

living planet symposium | BONN 23-27 May 2022

TAKING THE PULSE OF OUR PLANET FROM SPACE

Novel ocean color information from Sentinel-5P's high spectral resolution



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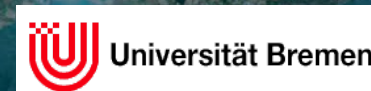
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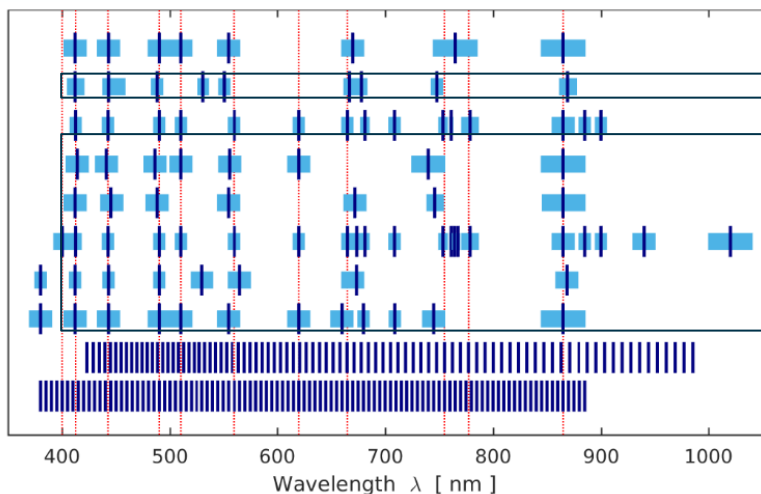
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24 May 2022

Ocean Colour beyond multispectral satellite data

-2



- SeaWiFS
- MODIS
- MERIS
- OCM-2
- VIIRS
- OLCI
- SGLI
- GOCI-2

Current multispectral

<1 km pixel

1.5-3 days global coverage

EnMAP 2022-, 30m pixel, 5000km/orbit, as DESIS 2018-, PRISMA 2019-

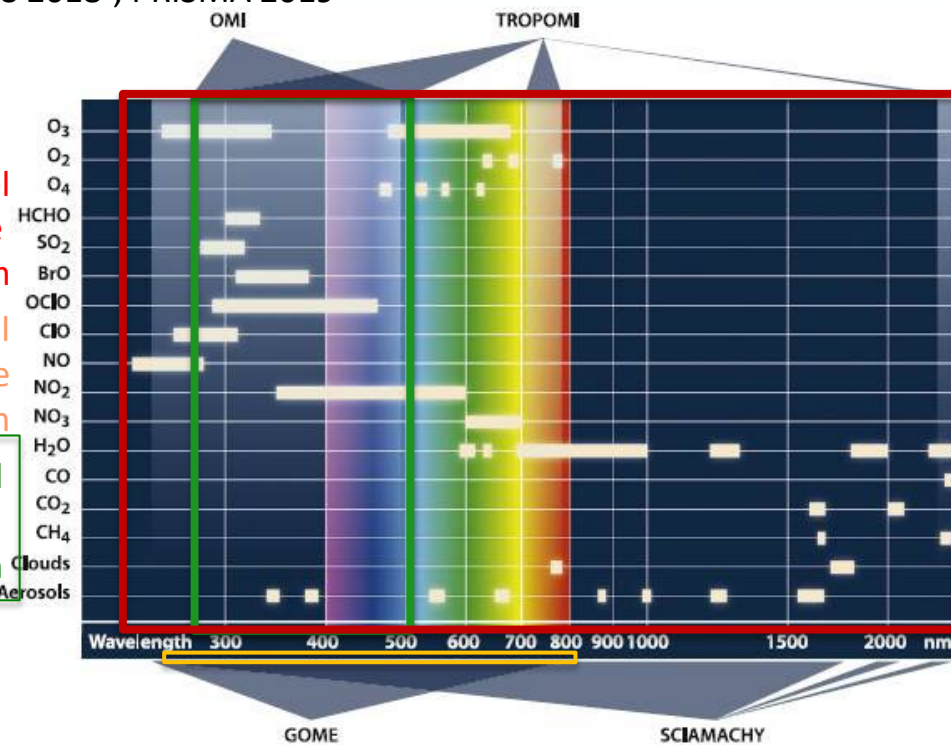
PACE/OCI 2024-, 1km pixel, 2 days

Hieronymi et al. (2019)

SCIAMACHY/ENVISAT: 2002-2012, 30 x 60 km pixel
6 days global coverage
240-2400 nm

