064

Range for East Gooses Cells: 0.00005 - 0.0272
Range for West Gooses Cells: 0.0418 - 0.1555

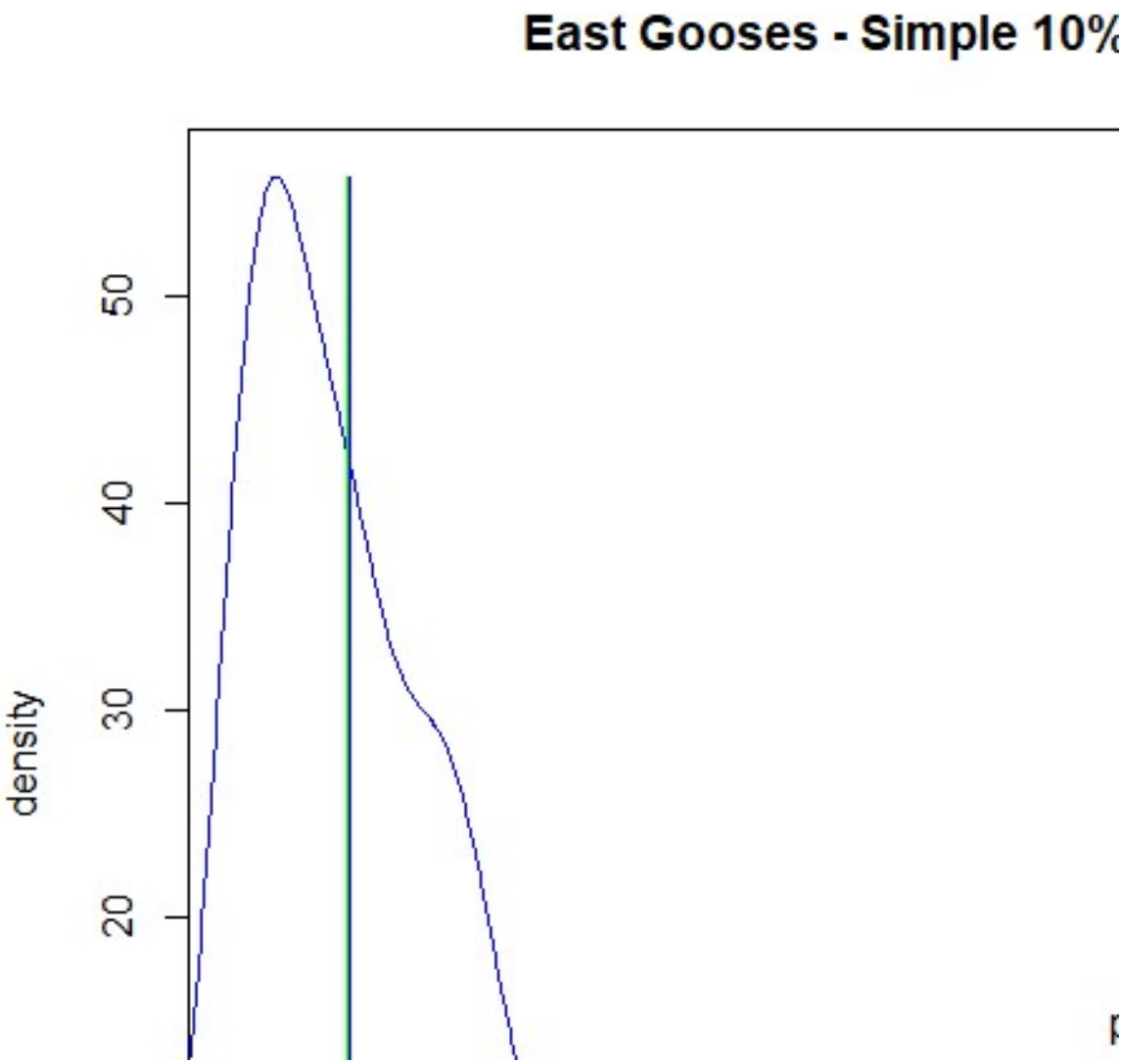


Figure 10. Density function (blue) estimate for interpolator predictions near the East Gooses array site with the mean observed violation rate based on array observations.

Using the 20 interpolator observations from the two interpolator cells paired with each vertical array site, density functions were estimated and plotted with the observed mean violation rate super-imposed (Figures 10 and 11). The observed violation rate for each array location is near the mean of the predicted simulation distribution for that location (compare green and blue vertical lines) and both the observed mean (green vertical line) and the mean of the simulated values (blue vertical line) are below the 10% threshold for each site.

For the East Gooses Bottom site, the simulation frequencies show that the likelihood of exceeding the 10% threshold is very small (<0.0001). This implies that DO in the vicinity of East Gooses is clearly in compliance with the weekly mean criterion.

