Ocean Carbon From Space 2022 Workshop

A new method to estimate DOC in the global open ocean

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ACRI ST

DOM

Organic compounds that pass through a submicron filter
(proteins, lipids, polysaccharides, etc.)

DOC

~ 90% of TOC's bulk

(e. g. Kumari and Mohan, 2018; Maciejewska and Pempkowiak 2014; Sanders et al., 2014; Santana-Falcón et al., 2017)

> 200 times the carbon stock of marine biomass

(Hansell et al., 2009)

~ 50% of DOM's bulk

(Cmoody & Worrall, 2017)

CDOM

Fraction of DOM that interacts with light.

Passes through a 0.2 µm filter (Nelson and Siegel, 2013)

Humic and fulvic acids (Harvey et et al., 1983)

In contrast to POC the DOC spatio-temporal variability is still not well characterized over the global open ocean

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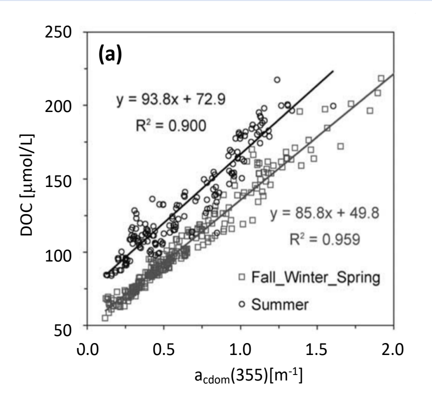
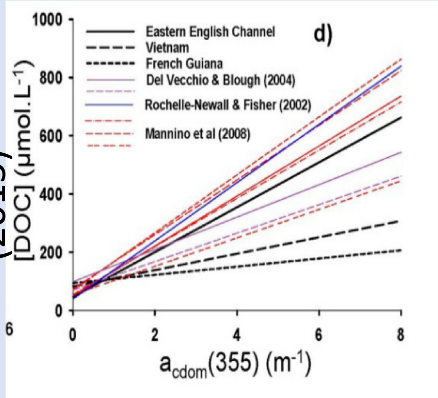
While CDOM can be used to estimate DOC from remote sensing in coastal waters (same dilution patterns), the different kinetics in the processes driving their distributions make the CDOM a poor proxy to estimate DOC.

CDOM – DOC correlation in COASTAL areas:

Mannino et al. (2008)

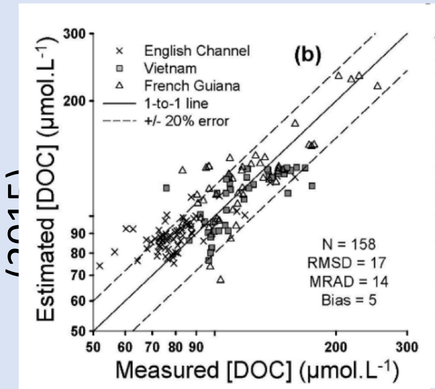


Vantrepotte et al. (2015)

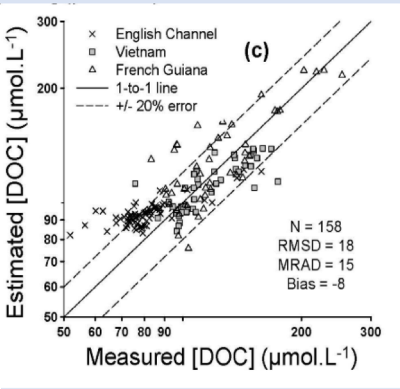


Using S_{cdom} reduces the spatio-temporal variability of CDOM vs. DOC

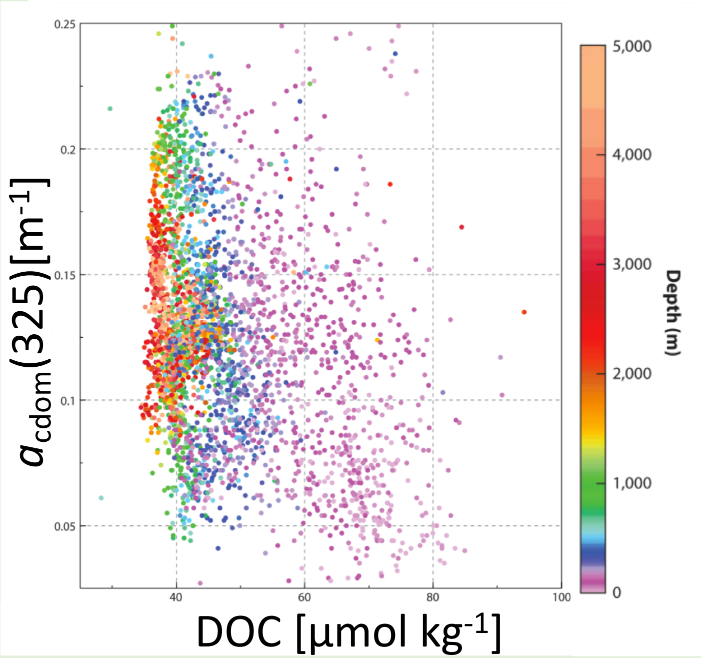
Vantrepotte et al. (2015)



S275-295 based method



$a_{cdom}(412)$ based method



Source: Nelson and Siegel (2013)

- ➢ The relation is more complex in open ocean than in coastal water (no direct correlation).
- ➢ CDOM and DOC sources and sink processes are not strictly covarying.

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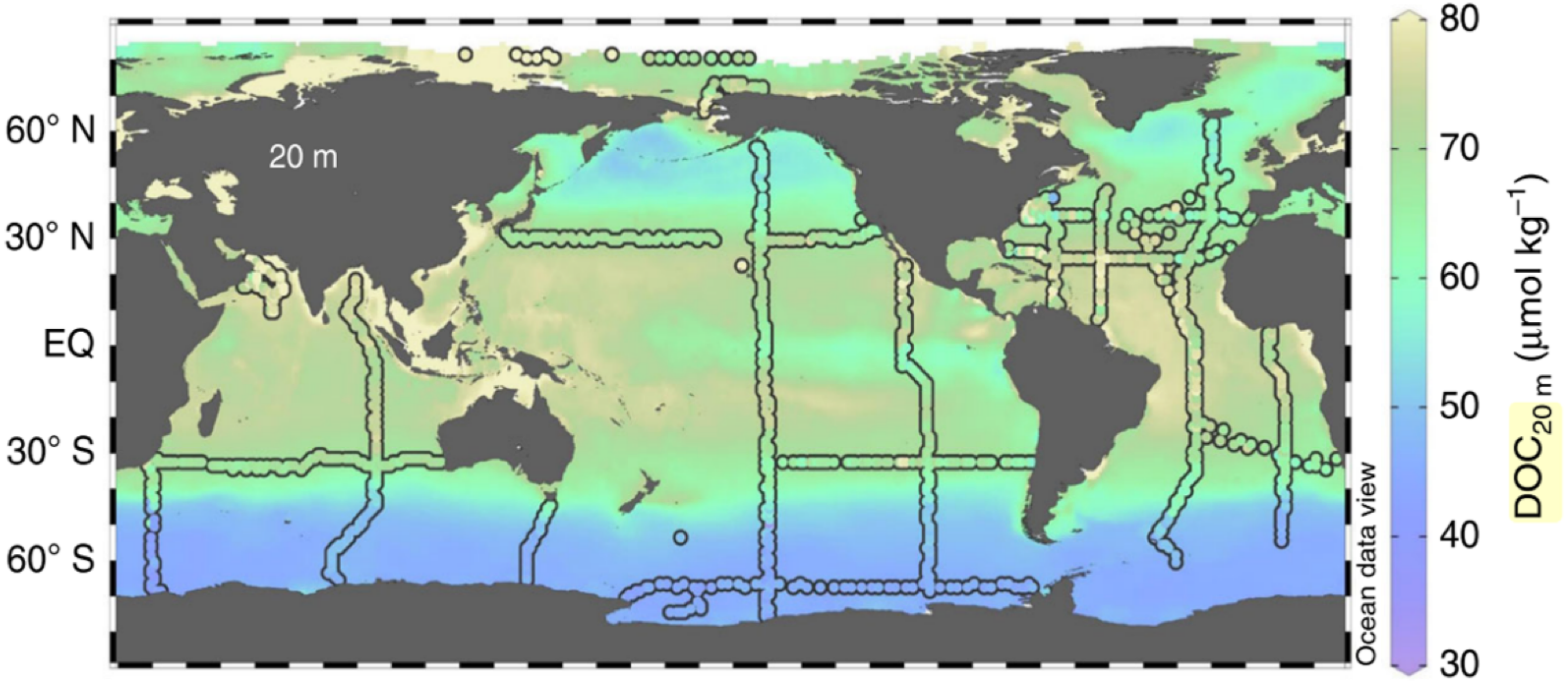
Based on a Artificial Neural Network approach, a global map of DOC has recently been obtained combining in situ DOC and other data collected over a long time period providing the first DOC spatial distribution (but no temporal information).



Global mean produced with an Artificial Neural Network
Validation subset with $R^2 \geq 0.95$
(Source: Roshan and DeVries, 2017)

DOC information from satellite data, would provide greater coverage and temporal variability information necessary for the validation of this kind of coupled models.

