

Pycnocline approach for 4-D interpolator

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For Bay Oxygen Research Group Development Team update

March 17, 2025

Outline today

- Background/current approach
- Decision points for pycnocline with 4-D interpolation tool
 - Overall approach
 - Temporal resolution
- Proposed method
- Example results
- Comparison to current approach
- Next steps

Background

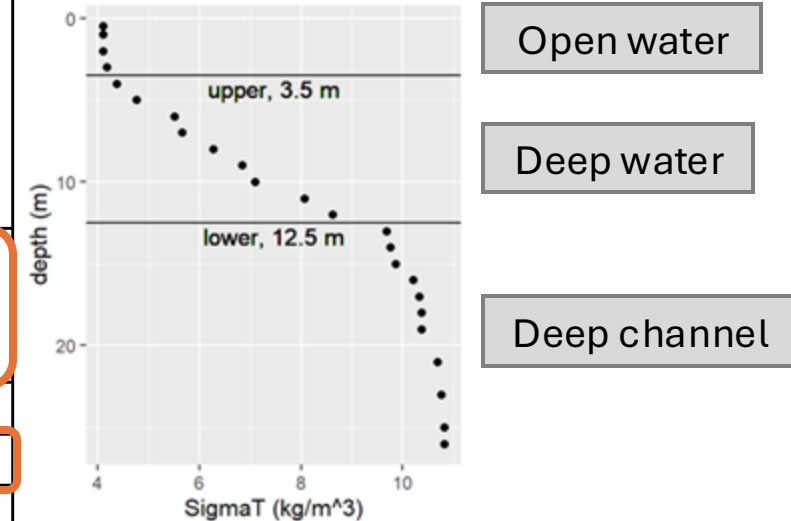
Table 1. Chesapeake Bay dissolved oxygen criteria.

Designated Use	Criteria Concentration/Duration	Protection Provided	Temporal Application
Migratory fish spawning and nursery use	7-day mean $\geq 6 \text{ mg liter}^{-1}$ (tidal habitats with 0-0.5 ppt salinity)	Survival/growth of larval/juvenile tidal-fresh resident fish; protective of threatened/endangered species.	February 1 - May 31
	Instantaneous minimum $\geq 5 \text{ mg liter}^{-1}$	Survival and growth of larval/juvenile migratory fish; protective of threatened/endangered species.	
	Open-water fish and shellfish designated use criteria apply		June 1 - January 31
Shallow-water bay grass use	Open-water fish and shellfish designated use criteria apply		Year-round
Open-water fish and shellfish use	30-day mean $\geq 5.5 \text{ mg liter}^{-1}$ (tidal habitats with 0-0.5 ppt salinity)	Growth of tidal-fresh juvenile and adult fish; protective of threatened/endangered species.	Year-round
	30-day mean $\geq 5 \text{ mg liter}^{-1}$ (tidal habitats with >0.5 ppt salinity)	Growth of larval, juvenile and adult fish and shellfish; protective of threatened/endangered species.	
	7-day mean $\geq 4 \text{ mg liter}^{-1}$	Survival of open-water fish larvae.	
	Instantaneous minimum $\geq 3.2 \text{ mg liter}^{-1}$	Survival of threatened/endangered sturgeon species. ¹	
Deep-water seasonal fish and shellfish use	30-day mean $\geq 3 \text{ mg liter}^{-1}$	Survival and recruitment of bay anchovy eggs and larvae.	June 1 - September 30
	1-day mean $\geq 2.3 \text{ mg liter}^{-1}$	Survival of open-water juvenile and adult fish.	
	Instantaneous minimum $\geq 1.7 \text{ mg liter}^{-1}$	Survival of bay anchovy eggs and larvae.	
	Open-water fish and shellfish designated-use criteria apply		October 1 - May 31
Deep-channel seasonal refuge use	Instantaneous minimum $\geq 1 \text{ mg liter}^{-1}$	Survival of bottom-dwelling worms and clams.	June 1 - September 30
	Open-water fish and shellfish designated use criteria apply		October 1 - May 31

¹ At temperatures considered stressful to shortnose sturgeon ($>29^{\circ}\text{C}$), dissolved oxygen concentrations above an instantaneous minimum of $4.3 \text{ mg liter}^{-1}$ will protect survival of this listed sturgeon species.

Summer designated uses are identified from the density-stratified layers of the water column

Density and Pycnoclines:
CB4.3C on 7-11-2017



Current approach

*Note: Only applies to summer and certain segments.
There are more details to these steps.*

Chapter 3 of the September 2008 Addendum to EPA's Criteria Assessment documentation (EPA 2008):

- **Density computation**
 - Compile the vertical columns of salinity and temperature data for each station for a cruise;
 - Compute water density from the salinity and temperature.
- **Pycnocline identification**
 - Throughout a vertical column of data, compute the density and salinity gradients with depth;
 - Using those gradients, for each column of data, identify the shallowest stable density slope $>0.1 \text{ kg/m}^3/\text{m}$ as the upper limit of the pycnocline;
 - If an upper pycnocline exists, identify a lower boundary to the pycnocline as the deepest stable density gradient $>0.2 \text{ kg/m}^3/\text{m}$,
- **Interpolate the upper and lower pycnocline boundary depths: for a bi-weekly cruise (or monthly average)**
 - Spatially interpolate the upper pycnocline depth on the segment's interpolation grid (using IDW);
 - Compute the fraction of the water column below the lower pycnocline at each monitoring station;
 - Spatially interpolate the fraction of the water column below the lower pycnocline. Note, this is 0 if there is no lower pycnocline;
 - Compute the depth of the lower pycnocline at each grid cell based on the fraction interpolated and the bottom depth.
- **Split each cruise or month's DO interpolation results into the designated uses by the pycnocline boundaries.**

4-D Pycnocline: overall approach

Options:

1. Compute density from vertical columns of data first, then interpolate the upper and lower pycnocline depths in space and time.
2. Interpolate salinity and temperature in space and time, then compute pycnocline boundaries.

→ To reduce how much is changed from the current approach, we moved forward with Option 1 in development.

→ Along with temporal considerations, Option 2 may be something to circle back to in the future once the 4D interpolator is established.

4-D Pycnocline: temporal approach

- High frequency data indicates pycnocline moves a lot, certainly at more than bi-monthly
- Use 2 vertical high frequency stations to explore this