GOME-2/METOP: 2007 - , 40 x 80 km pixel
3 days global coverage
240 - 800 nm

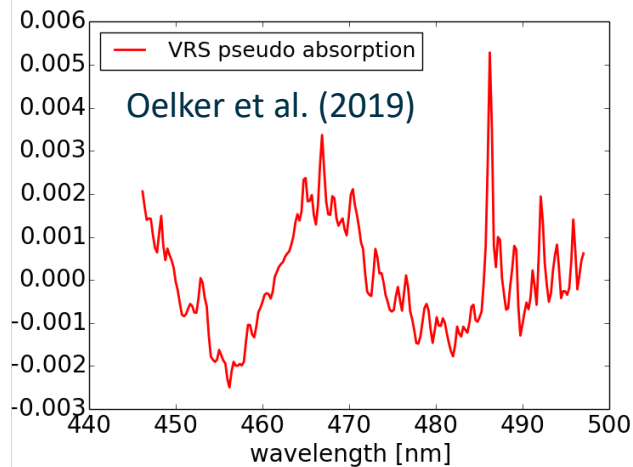
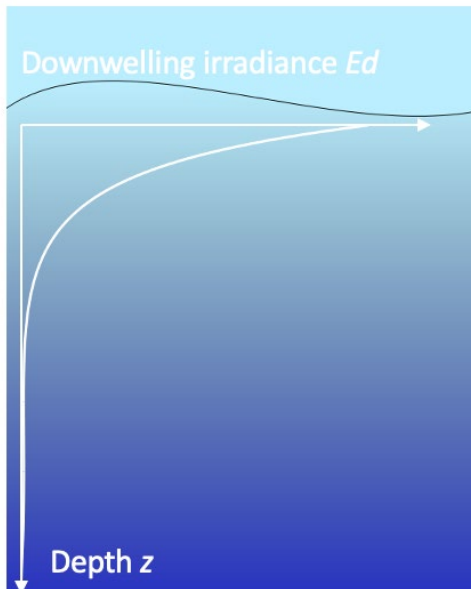
TROPOMI/S5P: 5/2018 -, 5.5 x 3.5 km pixel
daily global coverage
280 - 500 nm, 675-775 nm



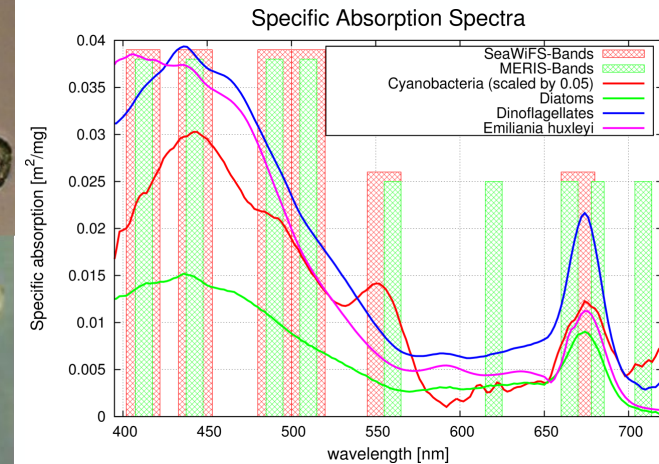
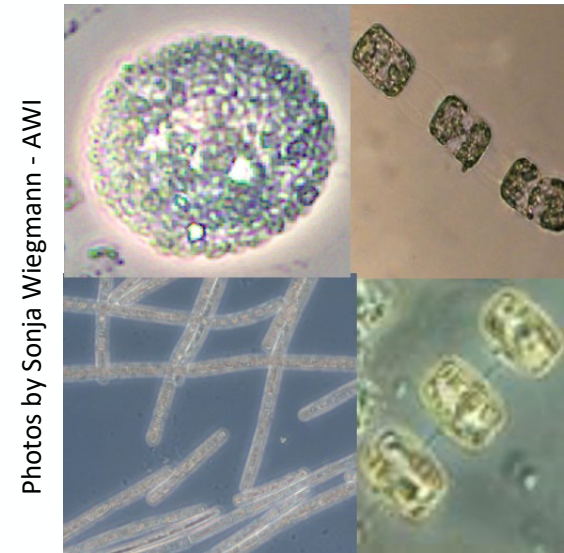
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Novel (missing) Ocean Color Products with TROPOMI

Diffuse attenuation K_d



PFTs: phytoplankton functional types

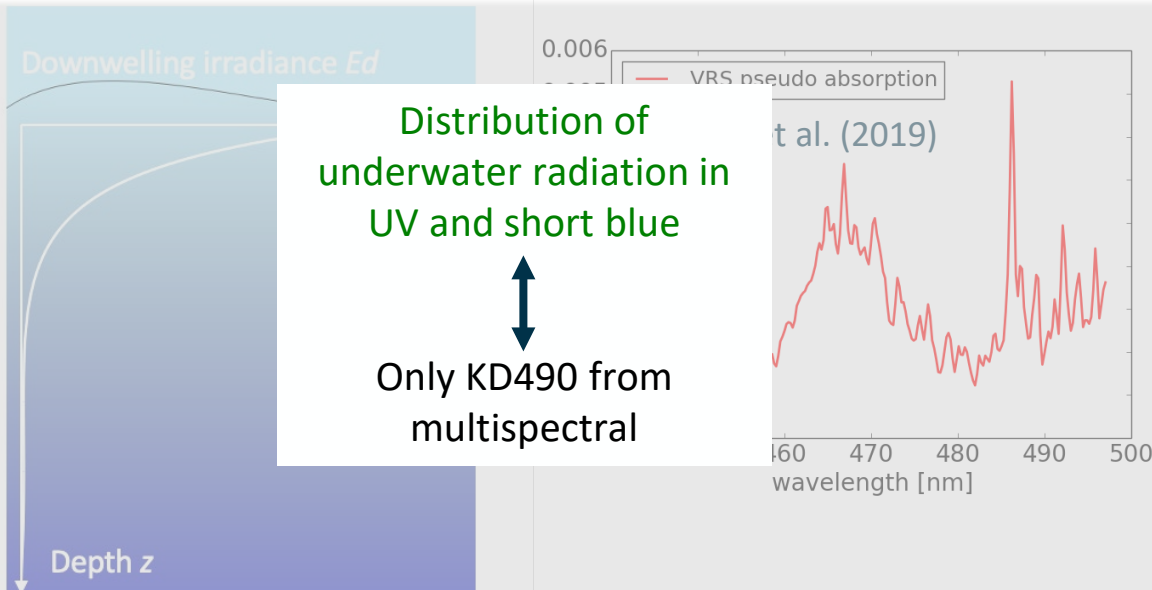


Vibrational Raman scattering (VRS) of H₂O molecules - causes filling-in in high spectrally resolved backscattered radiation
 ➤ related to the light availability (diffuse attenuation – see for SCIAMACHY (Dinter et al. 2015), for OMI and GOME-2 (Oelker et al. 2019)).