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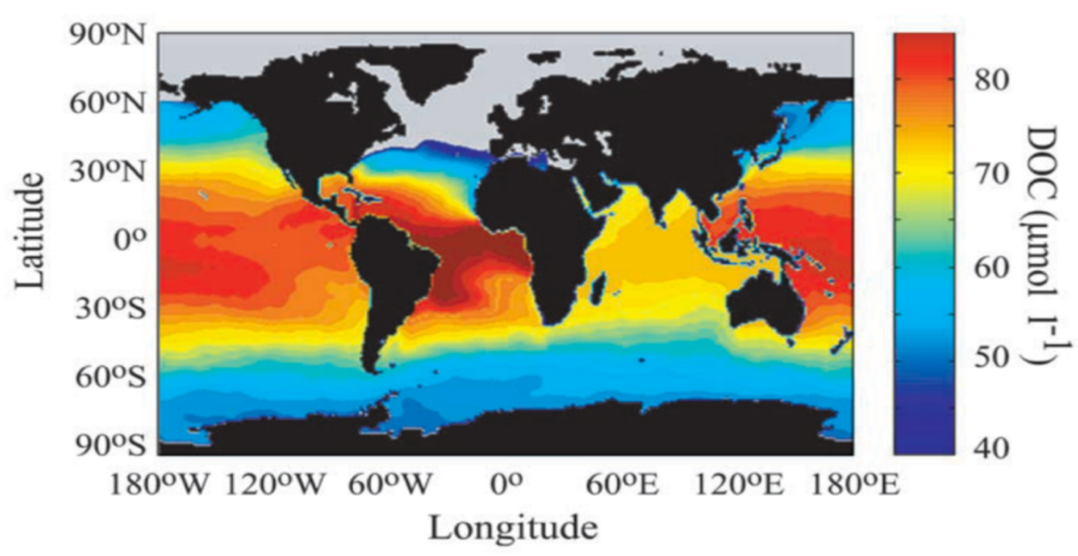
Some preliminary algorithms have been developed to estimate DOC concentration from space over open ocean waters.



SIEGEL ET AL. (2002)

Linear regression between DOC and Sea Surface Temperature (SST) from trans oceanic cruises samples.

Atlantic Ocean:

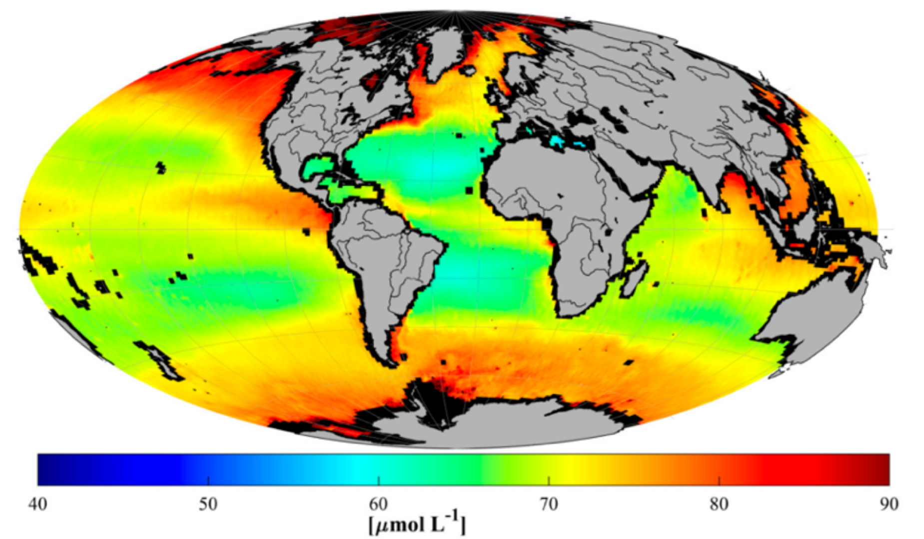
- DOC = 3.493(SST) – 9.79 (DOC< 85)
- DOC = 85

Indian Ocean:

- DOC = 0.795(SST) + 48.58

Pacific and Southern Ocean:

- DOC = 0.993(SST) + 52.05



AURIN ET AL. (2018)

Purely empiric model that estimates DOC concentration from SSS and a_{cdom} (350).

Developed trough a multiple linear regression.

$$DOC = 192.78 + 26.79 * ln(a_{cdom}(355)) - 3.558 * ln(SSS)$$

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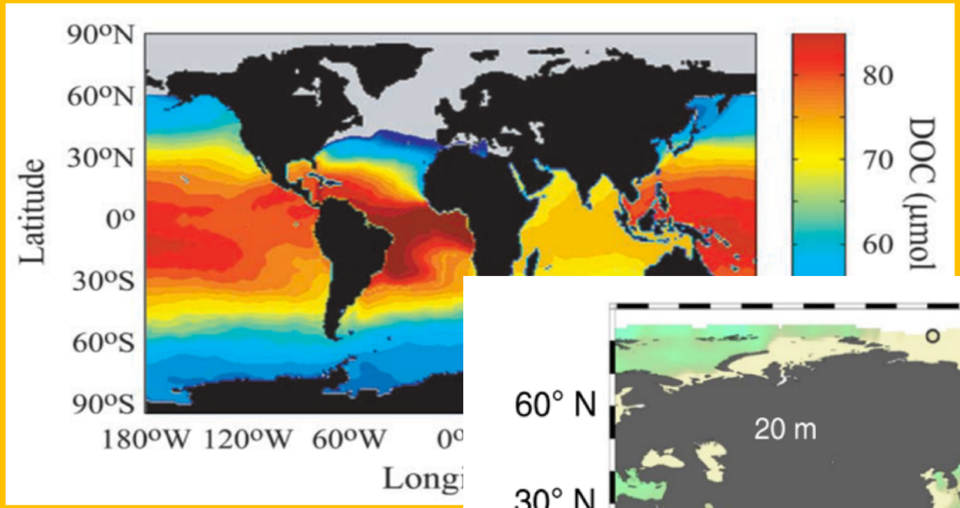
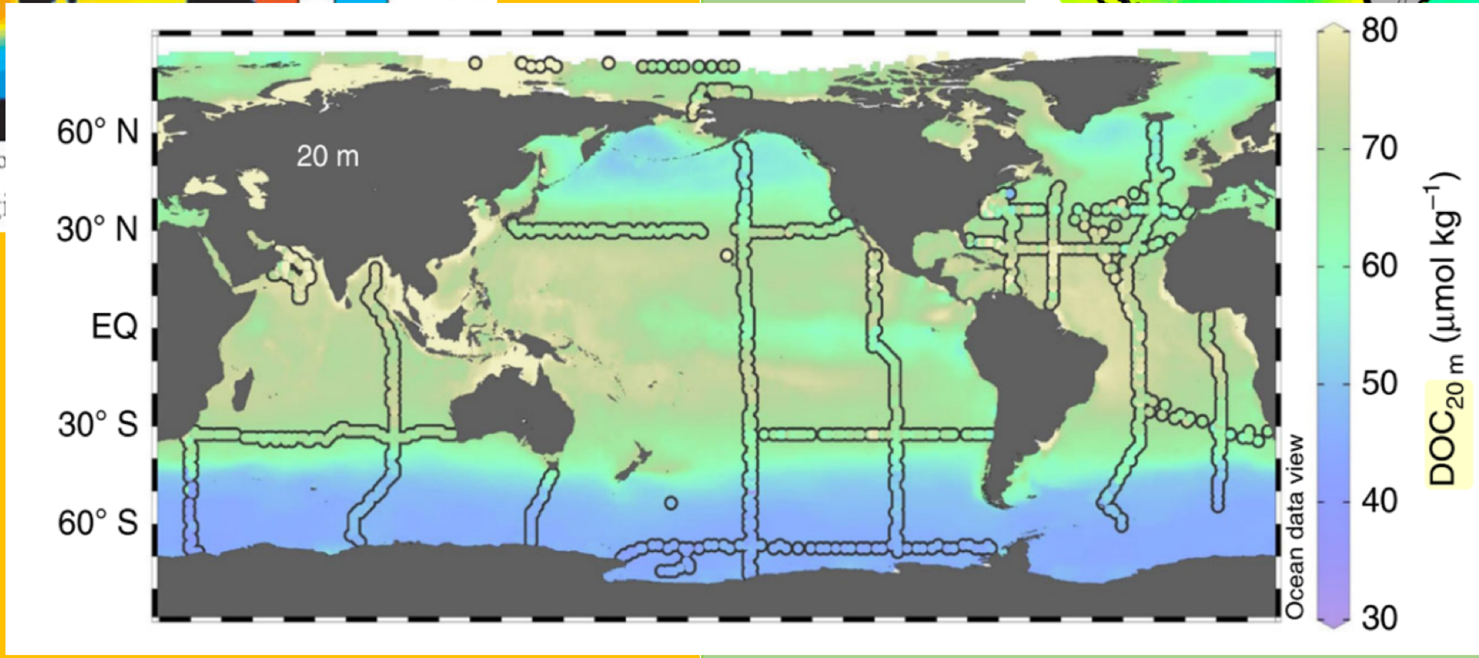
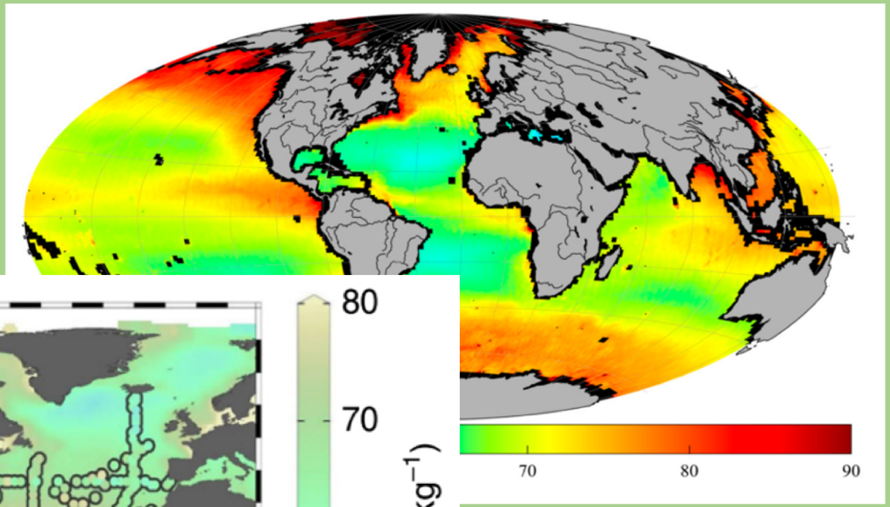
While the SST based approach provides the expected feature, but with too marked latitudinal gradient, the OCR based approach seems to present some wrong spatial patterns, especially in gyres, when compared with the global image of Roshan and Devries (2017).



