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Supporting Information for

Dissolved Organic Carbon Fluxes in the Middle Atlantic Bight: An integrated approach based on satellite data and ocean model products

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Additional Supporting Information (Files uploaded separately)

High resolution versions of the figures were uploaded separately. These can be discarded if not needed.

Introduction

The supporting information provides more detail on the development and evaluation of the neural net model used to generate vertical profiles of dissolved organic carbon (DOC). Additional figures are provided on the relationships of DOC to CDOM optical properties and the monthly cross shelf (CS) flux of DOC and net community production (NCP).

Text S1.

The neural net model (NNet) was developed and evaluated with DOC profile measurements from field observations. A total of 912 DOC field measurements (Fig. S1) along with corresponding depth, temperature, salinity, latitude and longitude were inserted into the neural net to develop a model that generates DOC vertical profiles from the input parameters. The neural net analysis was iterated ten times with 80% of the stations randomly selected for each iteration and the remaining 20% applied to evaluate the neural net model. The iteration yielding the greatest skill (lowest error) was selected. Figure 3 shows how well the neural net model was able to predict DOC for all the field measurements entered into the neural net analysis. Figure 4 demonstrates that the neural net is able to represent the vertical profile of DOC with only the input parameters

of T, S, latitude and longitude. The statistics comparing the observed DOC values versus the neural net output are included in Table S1. The correlation coefficient (R) and RMSE between observed values and the neural net model decrease with increasing depth. The mean absolute percent difference (MAPD) between the observed and predicted DOC for various depth layers ranged from 6.7% to 8.1%. Our study region and model domain was limited to a bathymetry of 100m, so deep waters were not part of our study though the neural net was evaluated for waters deeper than 100m. A minimum DOC threshold value of 48 μmol L^{-1} was established within the NNet.

As described in sections 2.5 and 2.6, the ESPreSSO model provided the input parameters for the NNet and the satellite surface DOC value was applied to the normalized DOC profiles produced from the NNet to generate the DOC profiles used in the MAB fluxes and stocks computations.

Text S2

DOC was strongly correlated to CDOM absorption coefficients across a wide spectral range from the ultraviolet to blue wavelengths within the MAB and across the bay mouths (lower bay to plumes) of the MAB estuaries studied. Thus, DOC can be computed from a_{CDOM} at various ultraviolet and blue wavelengths (250-450 nm) as demonstrated by the strong correlation between DOC:a_{CDOM} ratio and wavelength (Fig. S2).