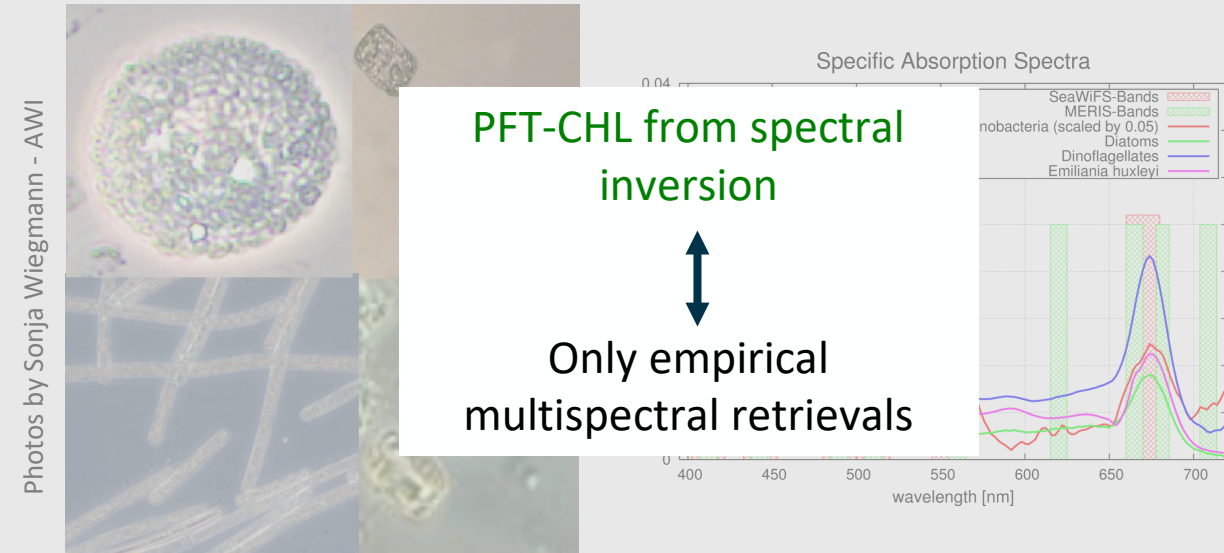
PFT specific absorption can be identified in high spectrally resolved SCIAMACHY data (Bracher et al. 2009, Sadeghi et al. 2012).

Novel (missing) Ocean Color Products with TROPOMI

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PFTs: phytoplankton functional types



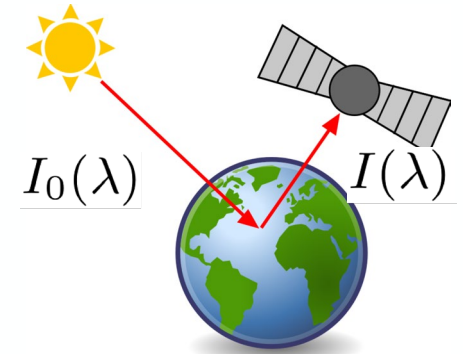
- ✓ KD : Sources of CDOM, UV-absorbing compounds
- ✓ KD : Shortwave radiation budget in the ocean (PP, photodamage, -degradation processes)

Effects of Climate Change

- ✓ PFTs: Indices of biodiversity & more precise descriptors of primary production (PP) ocean carbon pool

TROPOMI Retrievals: PhytoDOAS

DOAS applied to retrieve ocean products: Vountas et al. 2007, Bracher et al. 2009, Sadeghi et al. 2012, Dinter et al. 2015, Losa et al. 2017, Oelker et al. 2019, Oelker et al. 2022



Based on Beer-Lamberts law $I(\lambda) = I_0(\lambda) \cdot \exp(-\tau(\lambda)) \Rightarrow \tau(\lambda) = \ln \frac{I_0(\lambda)}{I(\lambda)}$

DOAS equation

$$\tau(\lambda) = \underbrace{\sum_{i=0}^I S_{a,i} \sigma_{a,i}}_{\text{Atmospheric absorbers}} + \underbrace{\sum_{j=0}^J S_{o,j} \sigma_{o,j}}_{\text{Oceanic absorbers (phytoplankton, liquid water)}} + \underbrace{\sum_{k=0}^K S_{p,k} \sigma_{p,k}}_{\substack{\text{Pseudoabsorption} \\ \text{(inelastic scattering:} \\ \text{VRS, RRS)}}} + \underbrace{\sum_{l=0}^L S_{e,l} \sigma_{e,l}}_{\text{instrumental effects}} + \underbrace{\sum_{m=0}^M x_m \lambda^m}_{\text{Polynomial (elastic scatt., CDOM+NAP absorption)}}$$