SIEGEL ET AL. (2002)
Linear regression between DOC and SST from trans oceanic cruises samples.





AURIN ET AL. (2018)
Purely optic model that estimates DOC concentration from SSS and a_{cdom} (350).

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The DOC algorithm should include, when possible, information on parameters linked to its dynamics.

SOURCE

COASTAL WATER

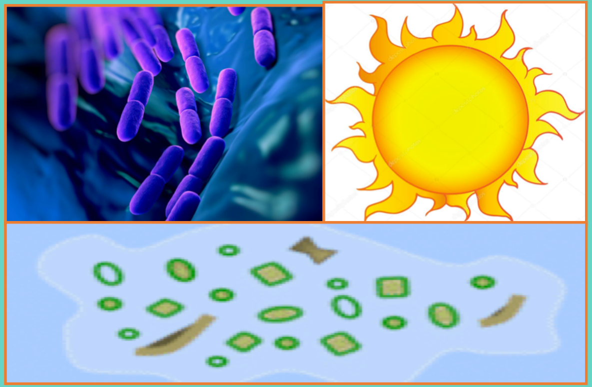
- Terrestrial origin
- Degradation of organic matter introduced by rivers runoff, landwashing, groundwater discharge.
- High biological activity

OPEN OCEAN

- Local production by autotrophs in the euphotic zone.
- Phytoplankton and bacterial excretion.
- Viral lysis, grazing.
- Horizontal and vertical advection

SINK

- Photochemical degradation
- Microbial remineralization
- Aggregation into microparticles
- Grazing/sinking of aggregated DOC
- Horizontal and vertical advection



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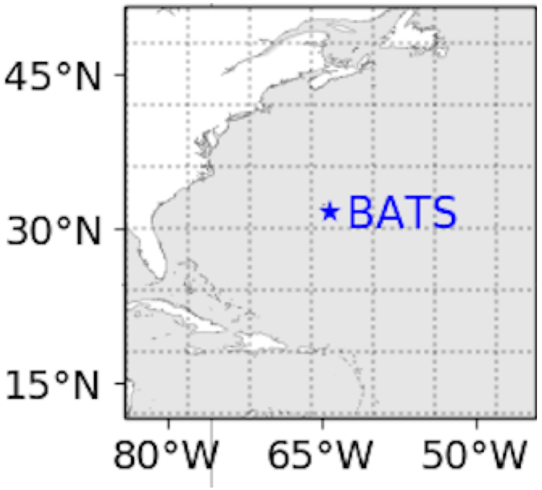
Based on literature review, and among the different parameters that are available, we decided that the algorithm should accounts for the mass history (i.e. Time Lag), Dynamics (SST, MLD), and bio-optics (Chl and a_{cdom}).

Possible variables:

Chl-a: Primary producers generate between 30-50 % of DOC

MLD: The mixing processes work as source and sink of DOC

Temporal lag?



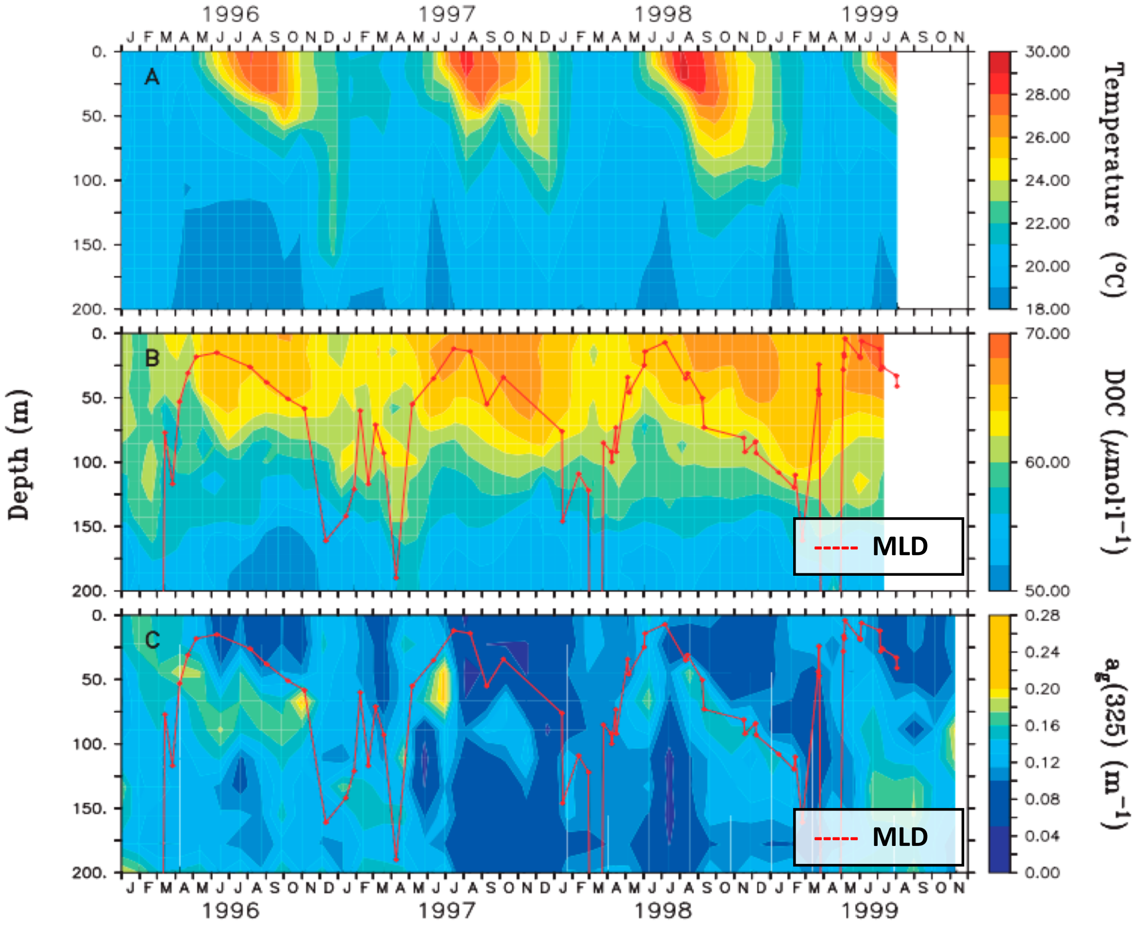


Figure 8. Time-depth distribution of (a) temperature (°C), (b) concentrations of dissolved organic carbon (DOC; μmol kg^{-1}), and (c) CDOM (a_g(325); in units of m^{-1}) measured at the BATS site (32.1°N, 64.5°W). The red lines in Figures 8b and 8c show the mixed layer depth calculated from potential density. Methods used for the determinations are documented in the literature [*Michaels and Knap*, 1996; *Nelson et al.*, 1998; *Hansell and Carlson*, 2001].

Siegel et al. (2002)

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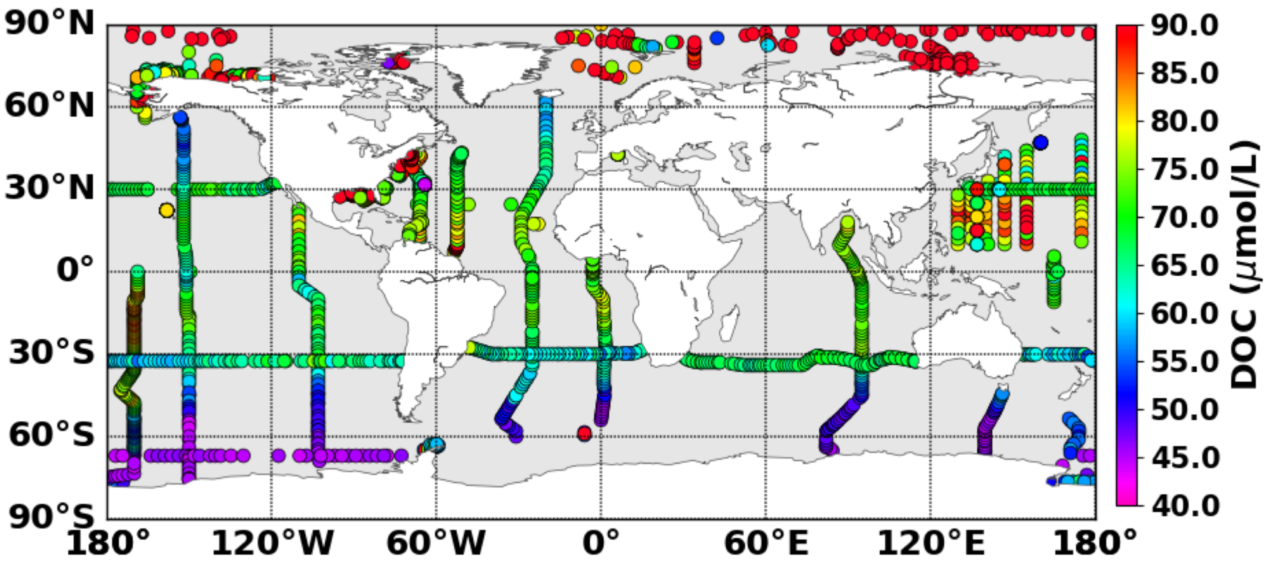
A match-up data base has been built between in situ DOC measurements, and the different possible inputs of the algorithm at different time lags.