NOAA data from East Goose vertical array in 2022

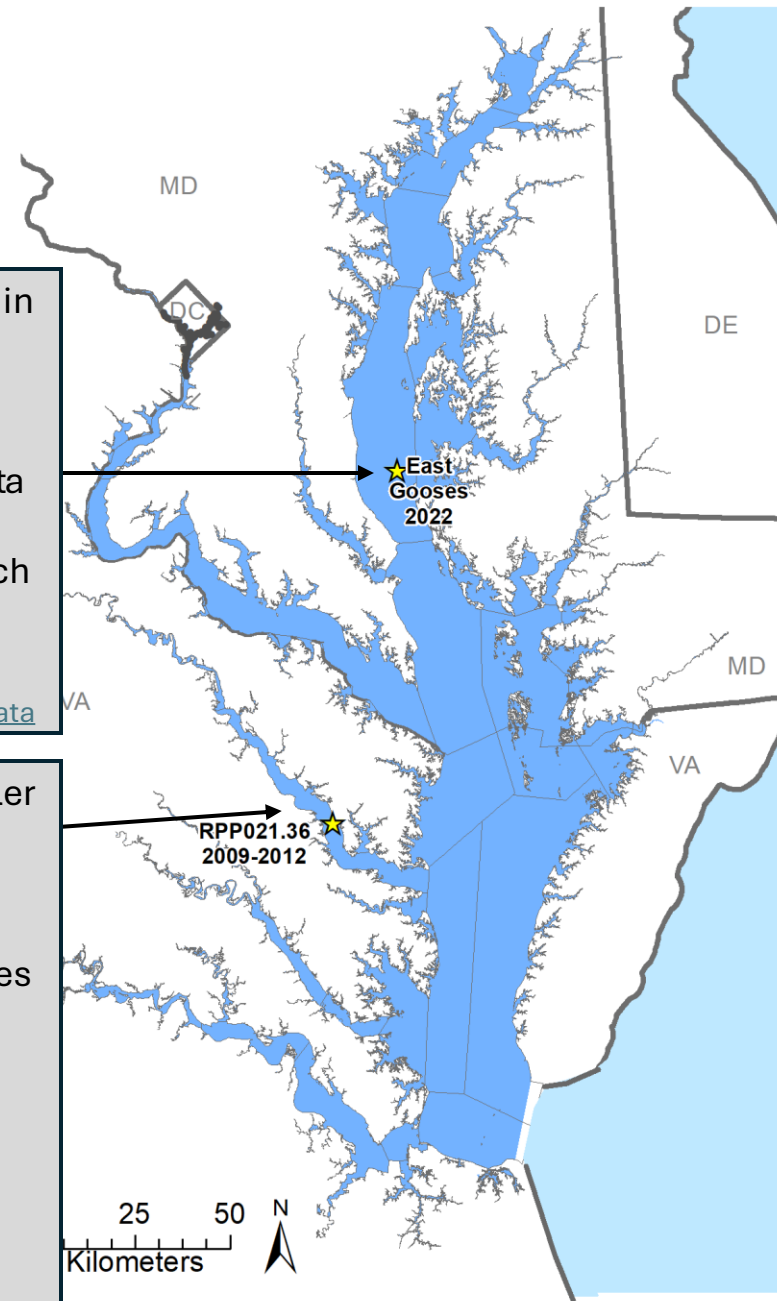
- 10-minute data, 21m deep.
- 2m = distance between observations.
- May 16 – July 5 has enough vertical data to compute pycnocline.
- Data collected at the same time at each depth with vertically arrayed sensors.

Data from: <https://sensors.ioos.us/#metadata/114122/station/data>

VECOS data from RPP021.36 vertical profiler in 2012

- Hourly data, 13m deep.
- 1m = distance between observations.
- June 8-Sept 30 used (although data goes into Oct and other years could be evaluated too).
- Profiler moves up and down water column, so samples are grouped over the ~20 minutes of collection for each profile.

Data from: <http://vecos.vims.edu/>

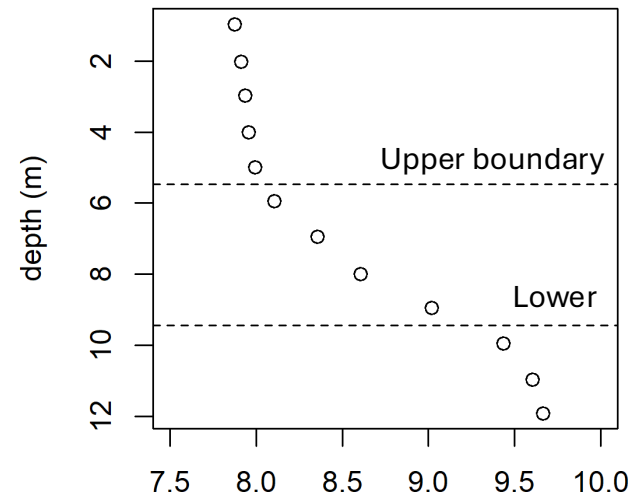


Temporal examples

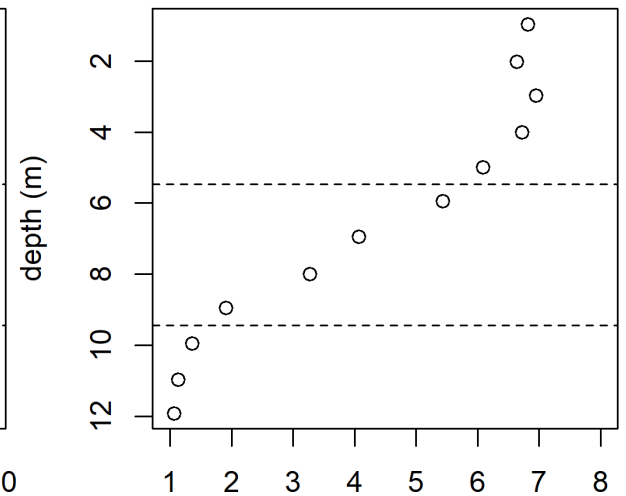
- Pycnocline identification can be done on the high frequency vertical data.



Density 7-22-2012, 3pm



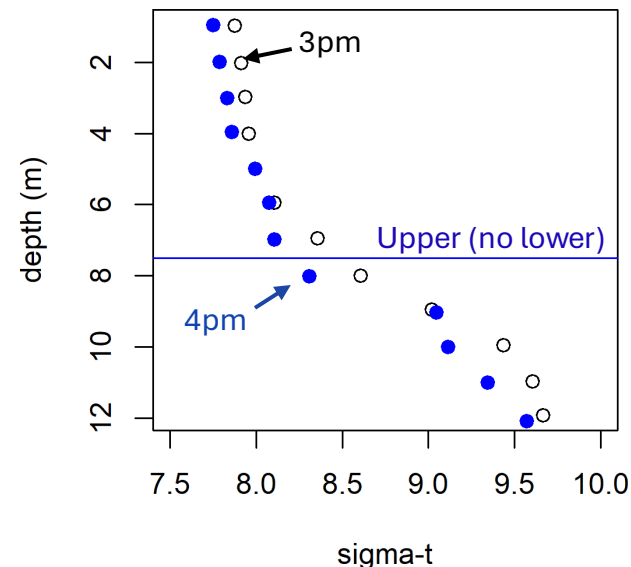
DO 7-22-2012, 3pm



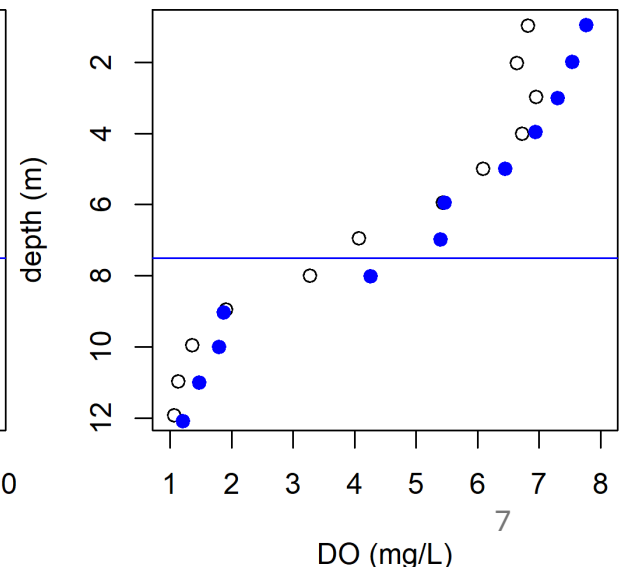
- Examination of the high frequency density and pycnoclines show that the boundaries change within a day.