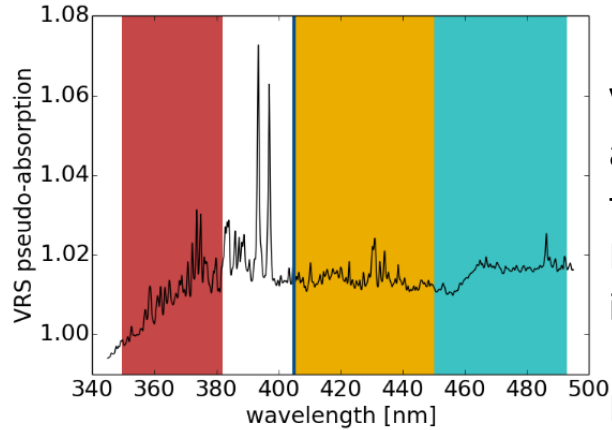
$I^{+,-}$ = modeled radiance with, without inelastic scattering
 S = fit factor, σ = reference spectrum
 VRS/RRS=vibrational/rotational Raman scattering

Solved for fit factors and polynomial coefficients via Levenberg Marquard LSM.

Diffuse attenuation (K_d) in three spectral bands from S5P's instrument TROPOMI (Oelker et al. 2022)



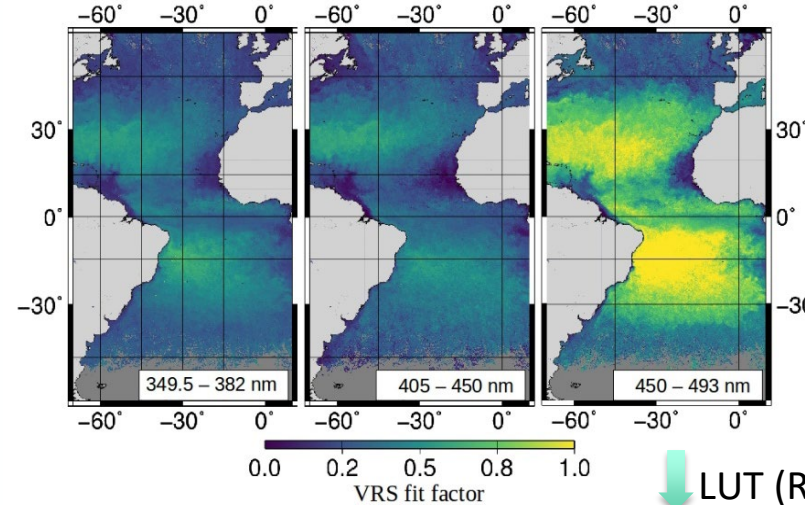
PhytoDOAS* K_d -retrieval (basis Vountas et al. 2007, Dinter et al. 2015, Oelker et al. 2019)



VRS pseudo-absorption derived from coupled O-A RTM SCIATRAN used in PhytoDOAS.

LUT: Look-Up Table links VRS-Fit factor + SZA + VZA to K_d .

TROPOMI Inelastic Scattering (VRS)



<https://doi.org/10.1594/PANGAEA.940352>

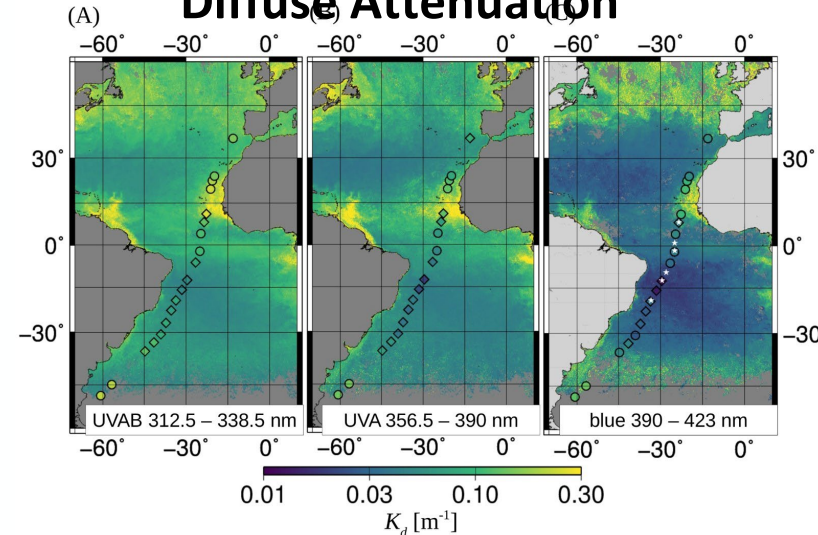
TROPOMI-retrieved underwater light attenuation in three spectral regions: ultraviolet to blue

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LUT (RTM)

Diffuse Attenuation

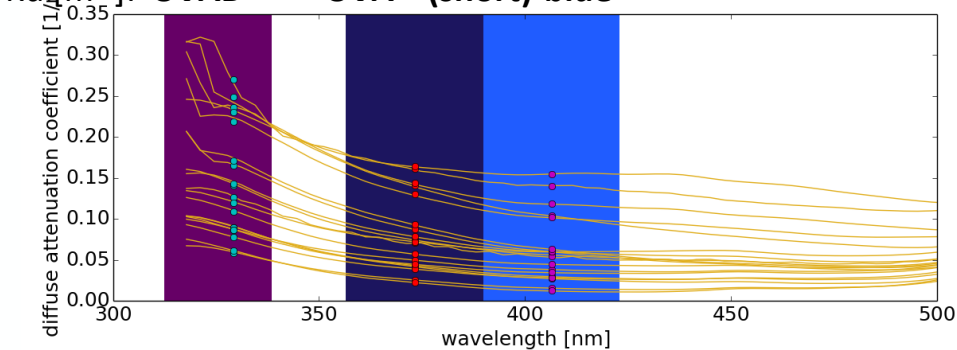


First time K_d retrievals in UV-AB & UV-A from satellite UV data (globally, via inversion).