DOC DATABASE (1991 – 2015)

- ANTARES
- BATS
- GLODAP
- GOCAD
- POLARSTERN
- TRANSDRIFT_VB
- TRANSDRIFT_YS
- GoMX
- HOTS
- K2

Match up variables

The match up was performed at 5 time steps (0,-1, -2, -3 and -4 weeks)

Remote sensing reflectance (Rrs) [412, 443, 490, 510, 590, 665]
Photosyntetical Available Radiation (PAR)
Chlorophyll-a (Chl)
a_{cdom} (443) (Bonelli et al. 2021)
GlobColour L3 merged daily (4km)

Sea Surface Salinity (SSS)
ESA Climate Change Initiative. Weekly (25km)

Sea Surface Temperature (SST)
NOAA Optimum Interpolation (OI) SST-V2
Weekly (1 degree)

Mixed Layer Depth (MLD)
MILA GPV (Argo, Grid Point Value)
10 days averaged (1 degree)

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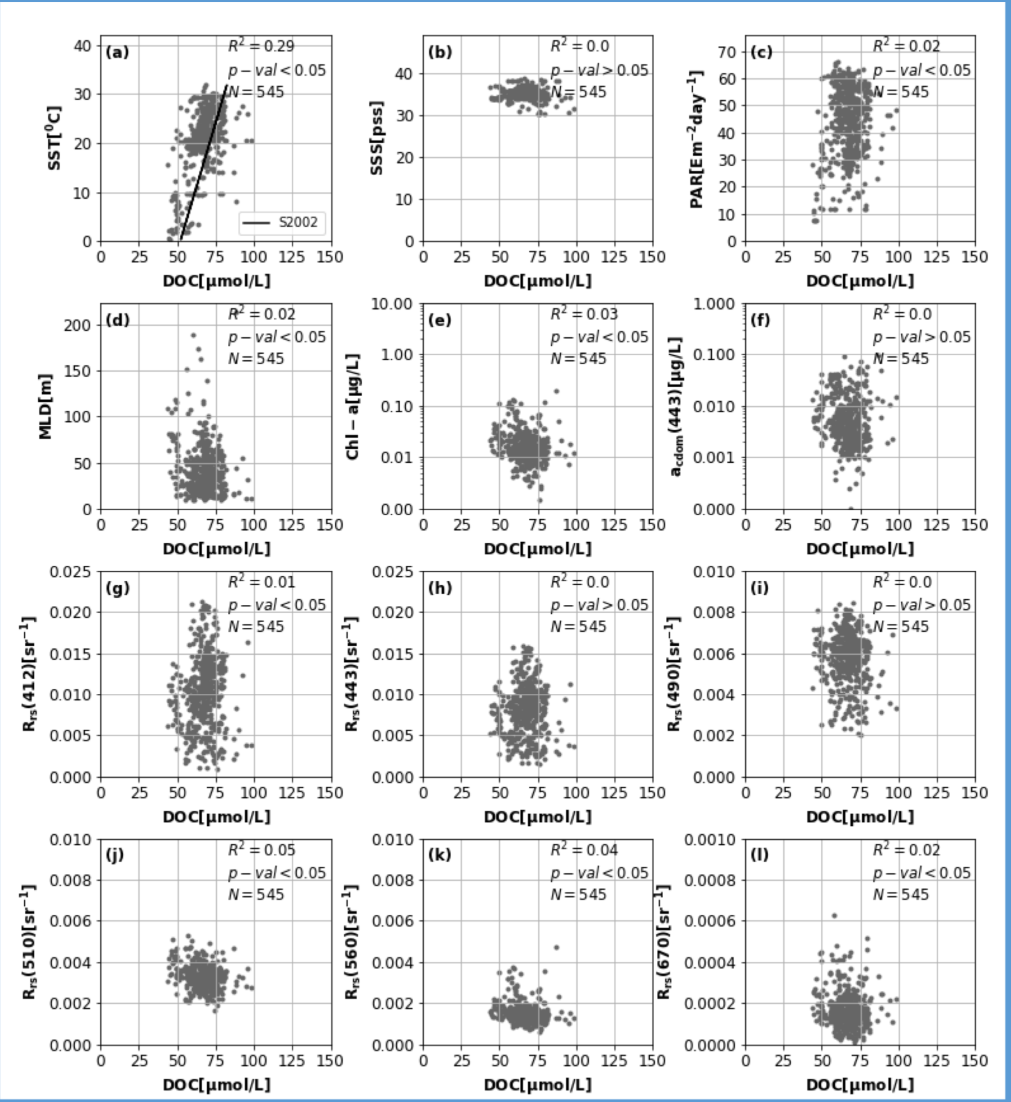
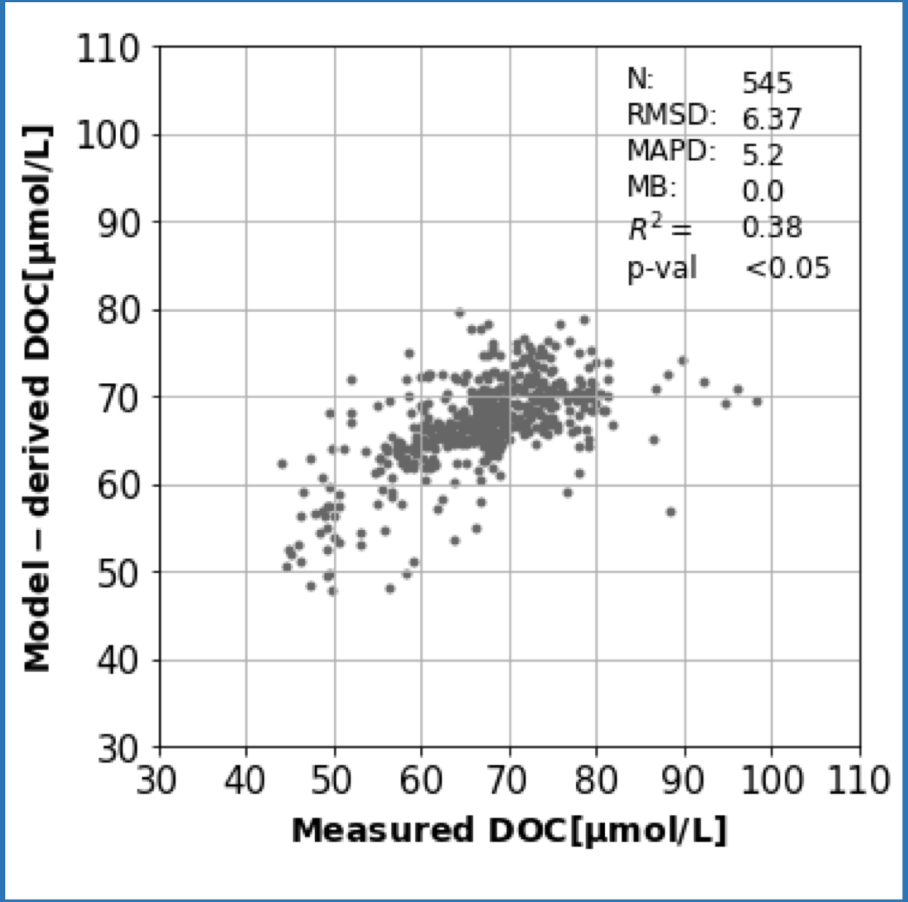
DOC does not covary with any of the individual input parameters. Nevertheless, the combination of parameters (MLR) shows great potential to estimate DOC.

Simple correlation



Multi Linear Regression



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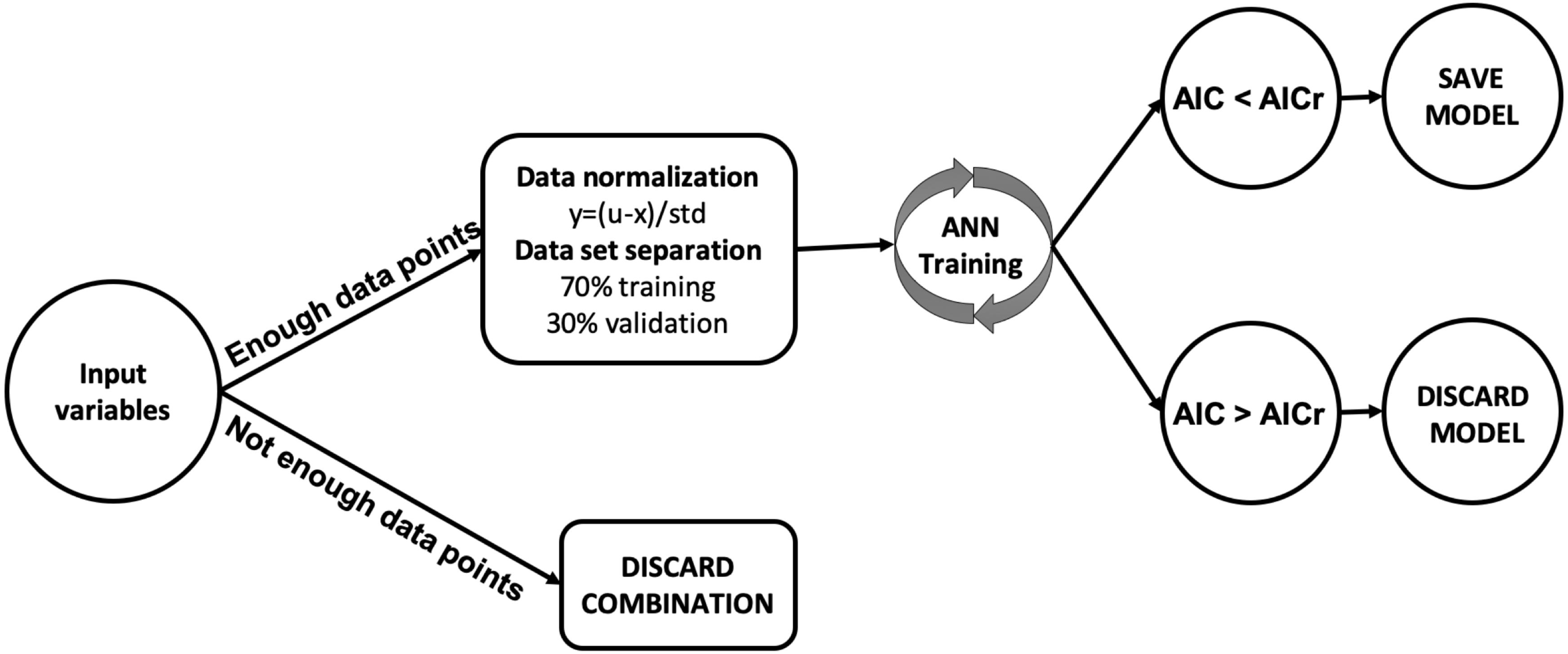
The model was built as a 2 steps iteration process to first select the most suitable inputs and then the best structure of the ANN.