Density 7-22-2012, 4pm

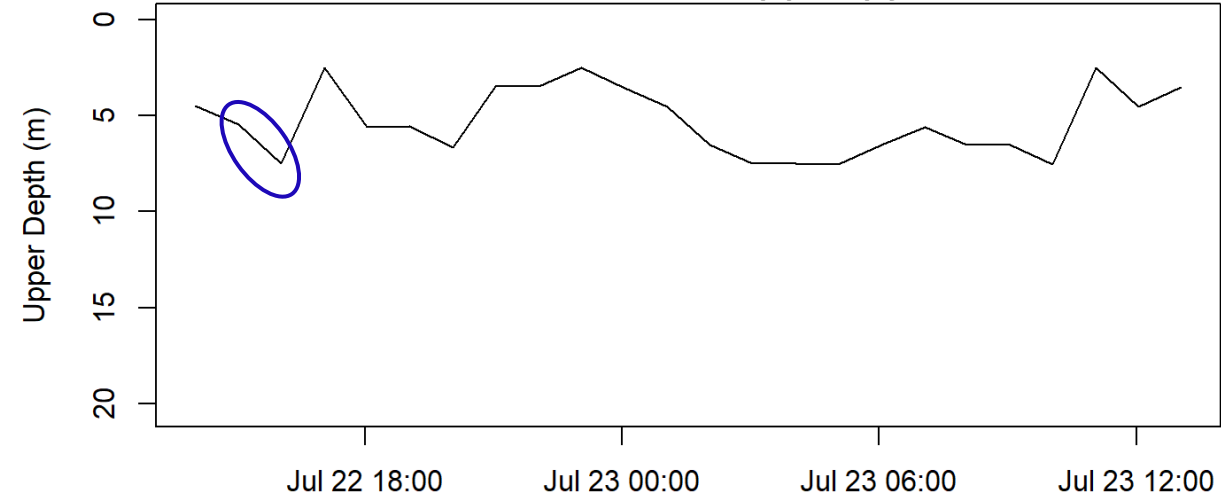


DO 7-22-2012, 4pm



Temporal examples

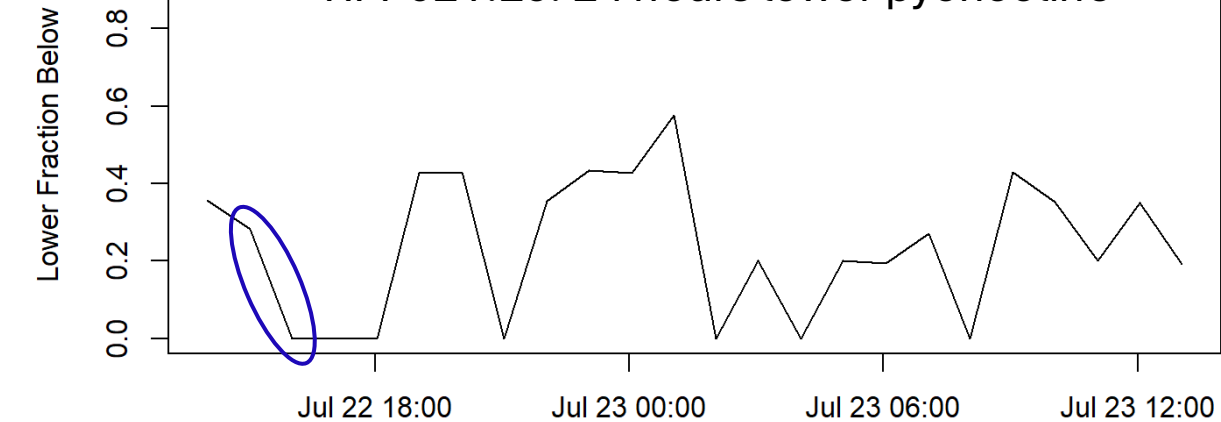
RPP021.26: 24 hours upper pycnocline



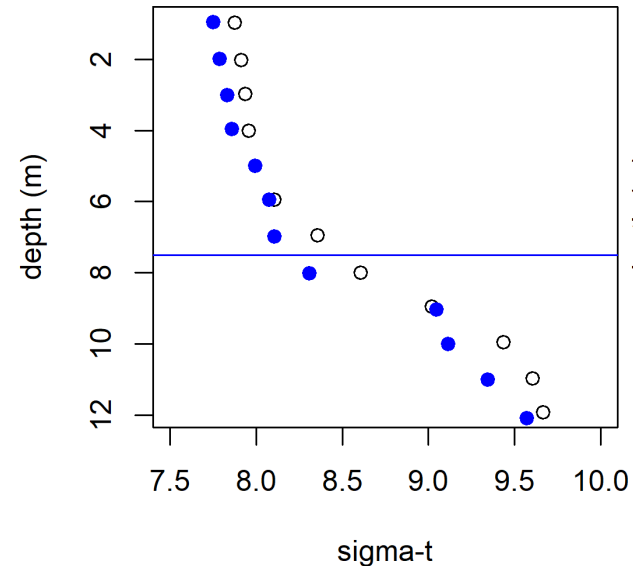
24 hours of upper and lower pycnocline boundaries at this station