VRS fit: UV short-blue blue

LUT (RTM)

K_d [m⁻¹]: UVAB UVA (short)-blue



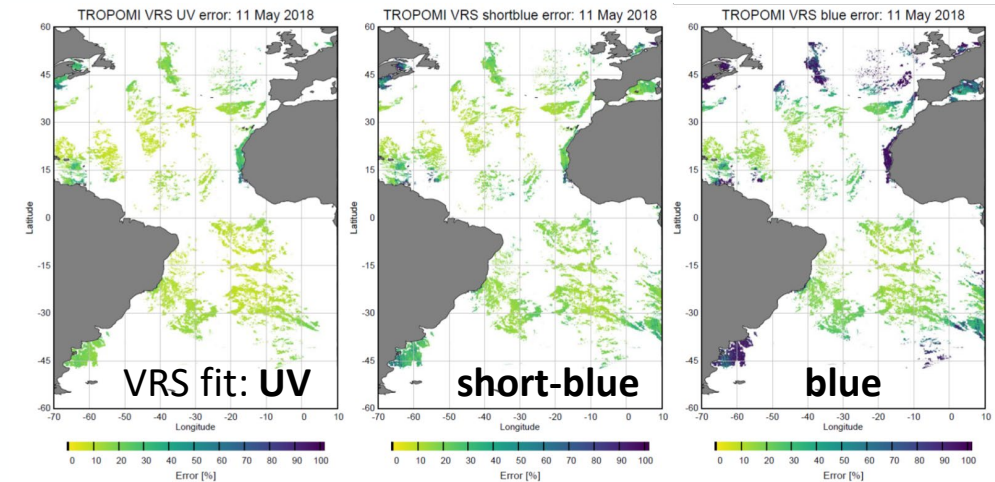
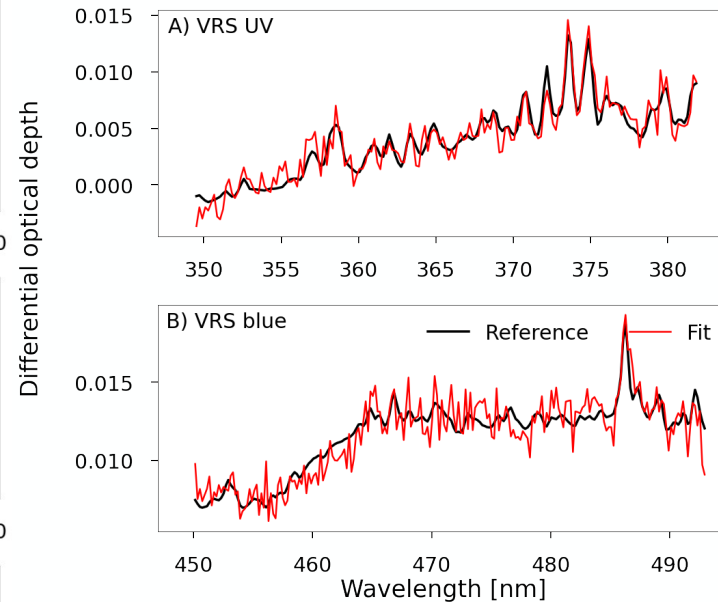
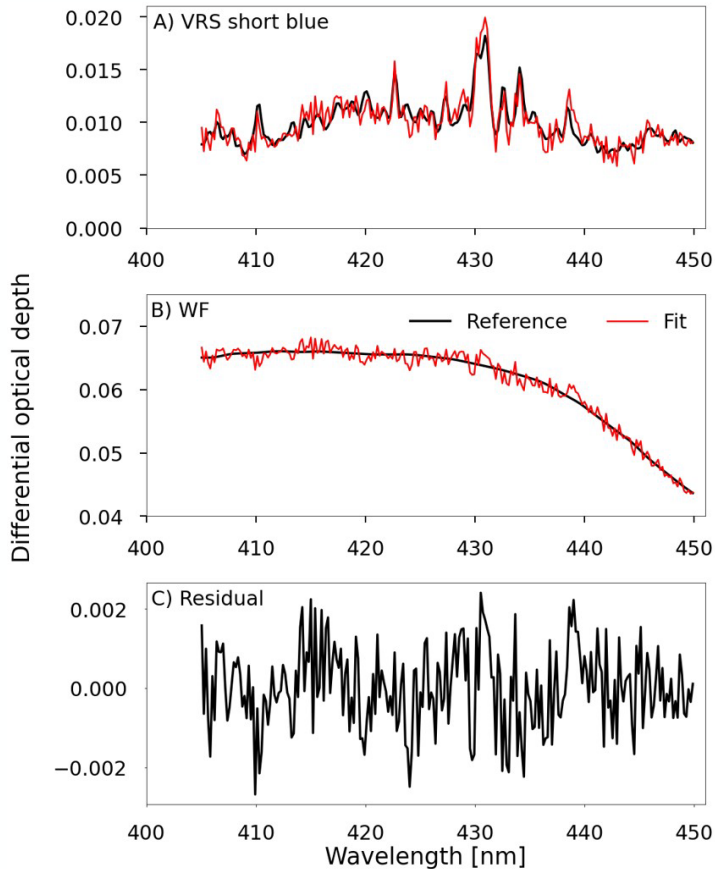
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TROPOMI diffuse attenuation (K_d) in UV and short blue: VRS (inelastic scattering) fit sensitivity & error (Oelker et al. 2022)