STEP 1: selection of the most suitable inputs

STEP 2: selection of the best structure (neurons, hidden layers, activation function, etc.)



STATISTIC USED FOR THE SELECTION:
Akaike Information Criterion (AIC; Akaike 1974)

$$AIC = n * ln\,(MSE) + (n + p\,)/(1 - (p + 2)/n)$$

p = number of weights and bias
n = number of data points in the training dataset
MSE = Mean square error of the estimation.

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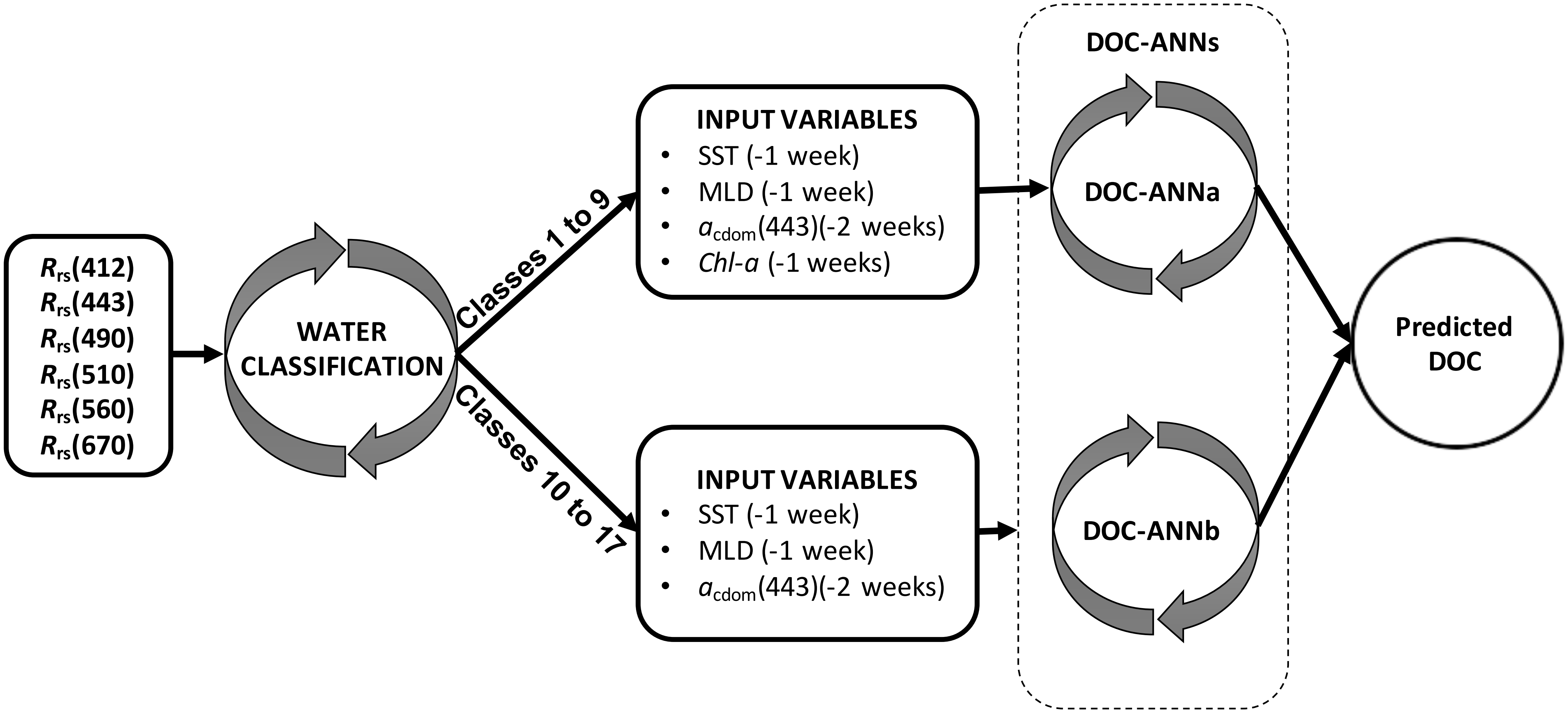
The final model (DOC-ANNs) combines two different ANN according to the optical water class the pixel belongs to. Each ANN uses different inputs with different time lags.



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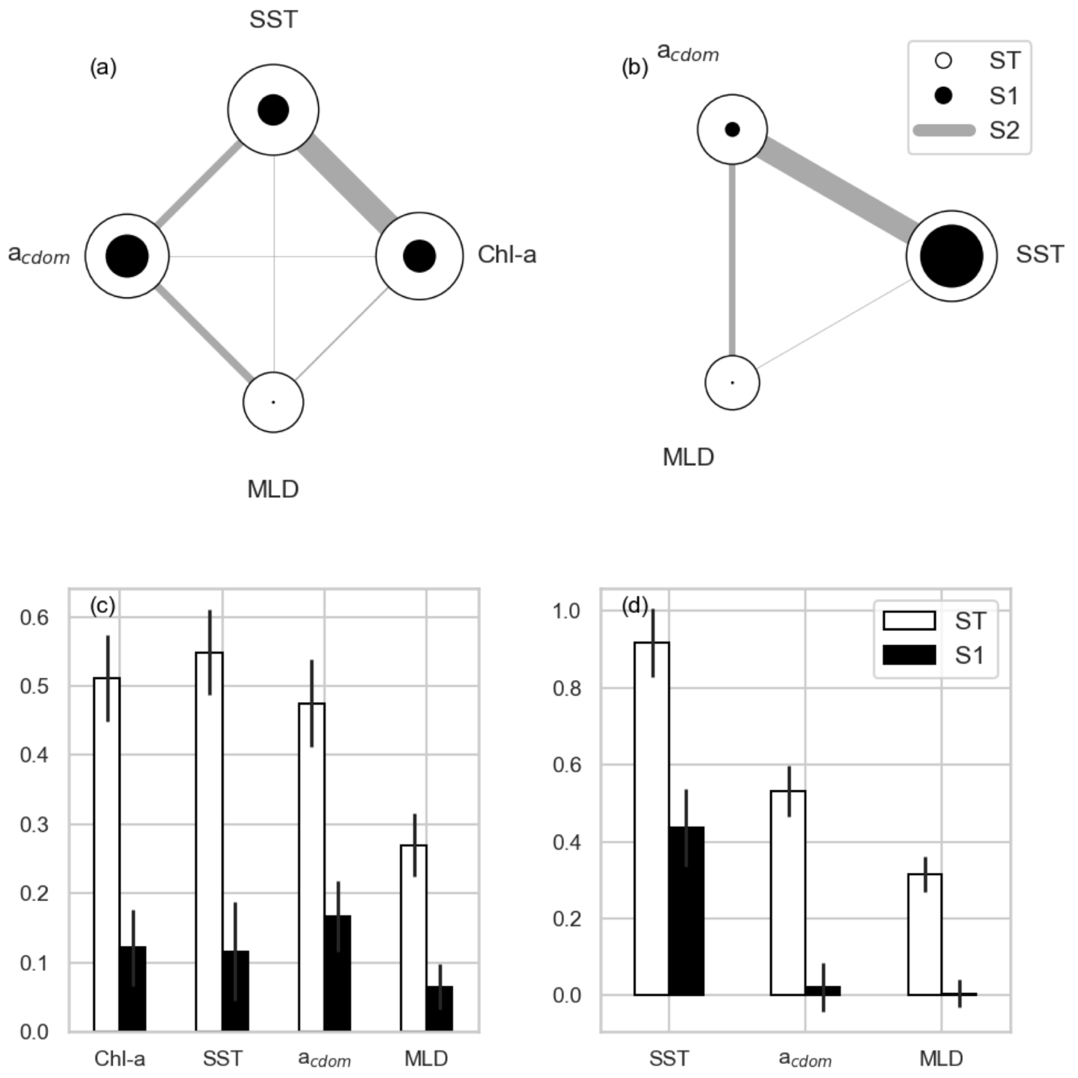
Based on a SOBOL sensitivity analysis, DOC-ANNs in open ocean is very sensitive to SST changes, followed by $a_{cdom}(443)$ variability. For OWC 1 to 9, SST, Chl-a, and $a_{cdom}(443)$ equally contribute to the variance of the model. In all cases MLD variability presents the lower impact on DOC-ANNs predictions.