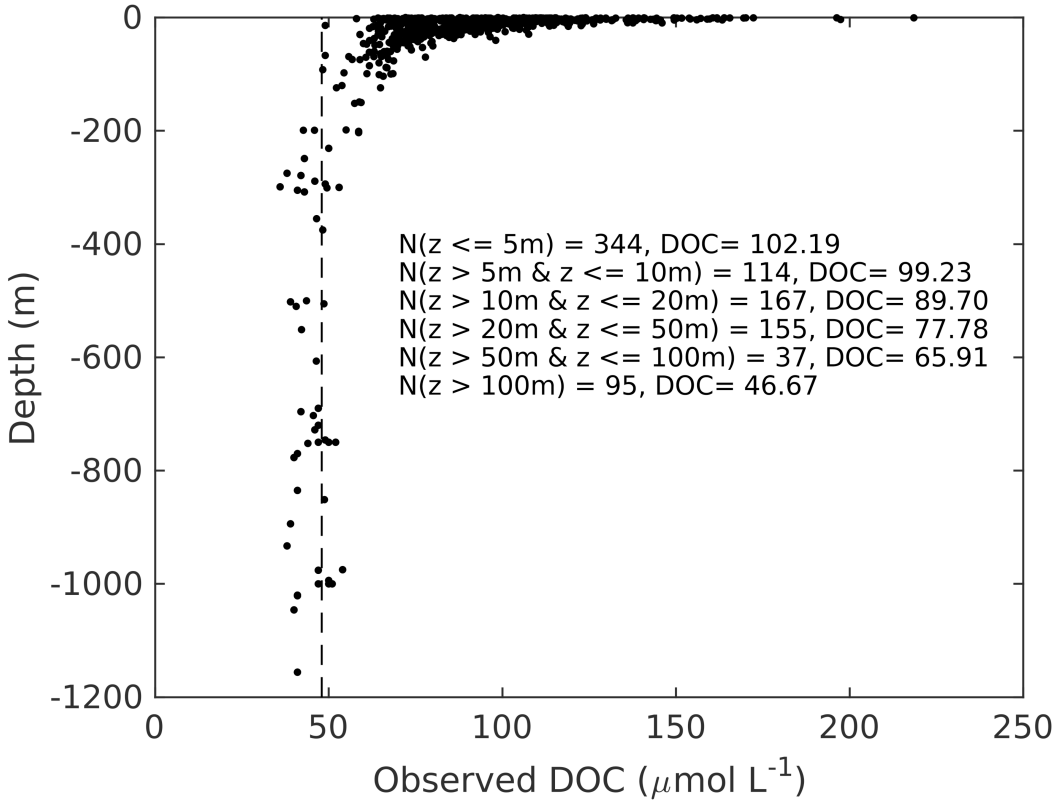

Figure S1. Vertical profiles of DOC field data from the MAB and adjacent continental slope and lower estuarine waters that were inserted into the neural network analysis. N = sample; z = depth; DOC = mean DOC for depth range listed. The MAB study domain was constrained to a bathymetry region of ~100 m and shallower. The neural net model excluded values below 48 μmol L^{-1} (dashed line), which were found onluy below 200 m depth within the *in situ* datasets.

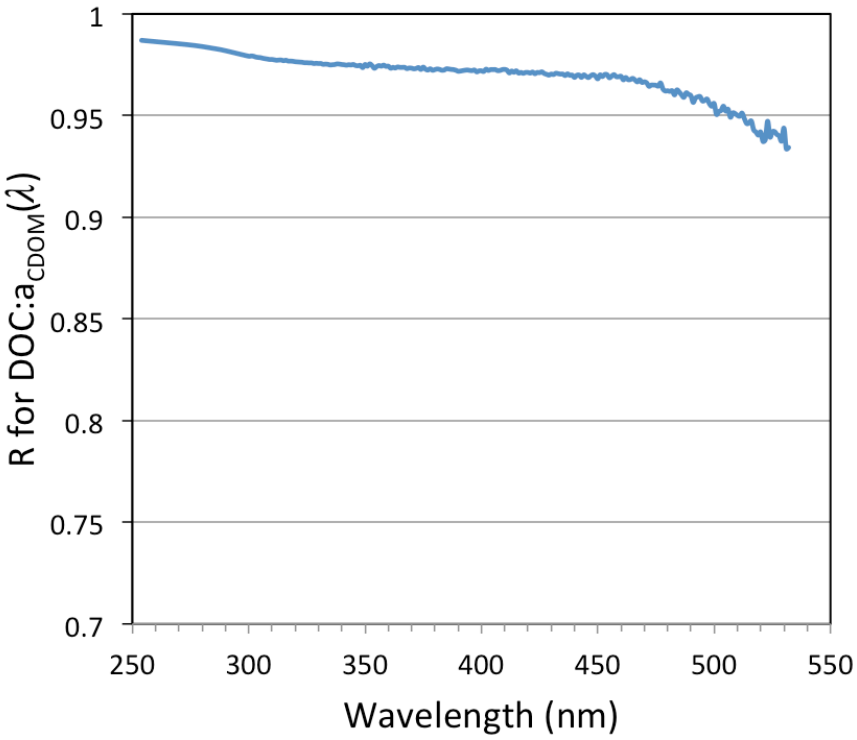

Figure S2. Pearson correlation of the DOC and $a_{CDOM}(\lambda)$ *in situ* measurements for a range of wavelengths (λ) from 254 to 532nm within the southern MAB during fall-winter-spring.