→ The 3-4pm example represents common density gradient shifting

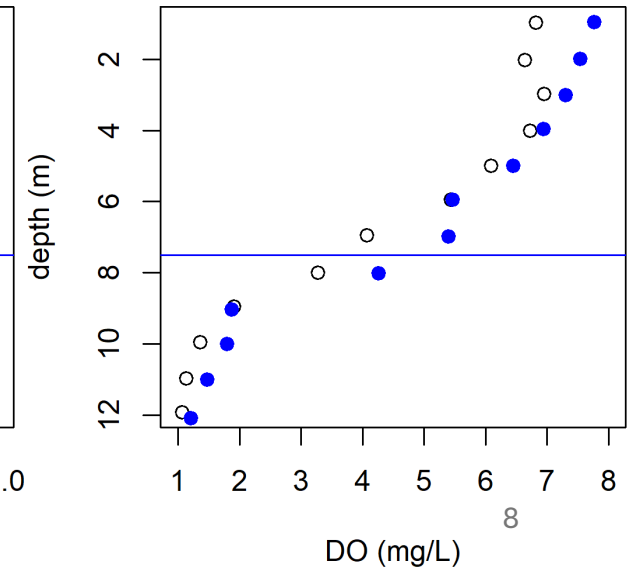
RPP021.26: 24 hours lower pycnocline



Density 7-22-2012, 4pm

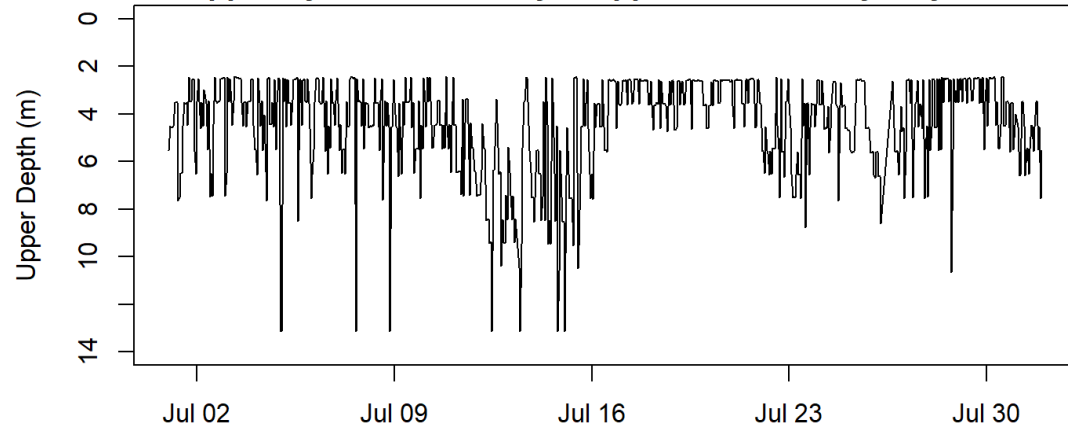


DO 7-22-2012, 4pm

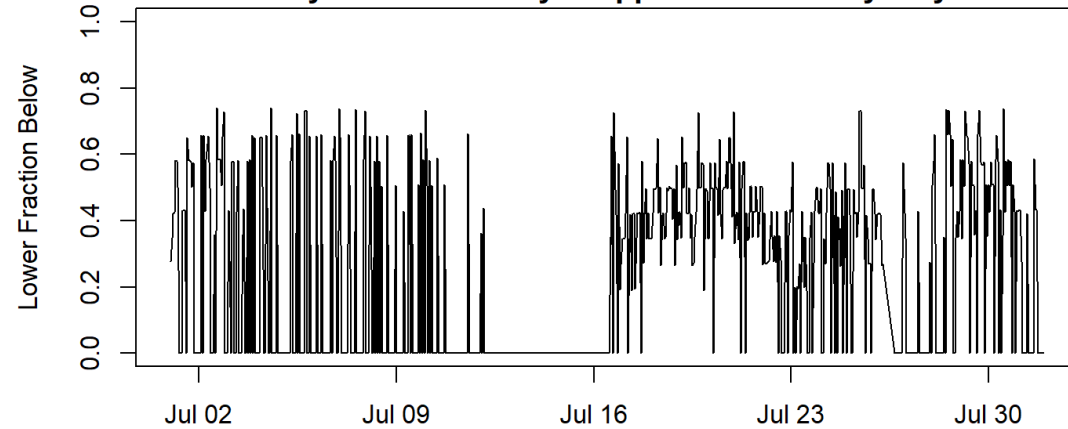


Rappahannock: Full month hourly variability

Upper Pycnocline Hourly: Rappahannock array July 2012

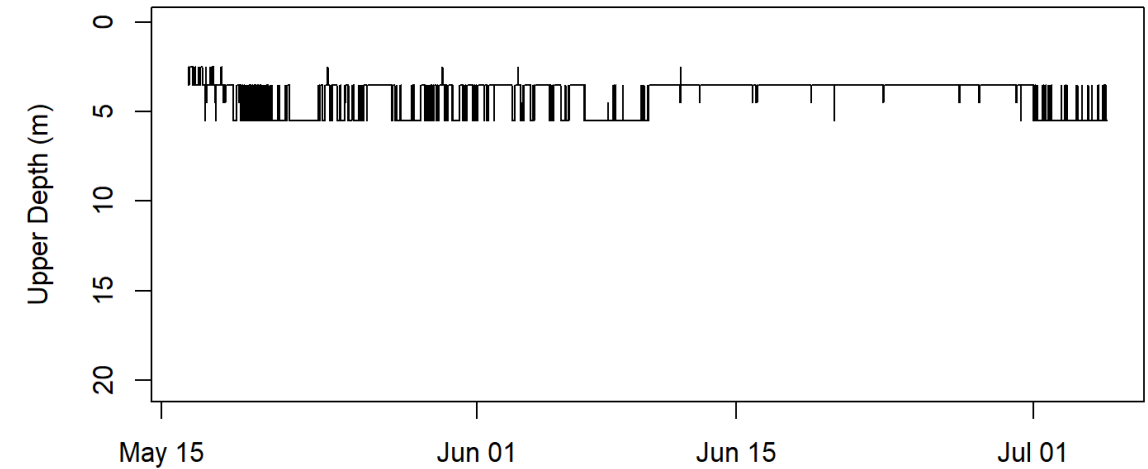
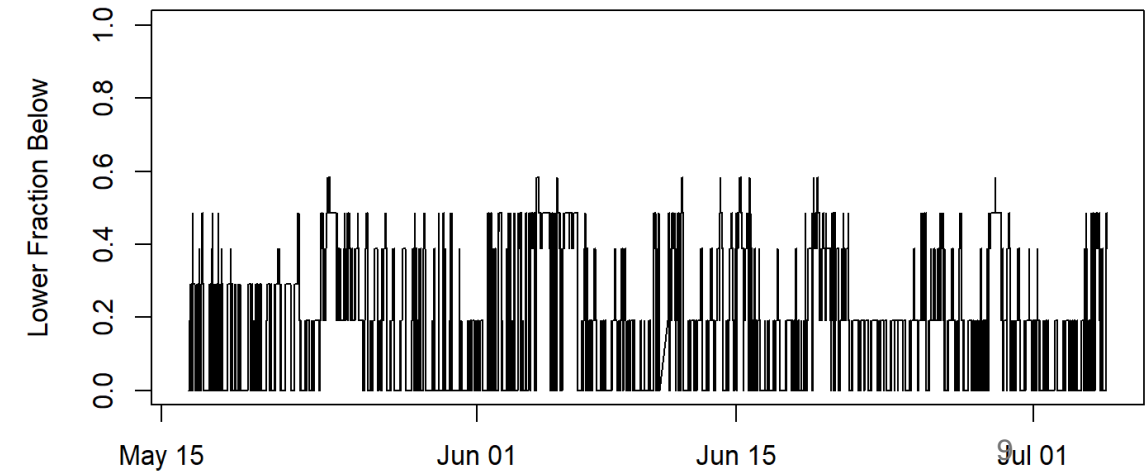


Lower Pycnocline Hourly: Rappahannock array July 2012



Similar finding at East Goose vertical array 2022,
10 minute computations (May 16-July 5)

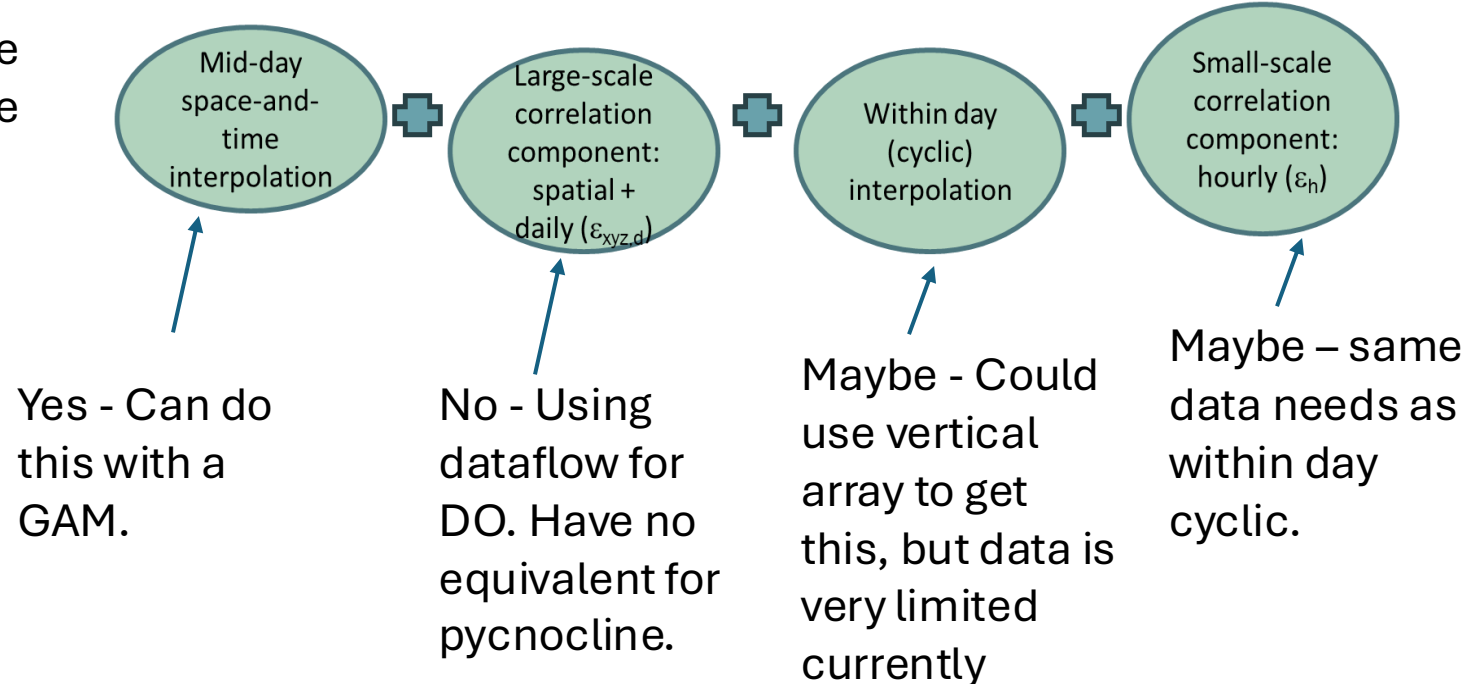
*Note: upper is limited by data and likely isn't as
constrained as it appears*



4d Pycnocline: temporal approach

- The data suggests that we should interpolate the pycnocline at a finer temporal resolution than bimonthly cruises.
- However, can we interpolate it hourly?