SOBOL SENSITIVITY ANALYSIS OF DOC-ANNs (Sobol, 2001)

ST: Contribution to the variance when interacting with other variables

S1: Individual contribution to variance

S2: Interaction between variables



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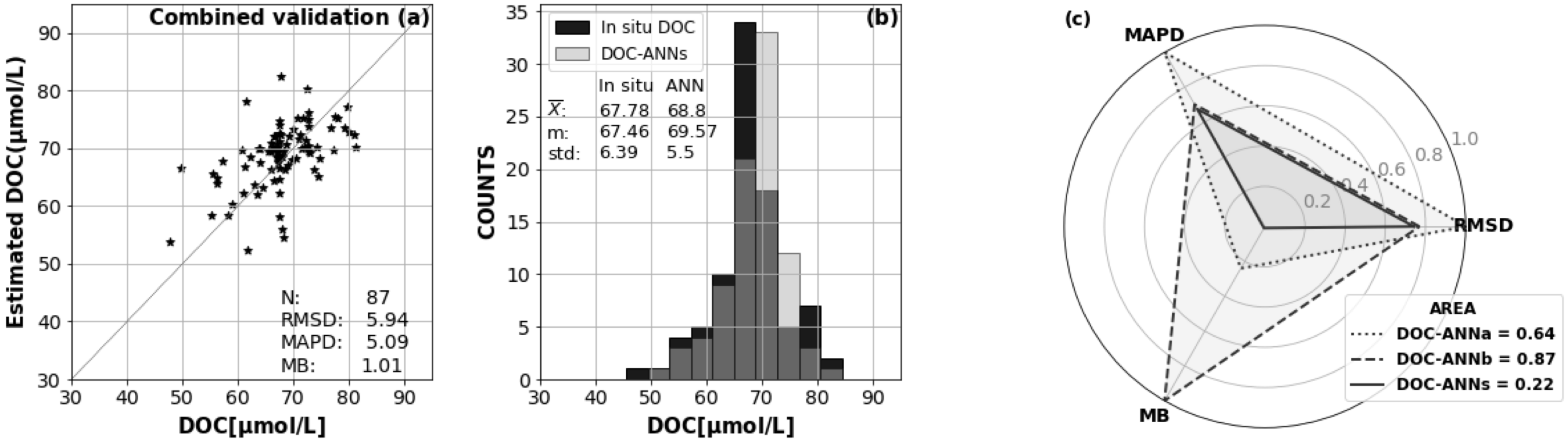
Based on the validation data set, DOC can be estimated with a MAPD of 5.09%. The implementation of a switch by water class improves the estimation of DOC by 65 % with respect to DOC-ANNa and 75 % with respect to DOC-ANNb.



Radar plot summarizing the statistics (normalized to 1) used for evaluating *DOC*-ANNa, *DOC*-ANNb, and *DOC*-ANNs over their respective validation data sets.
The smaller the area, the better is the performance.

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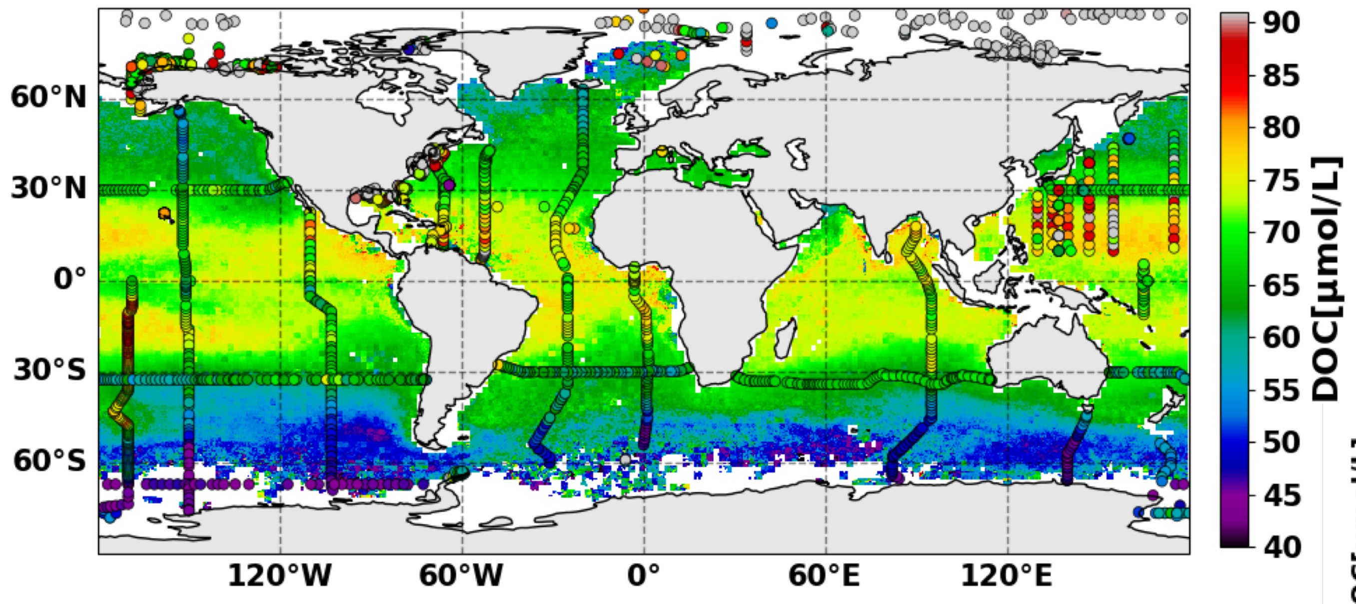
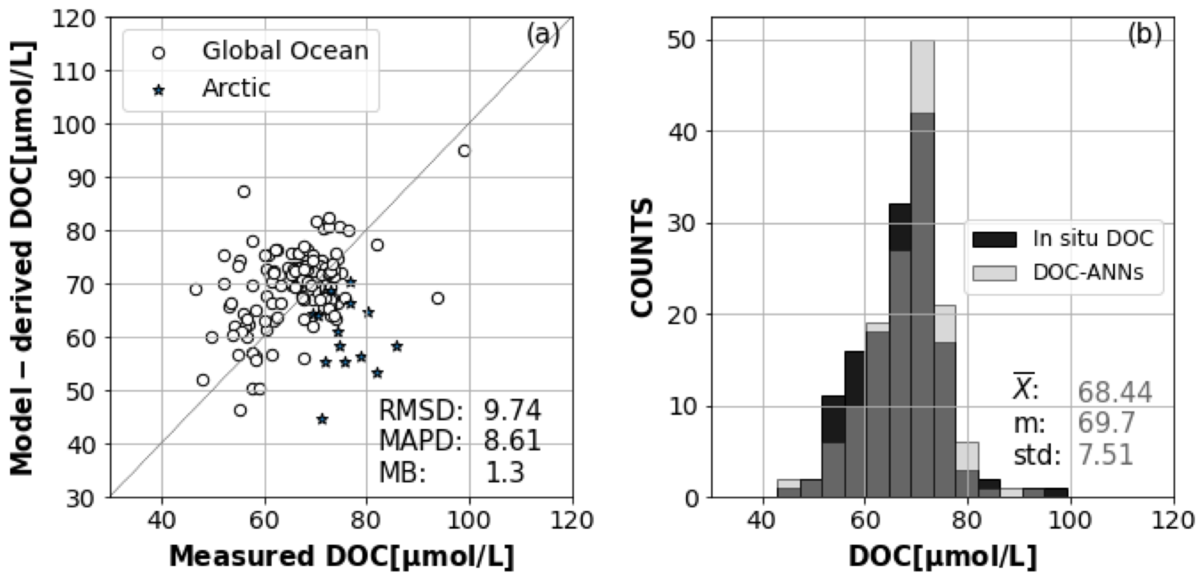
The DOC 10-year average map (2002-2012) produced with DOC-ANNs follows the expected DOC spatial patterns and is in general agreement with in situ DOC data collected between 1991 to 2015.

Further, the model-derivied DOC shows good accuracy with a new in situ independent data set (Hansell et al., 2021), with a small underestimation in the Arctic.





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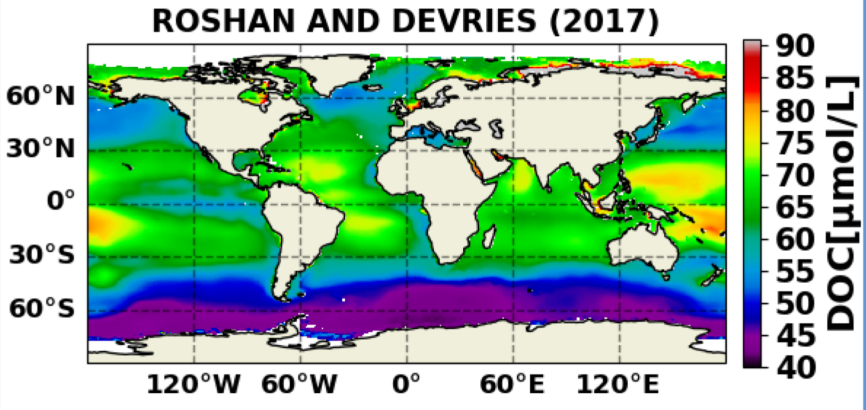
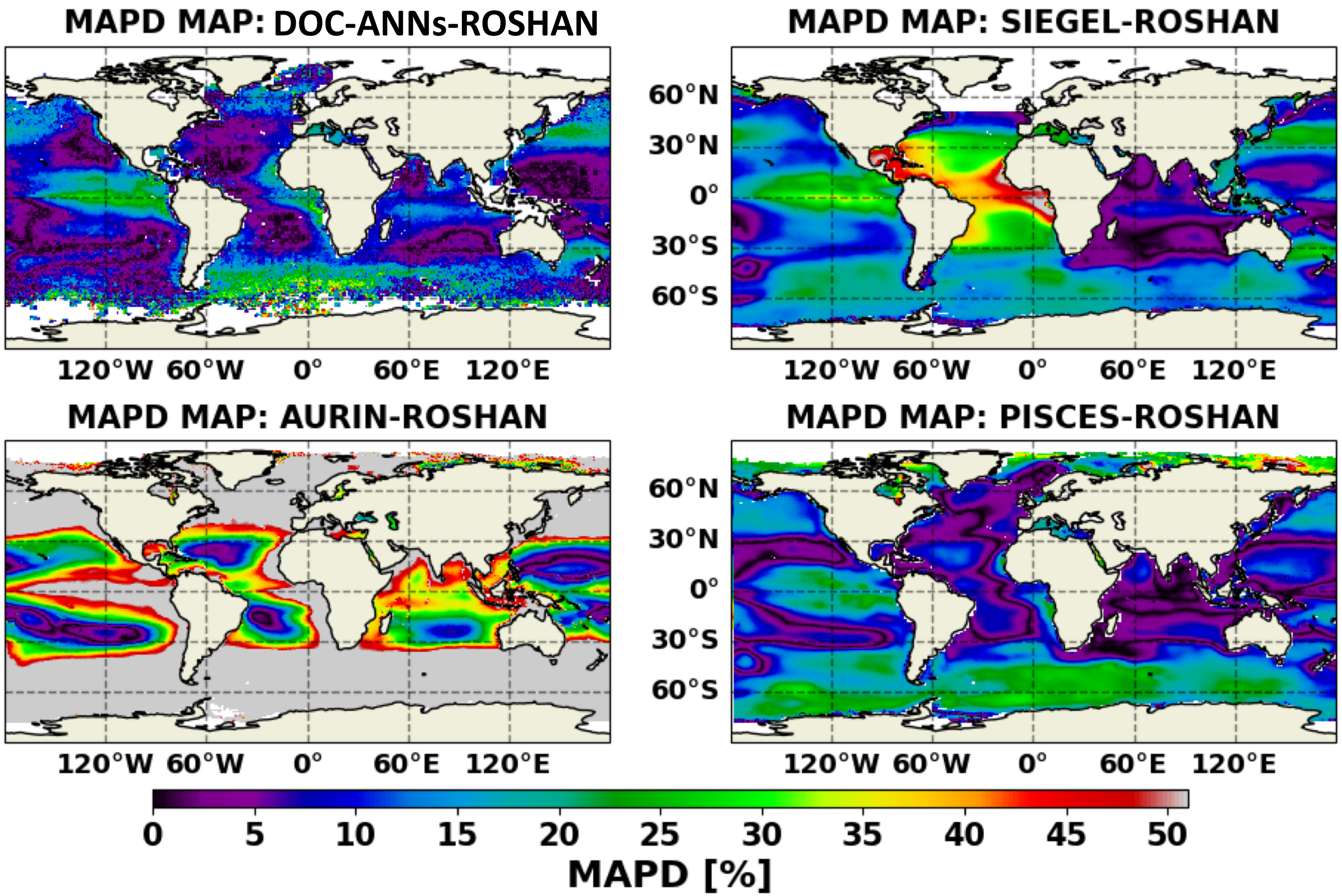
DOC-ANNs presents the greatest similarities with the annual average developed by Roshan and Devries (2017).