VRS fit with high fit factor

Specific fit factor error [%]



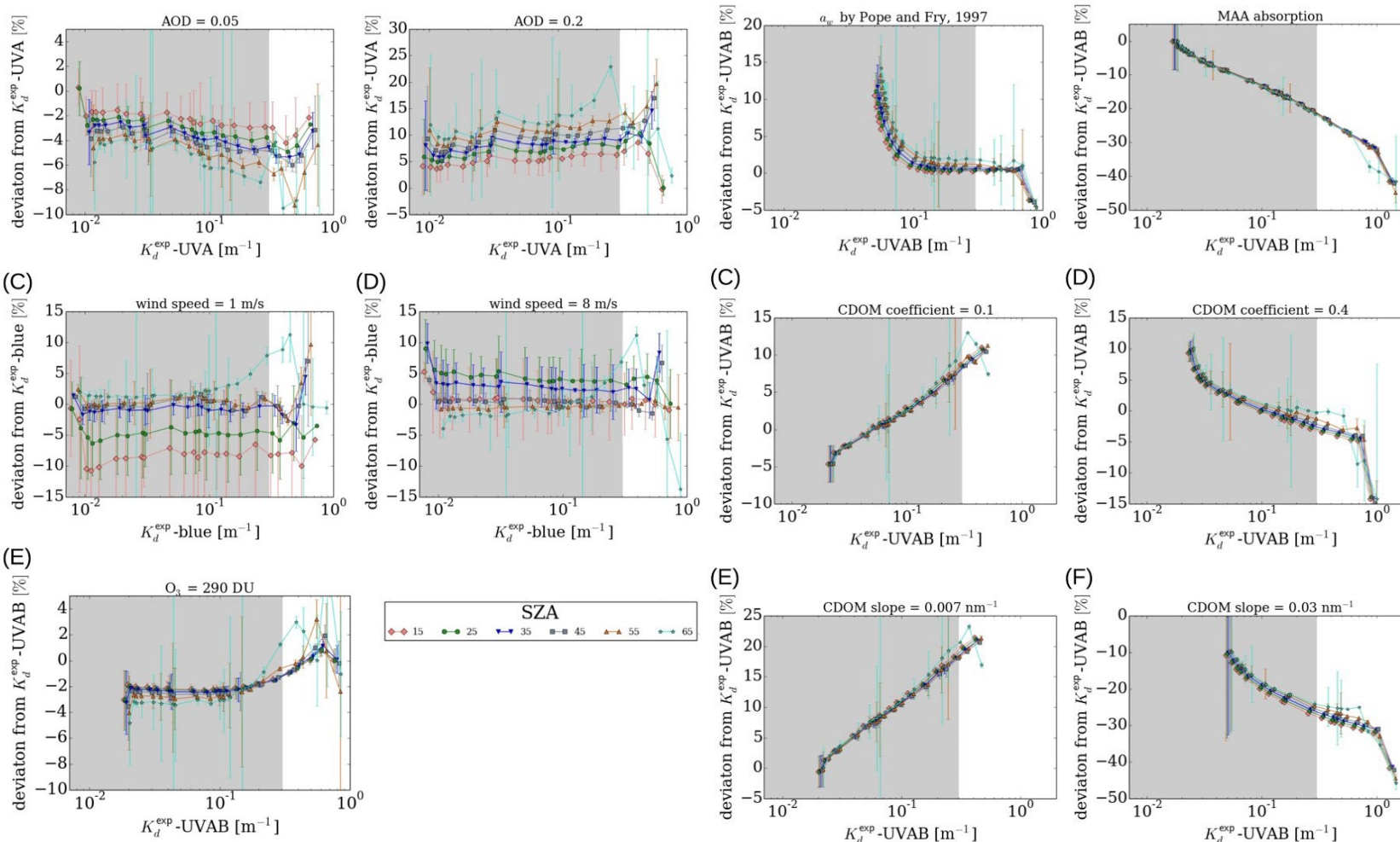
TROPOMI VRS fits:

High sensitivity (10^* more than SCIA)

Low errors: < 5% UVA, <10% short-blue, <15% blue

TROPOMI diffuse attenuation (K_d) in UV and short blue: K_d retrieval sensitivity & error budget (Oelker et al. 2022)

Retrieval sensitivity [%] to atmospheric (left) & oceanic (right) parametrizations using O-A RTM



Fit and model error of TROPOMI K_d (<0.3 m^{-1})

K_d	Fit	a_{CDOM}	CDOM-S	a_{ph}^*	AOD	WS	O_3
UVAB	10	10	30	20	5	3	3
UVA	15	10	25	20	15	5	0
blue	20	20	25	10	20	10	0

Error contributions as input for pixel-by-pixel uncertainty.