Consider the pieces of the tool:



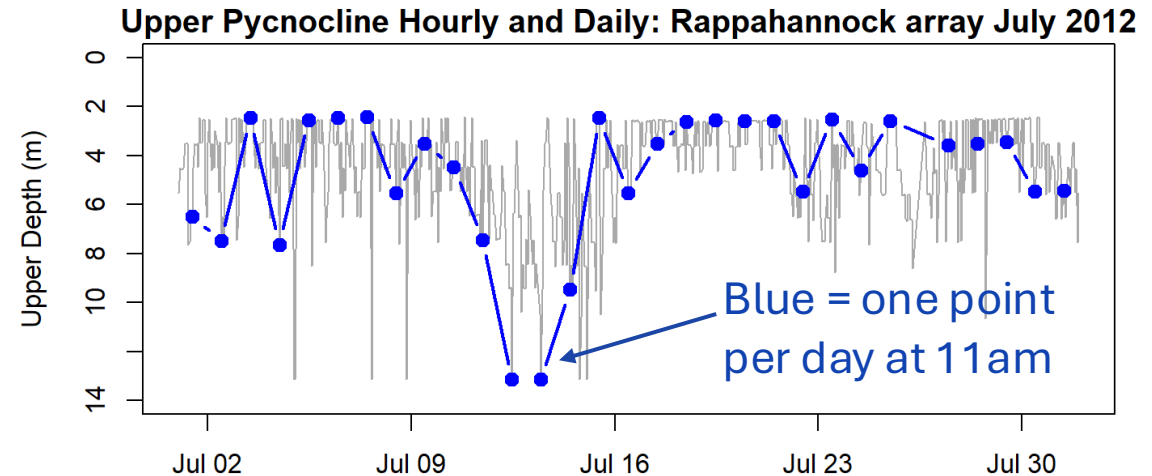
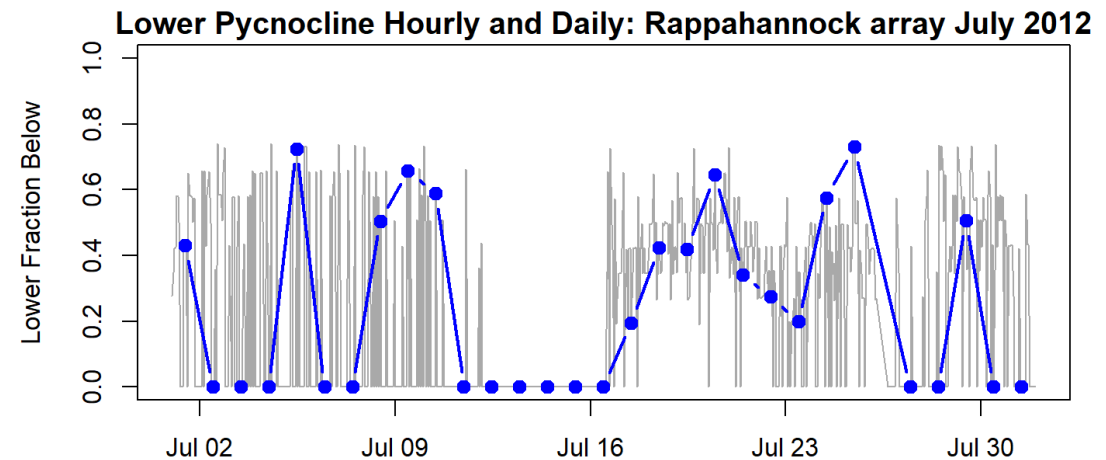
In summary, if we tried to do an hourly simulation for the pycnocline, we do not have all the pieces of data required.

Furthermore, there is a question of how to link pycnocline simulations to DO simulations.

4d Pycnocline: temporal approach

- At this point, daily pycnocline interpolation is likely the most feasible option, and an improvement from the current approach.
- We can evaluate the impact of this plan using the high frequency vertical arrays (next slides).

→ *NOTE: With increasing data from vertical arrays, we'd suggest that we continue to evaluate this choice in the future.*



Testing:

Impact of daily vs. instantaneous pycnocline

- Use 2 locations :
 - East Goose NOAA Vertical Array May 16-July 5, 2022
 - RPP021.26 VECOS profiler June 8-Sept 30, 2012
- Compare:
 - 1) **Instantaneous split:** Split the high frequency DO into DU bins using concurrent high frequency pycnocline computations
 - 2) **Daily split:** Split the high frequency DO into DU bins using each day's pycnocline computed at 11am.

Results: East Goose

Approach:

- Aggregate the high frequency DO into each DU determined by the pycnocline identified.
- Decide if conclusion would change if pycnocline was **daily instead of instantaneous.**

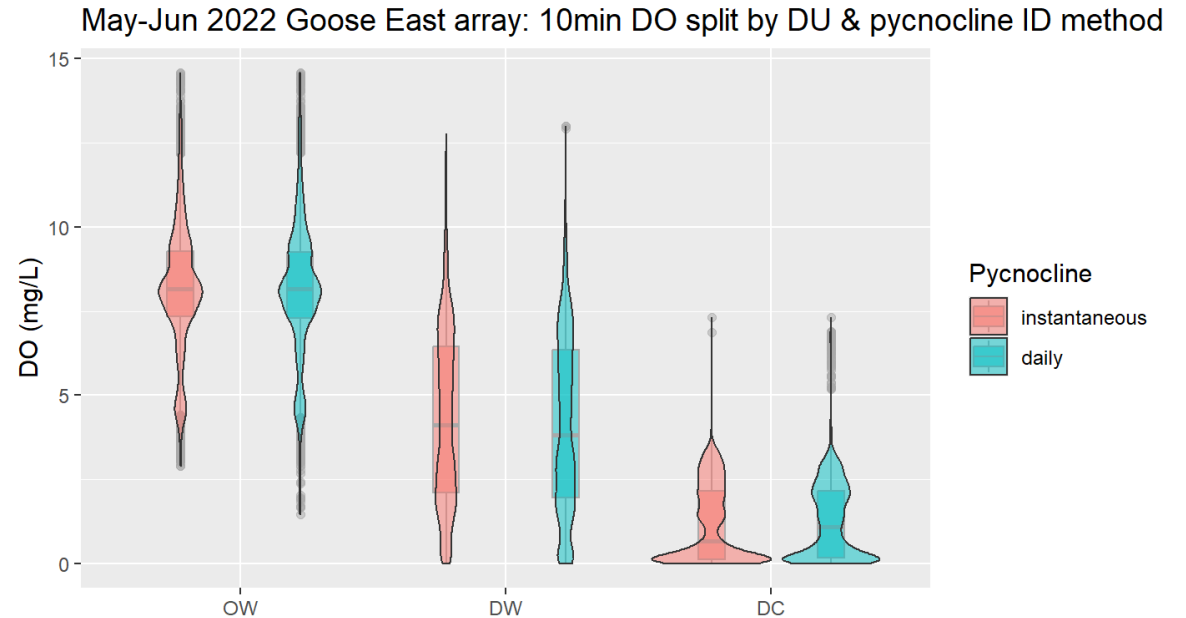
East Goose 2022, (May 16-July 5)