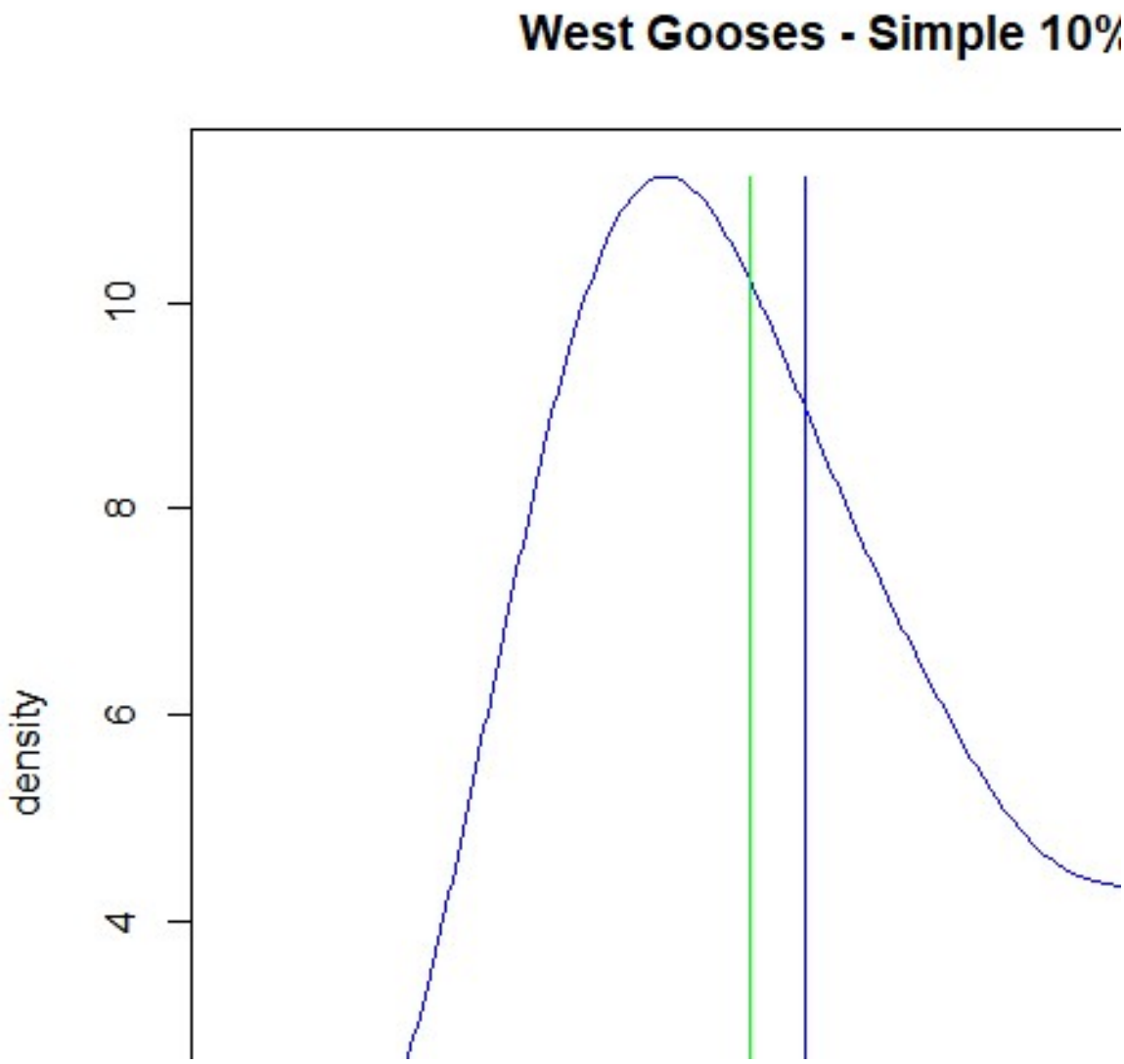


Figure 11. Density function (blue) estimate for interpolator predictions near the West Gooses array site with the mean observed violation rate based on array observations (green).

However, the simulation frequencies for the West Gooses site show that the likelihood of exceeding the 10% threshold is about one in three. This implies that DO in the vicinity of West Gooses Bottom has non-trivial likelihood of violating the 10% threshold.

This comparison to two high frequency data sets in one segment shows how variable DO conditions can be within a region and also serves as a good check on the interpolation method to ensure that it is capturing that variability in the data.

Citation:

[EPA] Environmental Protection Agency (US). 2003. Ambient Water Quality Criteria for Dissolved Oxygen, Water Clarity and Chlorophyll *a* for the Chesapeake Bay and Its Tidal Tributaries. Annapolis (MD): EPA. 219 p. EPA 903-R-03-002. (Available: http://www.chesapeakebay.net/search/pubs.htm)

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