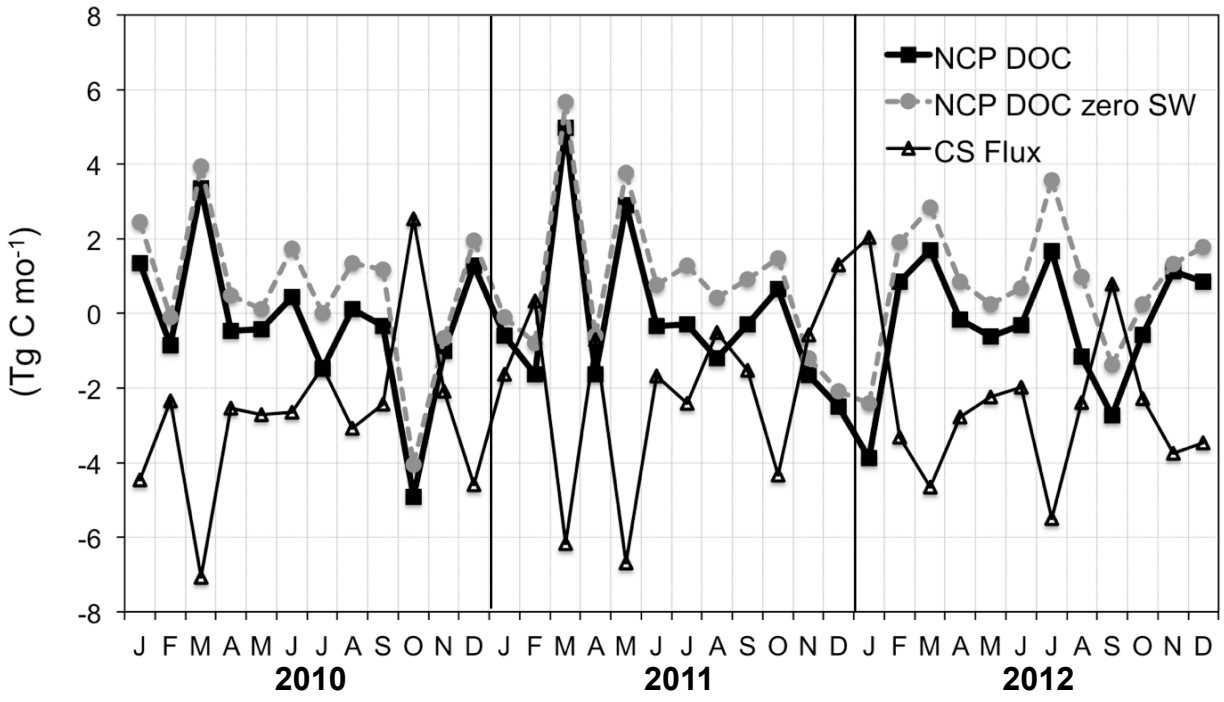

Figure S3. MAB monthly (a) NCP DOC, (b) NCP DOC with SW flux set to zero, and (c) CS flux.

Depth Range (m)	Mean Obs DOC (μmol L^{-1})	Obs vs. NNet (R)	MAPD (%)	RMSE (μmol L^{-1})
≤ 5	102.19	0.91 (0.89, 0.93)	7.27	10.67
> 5 & ≤ 10	99.23	0.83 (0.72, 0.89)	7.67	10.39
> 10 & ≤ 20	89.70	0.79 (0.72, 0.84)	6.75	7.91
> 20 & ≤ 50	77.78	0.60 (0.44, 0.71)	7.46	7.90
> 50 & ≤ 100	65.91	0.61 (0.33, 0.79)	6.66	5.75
> 100	46.67	0.69 (0.54, 0.82)	8.14	4.73

Table S1. Performance of the neural networks model between predicted vs. observed DOC concentration. The results were delineated by depth. The 95% confidence intervals for the correlation coefficient (R) are included between the parentheses.