	Open Water (inst criteria=3.2 mg/L)		Deep Water (inst criteria=1.7 mg/L)		Deep Channel (inst criteria=1 mg/L)	
	i. Instantaneous pycnocline	ii. One daily pycnocline (11am)	i. Instantaneous pycnocline	ii. One daily pycnocline (11am)	i. Instantaneous pycnocline	ii. One daily pycnocline (11am)
Percent of observations less than the criterion	0.19 %	0.29 %	18 %	21 %	53 %	49 %

Results: East Goose

Approach:

- Aggregate the high frequency DO into each DU determined by the pycnocline identified.
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East Goose 2022, (May 16-July 5)

	Open Water (inst criteria=3.2 mg/L)		Deep Water (inst criteria=1.7 mg/L)		Deep Channel (inst criteria=1 mg/L)	
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Percent of observations less than the criterion	0.19 %	0.29 %	18 %	21 %	53 %	49 %
10 th percentile (mg/L)	5.2	5.2	1.1	0.68	0.81	0.81
Median DO (mg/L)	8.2	8.2	4.1	3.8	0.68	1.1
90 th percentile (mg/L)	10.4	10.4	7.6	7.6	2.9	2.8
Count of DO observations	15,596	15,784	36,919	38,186	11,171	9,716

Results:

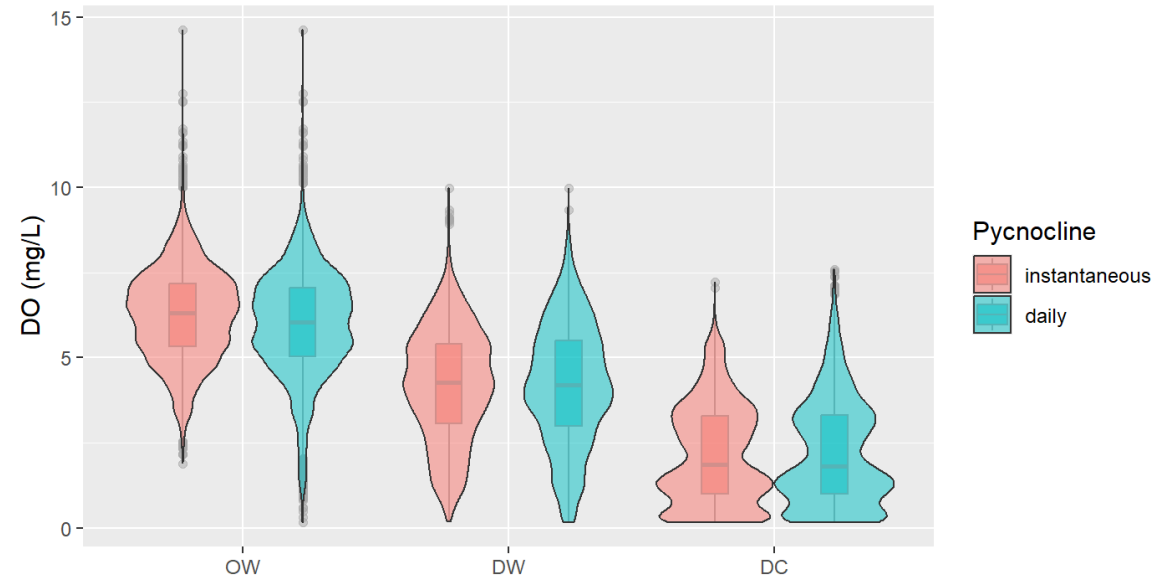
- The DO distributions and frequencies below the criteria suggest that the conclusion would not change if the 10-minute data was split into DUs every day instead of every 10 minutes.

Results: Rappahannock

Approach:

- Aggregate the high frequency DO into each DU determined by the pycnocline identified.
- Decide if conclusion would change if pycnocline was **daily instead of instantaneous**.

Jun-Sept 2012 Rappahannock array: hourly DO split by DU method



Rappahannock Vertical Profiler, (June 8-Sept 30, 2012)

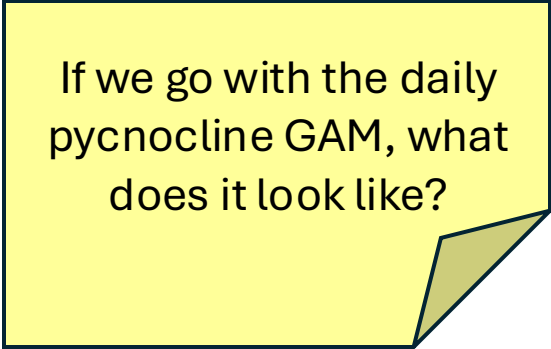
	Open Water (inst criteria=3.2 mg/L)		Deep Water (inst criteria=1.7 mg/L)		Deep Channel (inst criteria=1 mg/L)	
	i. Instantaneous pycnocline	ii. One daily pycnocline (11am)	i. Instantaneous pycnocline	ii. One daily pycnocline (11am)	i. Instantaneous pycnocline	ii. One daily pycnocline (11am)
Percent of observations less than the criterion	1.0 %	4.9 %	8.9 %	10 %	25 %	25 %
10 th percentile (mg/L)	4.5	4.1	1.8	1.7	0.30	0.30
Median DO (mg/L)	6.3	6.0	4.3	4.2	1.9	1.8
90 th percentile (mg/L)	7.9	7.8	6.3	6.5	4.1	4.3
Count of DO observations	12,028	13,046	11,026	10,702	6,077	5,383

Results:

- Similar findings to East Goose for this hourly data.
- The distributions of DO using the two pycnocline approaches are very similar.

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- Comparison to current approach
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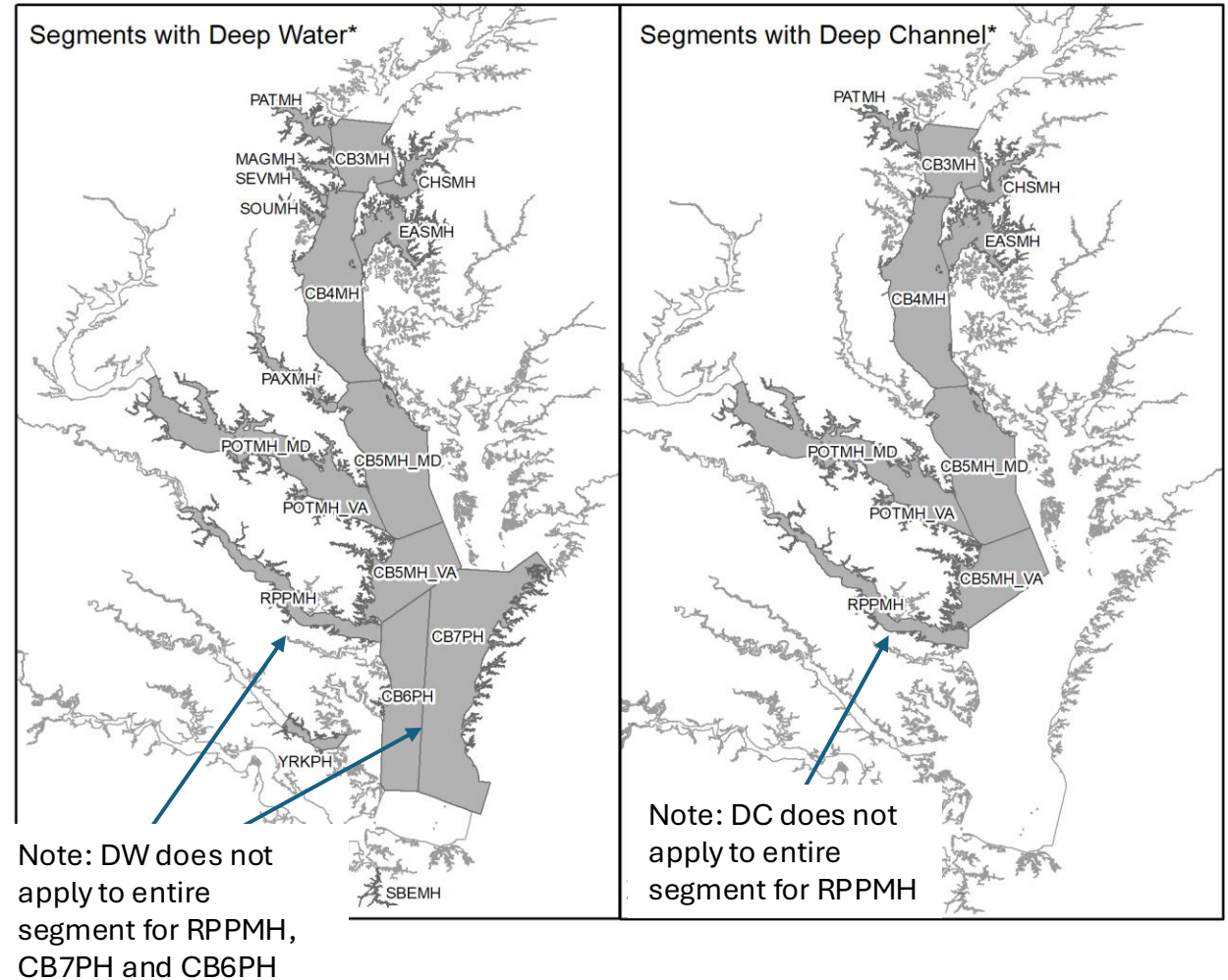
If we go with the daily pycnocline GAM, what does it look like?