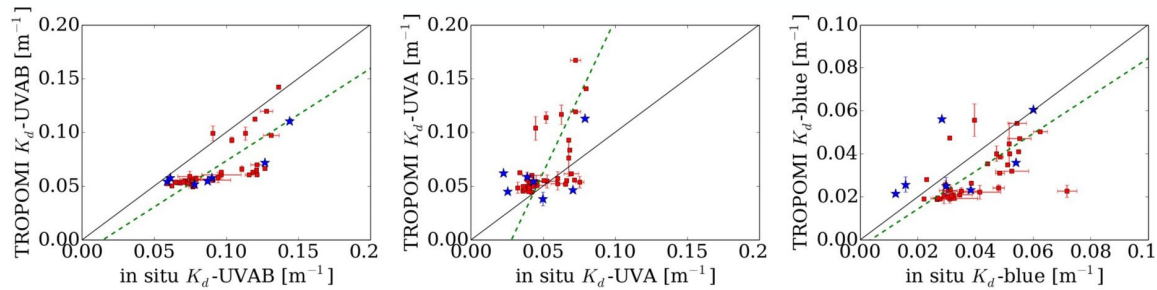
Overall reasonable uncertainty (max. 35%-45%)
 ~ multispectral K_d 490 & CHL retrieval errors.

TROPOMI K_d comparison to in-situ and OLCI & OC-CCI KD490

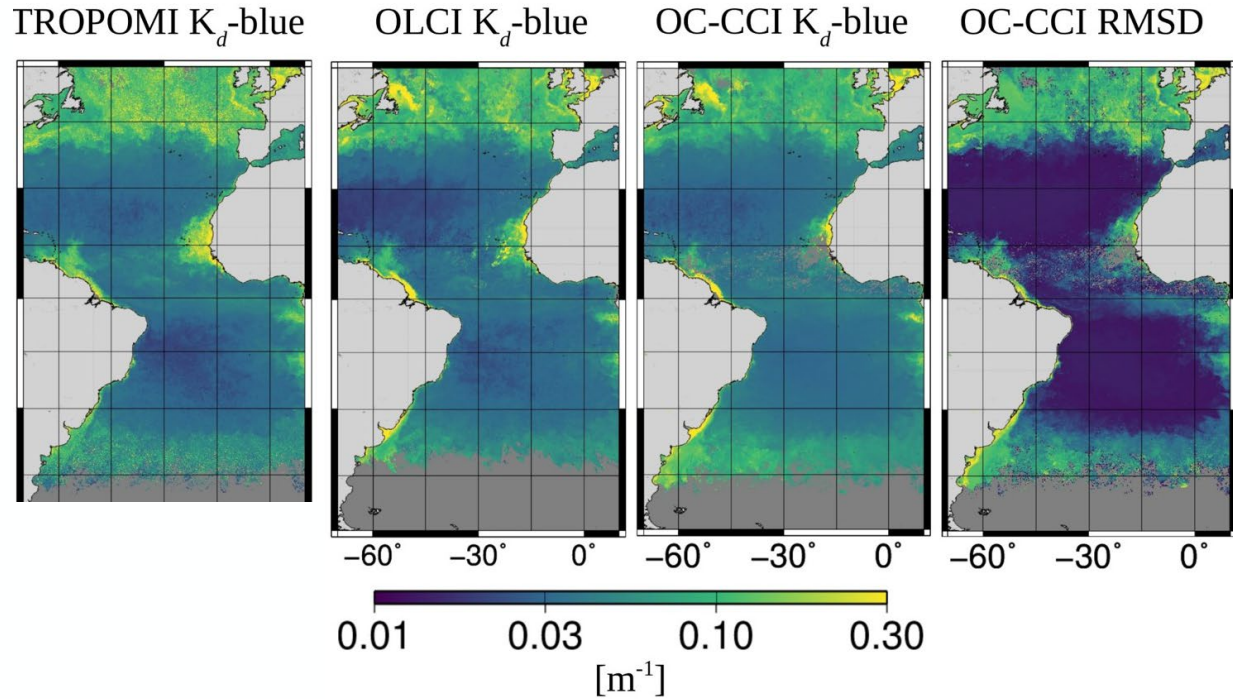


(Oelker et al. 2022)

TROPOMI K_d against in situ



Criteria	Kd-UVAB	Kd-UVA	Kd-blue
r	0.72	0.54	0.54
Bias (m ⁻¹)	-0.026	0.015	-0.008
MAE (m ⁻¹)	0.026	0.026	0.012
RMSD (m ⁻¹)	0.031	0.029	0.015
Unb.RMSE (m ⁻¹)	0.017	0.025	0.013



TROPOMI K_d-UVAB, -UVA and -blue agree well with in-situ (low # of matchups) and also K_d-blue within OCCCCI K_d.

TROPOMI PFT vs. OLCI-PFT vs. OCCCI-OCPPFT

TROPOMI

analytical

spectral decomp.

abundance-based

PhytoDOAS fit factor

TROPOMI

OLCI-PFT

OCCCI-OCPPFT

11 May- 9 Jun 2018

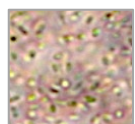
Circles: PFT from HPLC samples of RV Polarstern expedition PS113

Preliminary results indicate feasible retrievals of diatom and prokaryotic phytoplankton CHL.