Global average of DOC built by Roshan and DeVries (2017)

$R^2 \geq 0.95$ (In situ vs average map)

Only 6 % of the data used by Roshan and DeVries was included in the developing data set of DOC-ANNs



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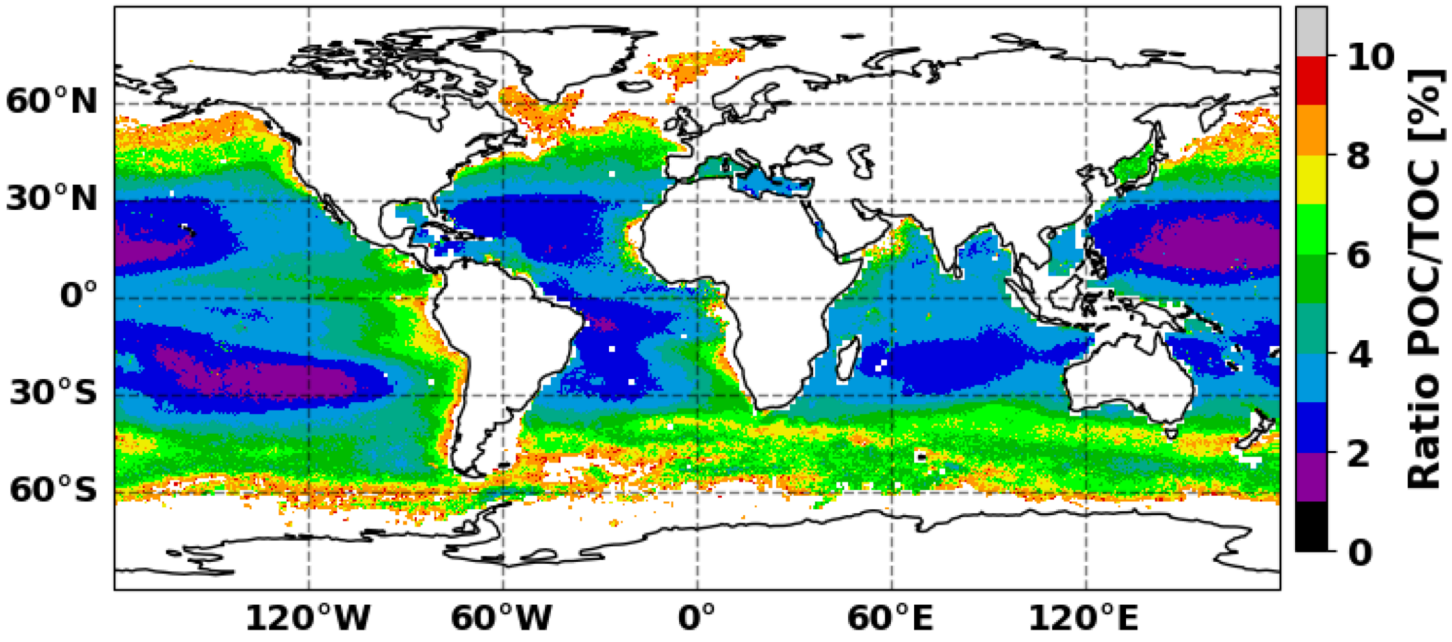
Ongoing work

Perform a deeper evaluation of DOC time series to test the temporal performance of the model.

Generate a longer satellite derived DOC dataset in order to provide better insight into DOC temporal dynamics (seasonality, inter-annual variability).

Study the contribution of DOC to the carbon budget (POC vs DOC) in the surface of the ocean and its temporal variability.



First global map of POC/TOC in good agreement with previous in situ studies (*F.Kumari and Mohan, 2018; Maciejewska & Pempkowiak, 2014; Sanders et al., 2014; Santana-Falcón et al., 2017*)

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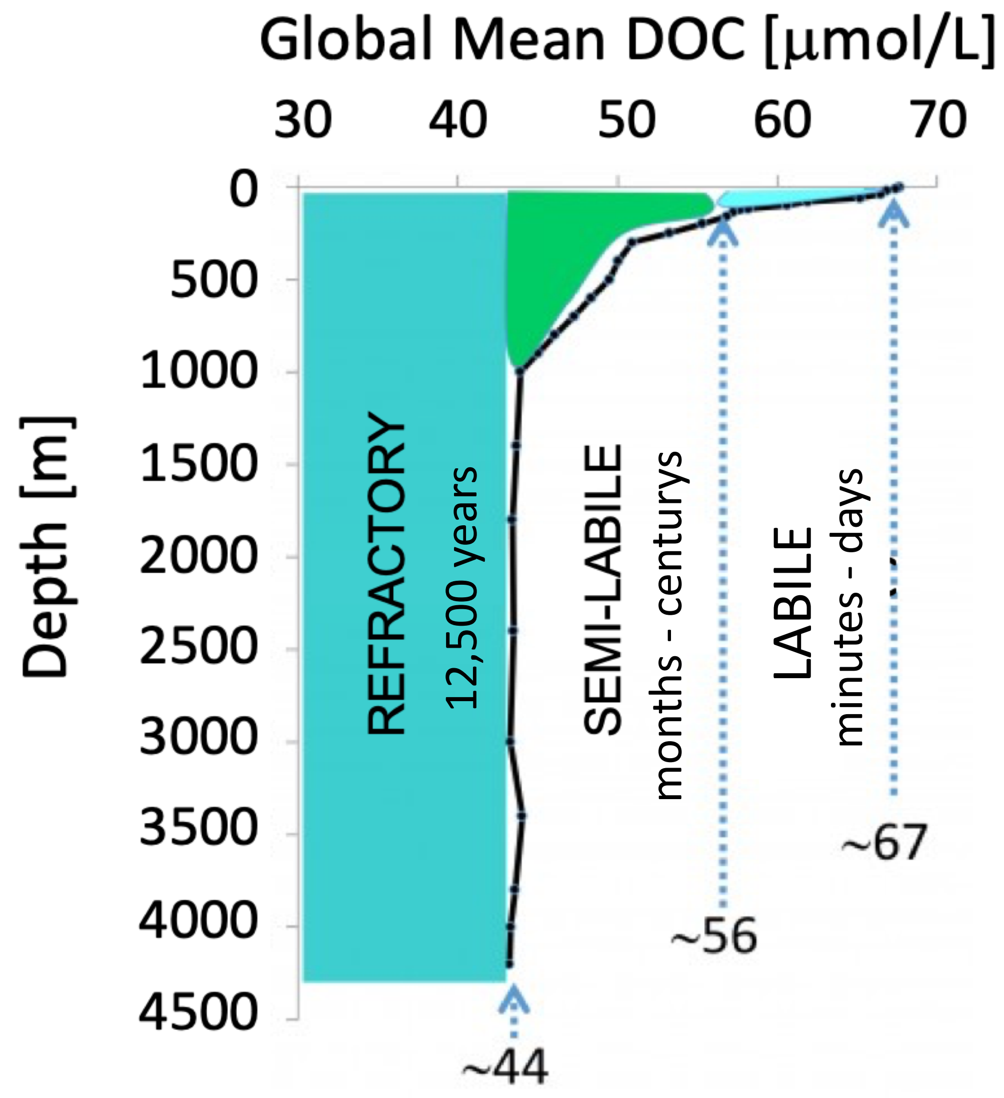
THANKS FOR YOUR ATTENTION

The DOC can be categorized in 3 types, depending on how resistant is to degradation.