Draft daily interpolation results: 2022

Some details that have been tested:

- Use a transformation of importance of interpolating “zero” values (Zero Beta)
- Fit GAMs to 3 separate overlapping regions, each with upper and lower pycnocline.

→ We have many results available on testing these items.
→ For today, we'll just show that it works.



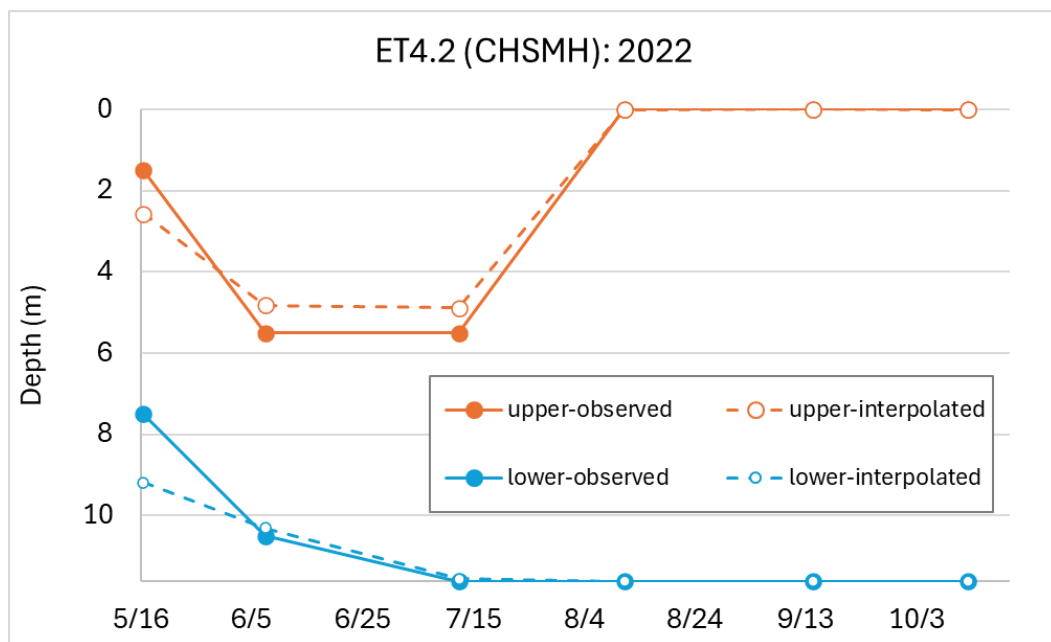
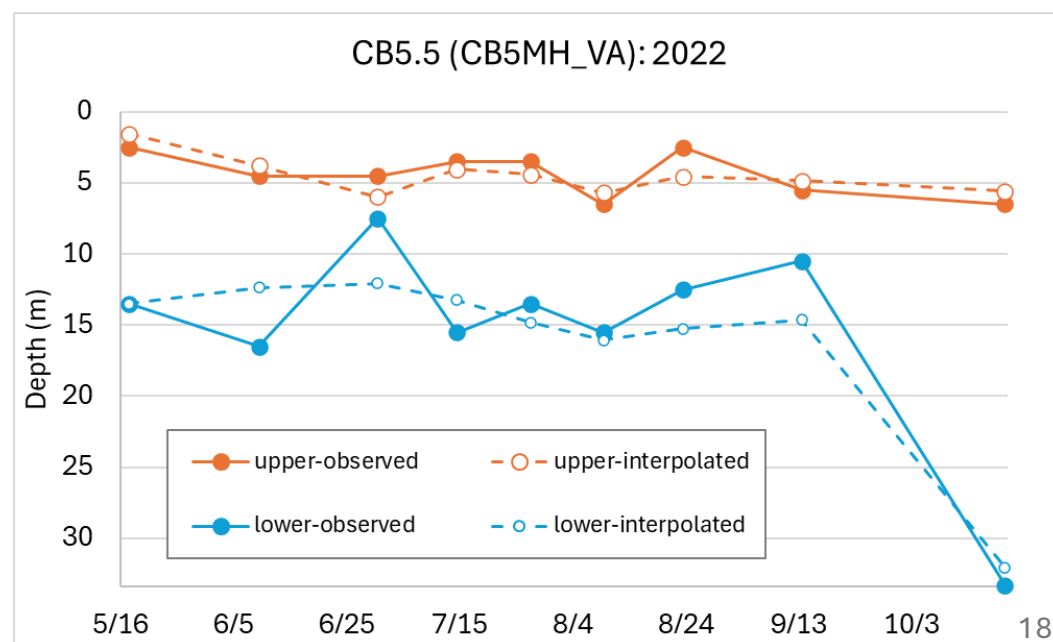
Draft: Pycnocline GAM fits

GAM structure: Allows for relationship with day, bottom depth, x-y location. Relatively high k-values used for closer match to observed values. Fit to only May-Oct of one year.

```
pycDepth ~ s(doy, k = 12)
+ s(wb_lat_km, k = 10) + s(wb_lon_km, k = 10) + s(depth_b, k = 10)
+ ti(doy, wb_lat_km, k = 8)
+ ti(wb_lat_km, depth_b, k = 8)
+ ti(wb_lat_km, wb_lon_km, k = 8)
+ ti(doy, depth_b, k = 8)
+ ti(wb_lon_km, depth_b, k = 8)
+ ti(doy, wb_lat_km, wb_lon_km, k = 9)
```