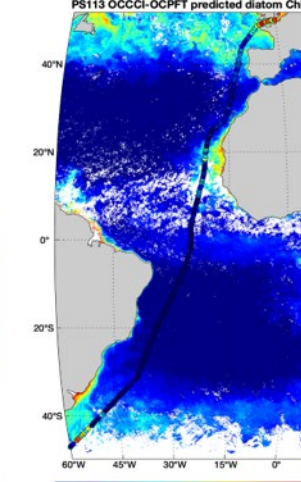
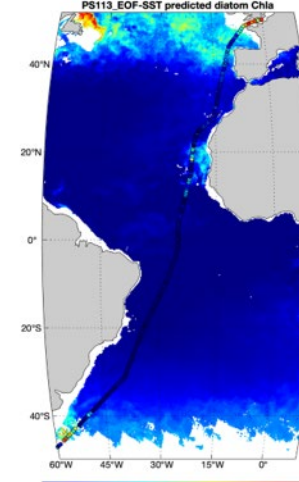
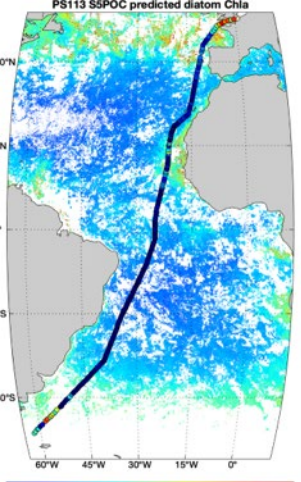
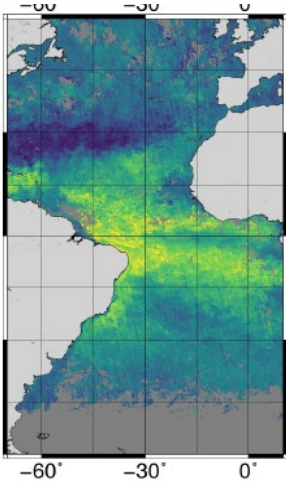
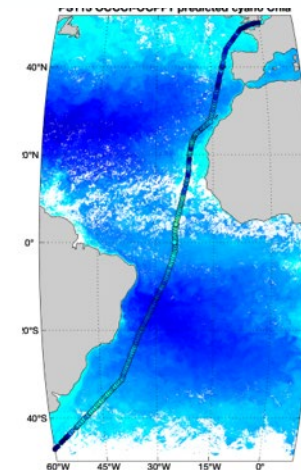
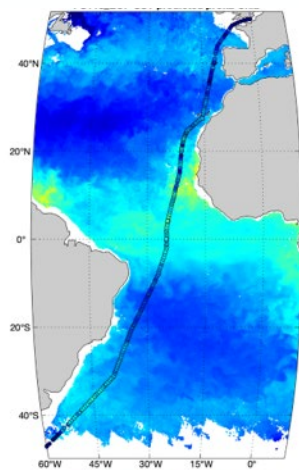
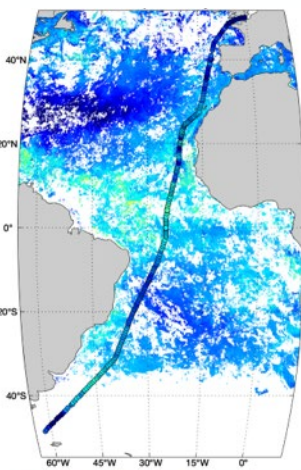
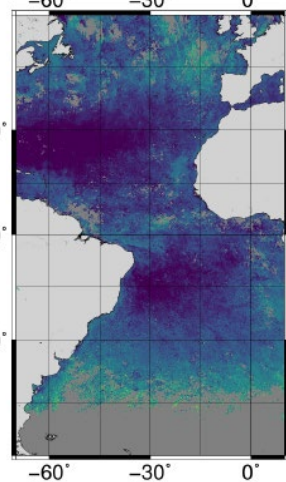
OLCI-PFT: Xi et al. 2021 <https://marine.copernicus.eu/>
 OCCCI-OCPPFT: CHL from OCCCI, PFT as in Losa et al. (2017)

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prokaryotic phyto.



diatoms



Conclusions & next steps for TROPOMI analytical OC products

Now:

- First time K_d in UVAB & in UV-A from satellite UV via [inversion with reasonable uncertainty](#).
- Potential of PFT-CHL [to improve empirical / statistical satellite PFT globally](#).

2-3 years:

[Global processing](#) (2018-) S5P K_d & (finalize retrieval) PFT-Chl incl. pixel uncertainty

[Combine](#) S5P-OC retrievals with [S3](#) (and similar data for long time series) to obtain

- $K_d(\lambda)$ at ≥ 9 -bands from 325-700 nm (325, 373, 405, [412](#), [443](#), [490](#), [510](#), [560](#), [665](#))
- higher quality cyanobacteria and diatom PFT-Chl from satellite (models)

[Demonstration of multiplatform](#) (bioARGO, towed, satellite) AOP & IOP [data fusion](#) for spectral K_D & 4D-PFT-Chl

TROPOMI-OC [know-how to new high spectral resolved](#) S4 (GEO), S5 - also PACE, EnMAP, DESIS, PRISMA

5 years:

New TROPOMI products: UV in water: MAAs, CDOM sources, photodegradation (PB), Chla fluorescence, DOC

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