LABILE
- Rapid mineralization
- < 1% of the ocean DOC stock

SEMI-LABILE
- More resistant
- Partially exported to deeper water

REFRACTORY
- Most resistant
- 94% of the oceanic DOC
- It is exported to deep ocean

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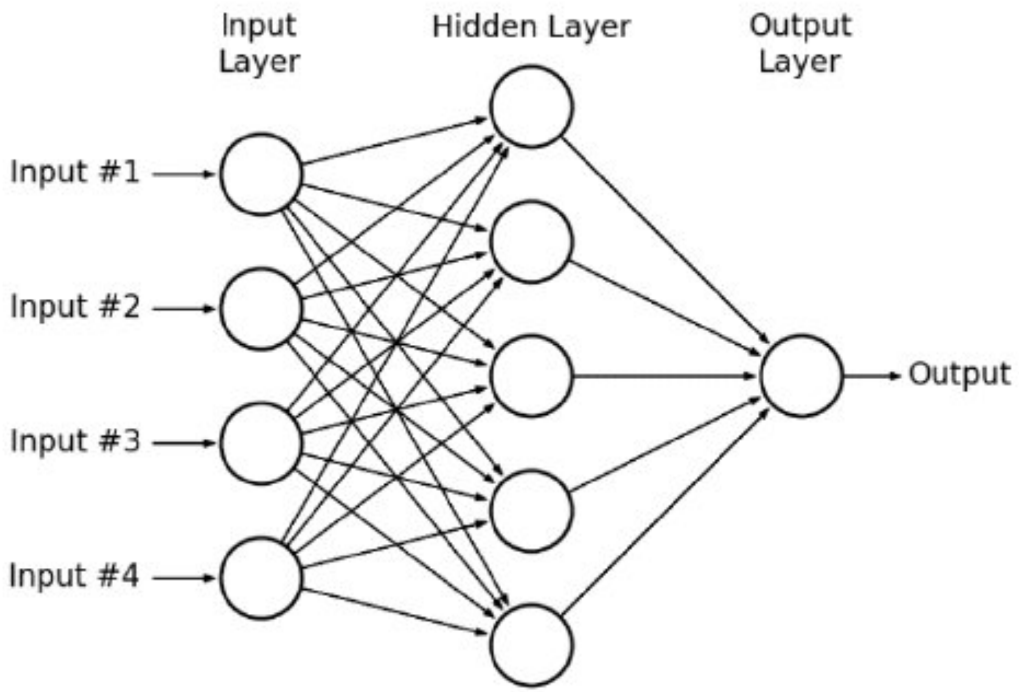
Artificial Neural Network: Set of functional units (neurons) organized in layers, interconnected to receive and transmit information (Jamet et al., 2012). The outer layer has non-linearity with the input layer (Sharma and Sharma, 2020).



Accuracy of the ANN

- **Architecture**
  - **Number of layers**
  - **Activation Function**
    Controls the amplitude of the output
- **Weights**

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Datasets distribution

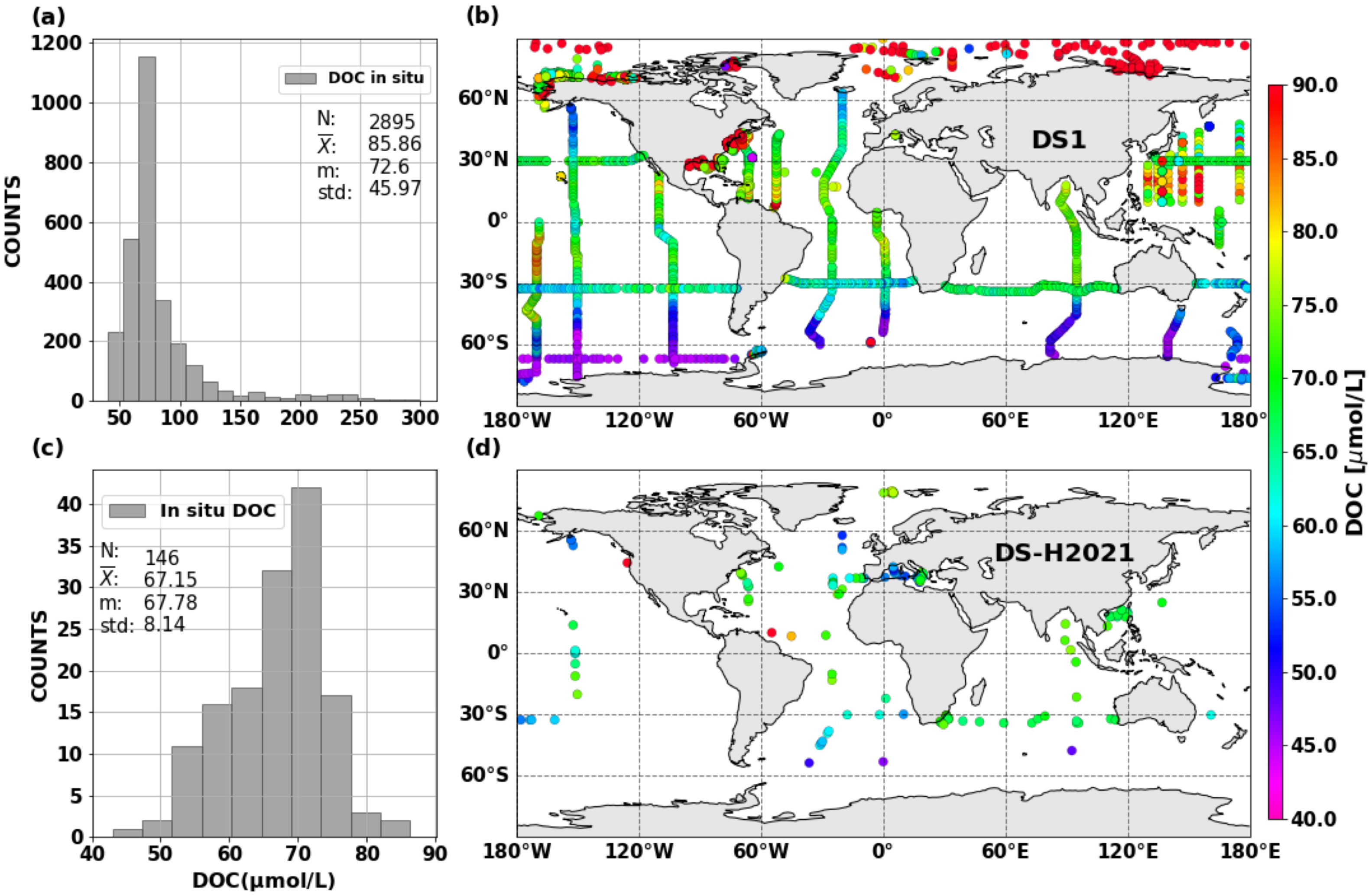

Figure. Histogram and spatial distribution of *in situ* surface *DOC* measurements for DS1 (a, b) and DS-H2021 (c, d). N, X, m and std correspond to the number of data points, mean, median and standard deviation, respectively.

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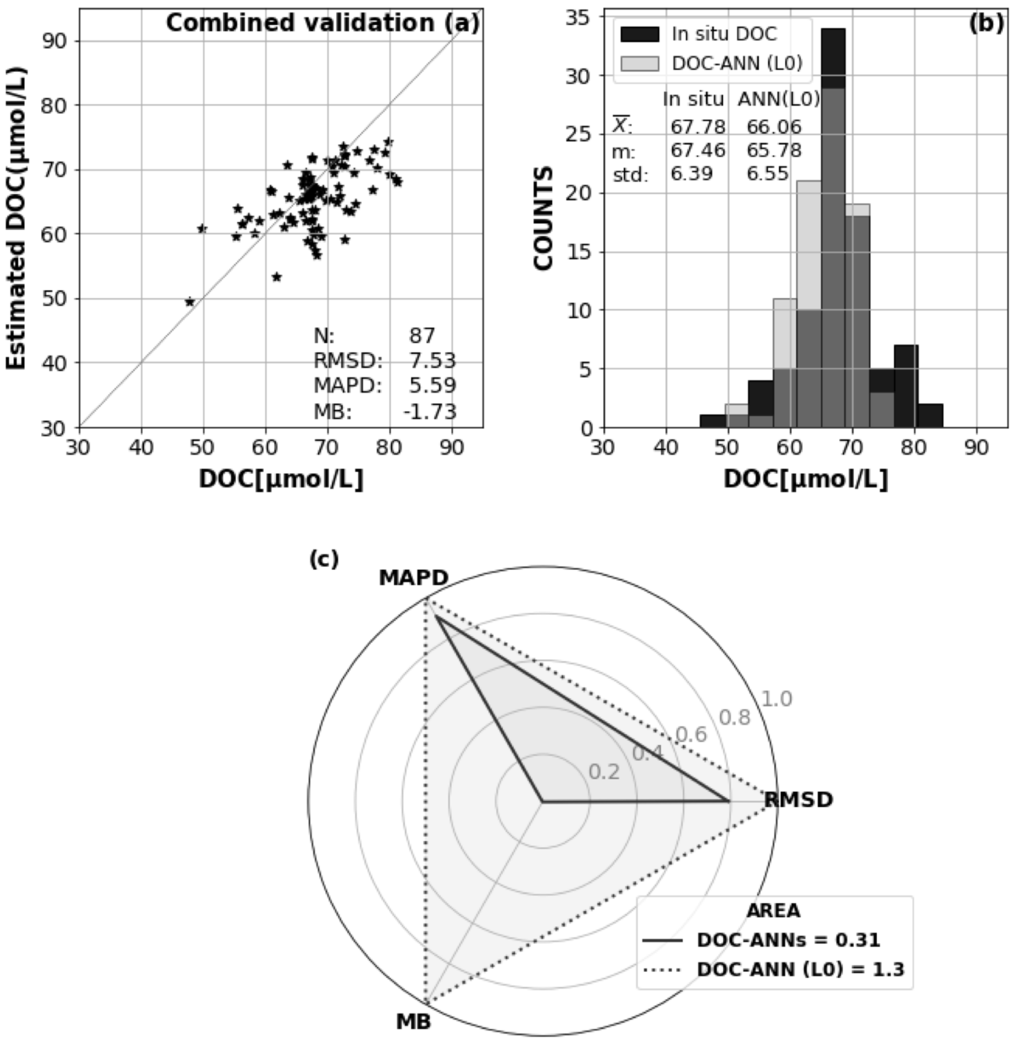
By training the neural network with the same inputs but at Lag 0 we observe that the performance considerably decreases



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