May-Oct 2022

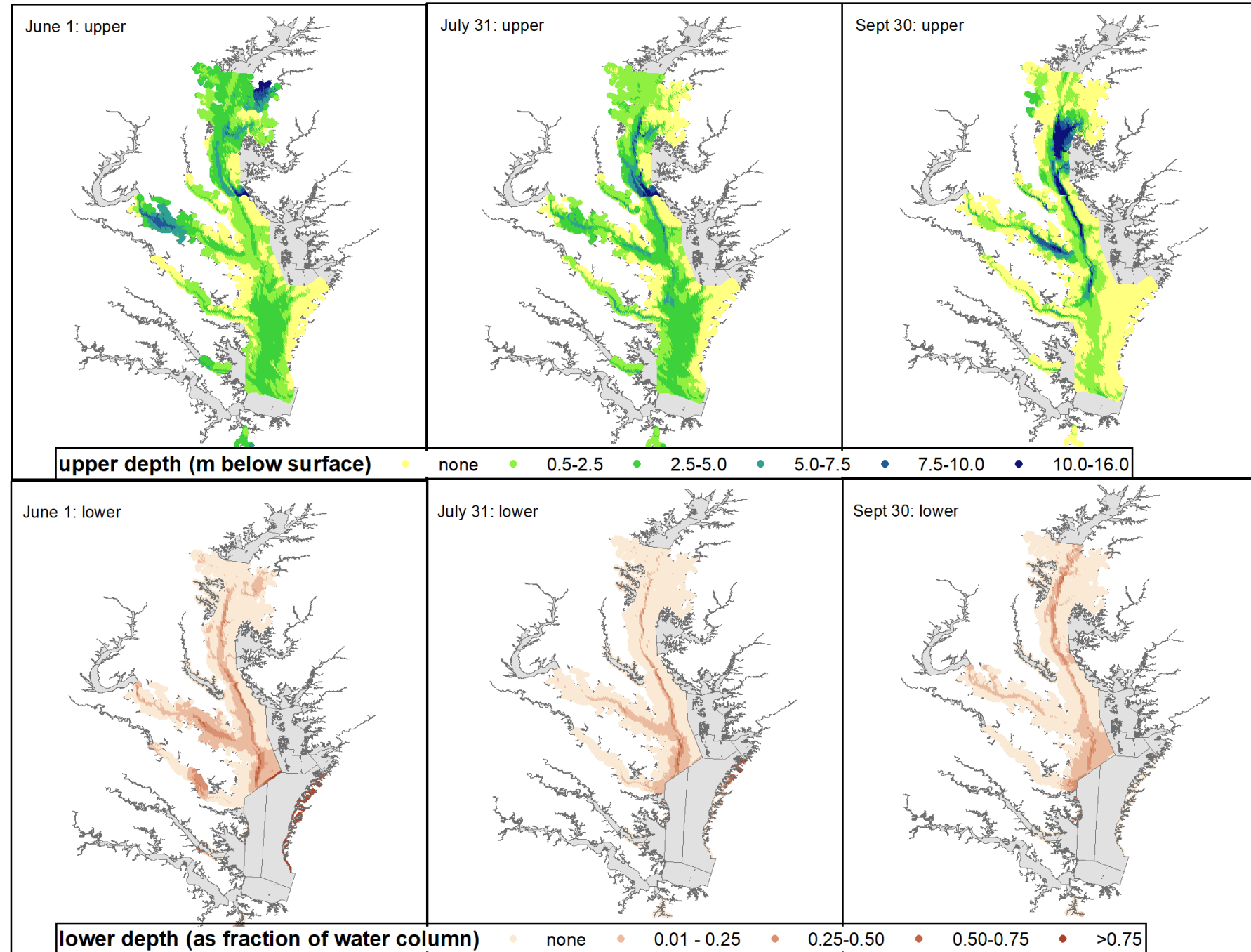
Region	Upper R ²	Lower R ²
1 (north)	0.67	0.58
2 (mid)	0.55	0.54
3 (south)	0.53	0.74



DRAFT: results

- Testing still underway.
- Results seem reasonable for first cut.

Grid predictions for 3 days in 2022 (expanded boundary, v2 GAM)

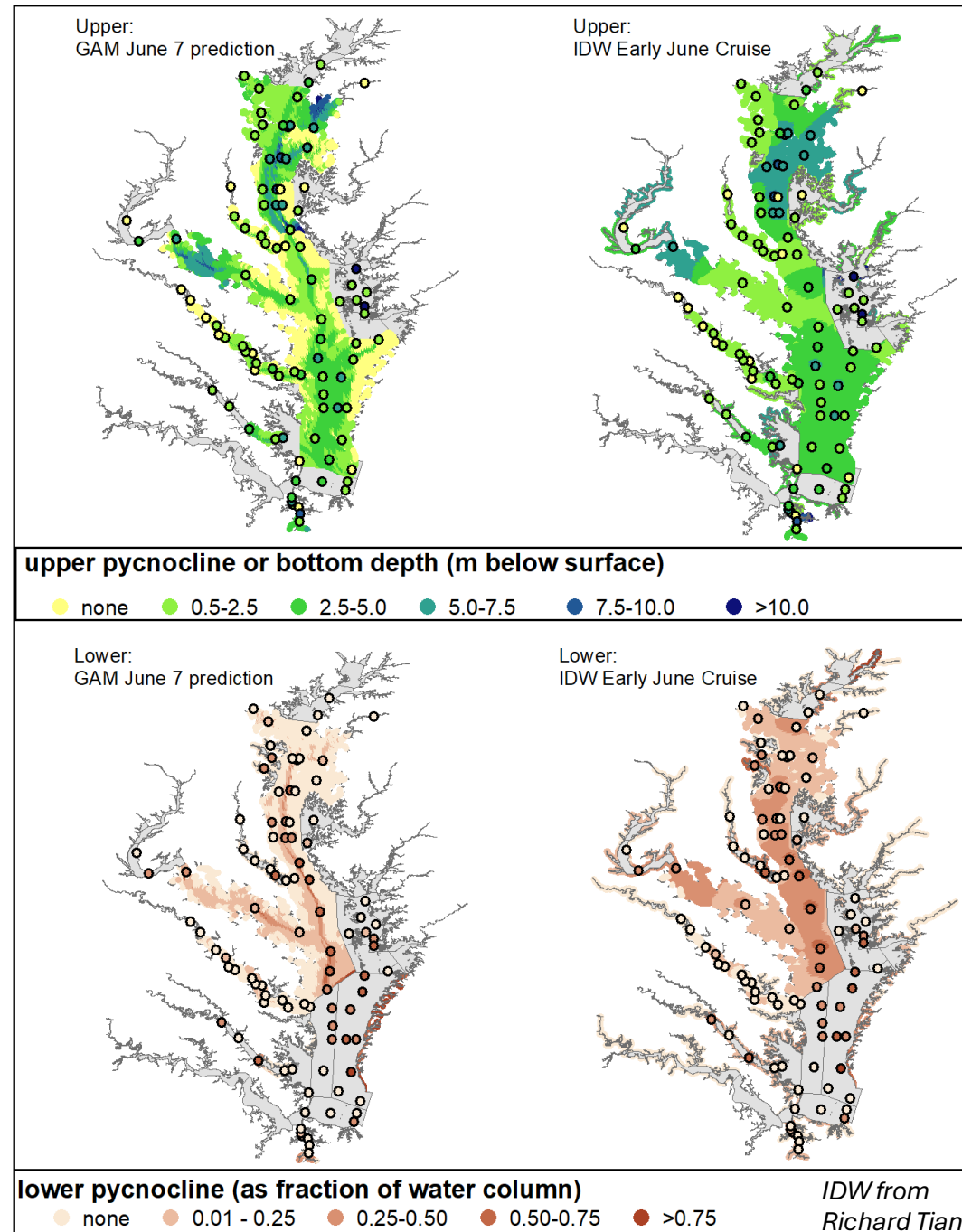


DRAFT:

Comparison with current IDW

- GAM June 7, 2022 interpolation, matched to early June cruise IDW.
- Note the distance-weighted interpolation between data for IDW, while GAM is using relationship with bottom depth and location to inform estimates.
- Investigation of differences underway still.

Compare GAM to IDW Pycnocline Interpolations: early June 2022



Next Steps

- Any adjustment based on BORG feedback.
- Finalize GAM equations/groupings with additional tests and comparison to daily pycnocline observations from arrays/profilers.
- Test using pycnocline in GAM for DO.
- Clean up functions and code to incorporate into work-flow for 4d tool.