

Enhancing ocean colour observation’s description of coloured dissolved organic matter by retrievals of the diffuse attenuation in the UV from Sentinel-5P TROPOMI

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Objectives

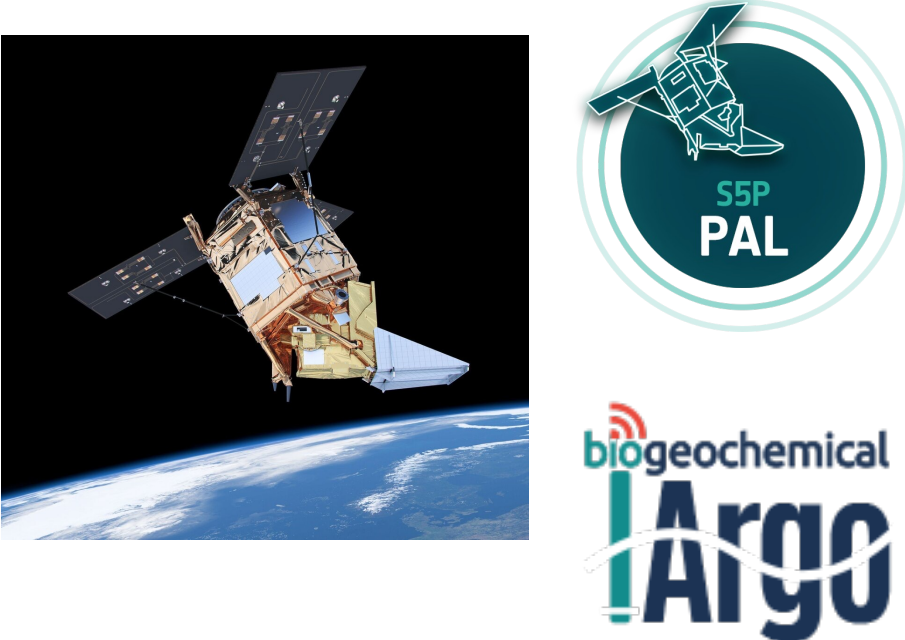
Light reflected from the ocean surface encodes essential information about phytoplankton, coloured dissolved organic matter (CDOM) and underwater light, relevant for estimating primary productivity or other biogeochemical processes. Atmospheric satellite sensors TROPOMI, SCIAMACHY, and GOME-2 have enabled **novel retrievals of diffuse attenuation (KD)** in the UV and short blue via differential optical absorption spectroscopy (DOAS) of Vibrational Raman Scattering (VRS) and radiative transfer modelling (RTM) [Dinter 2015, Oelker et al. 2019, Oelker et al. 2022]. Here we present updated TROPOMI KD-UVAB, KD-UVA and KD-blue products:

- Optimization** of retrieval by refining parametrization of phytoplankton and absorption and **extending Look-UP Tables (LUTs)** to include all viewing geometry effects.
- Implementation into operational processing** using ESA's operational prototype Copernicus Sentinel-5P Product Algorithm Laboratory (S5P-PAL).
- Comprehensive assessment of retrieval uncertainty and theoretical error budget** estimation for extending quality flags of KD products.
- Application of KD products for the Mediterranean Sea:**
 - Validation** against BGC-Argo Kd data
 - Classification of ecoregions** to improve the understanding of CDOM dynamics and contributing to a **refined view of carbon cycling** in the Mediterranean Sea.

Data sets

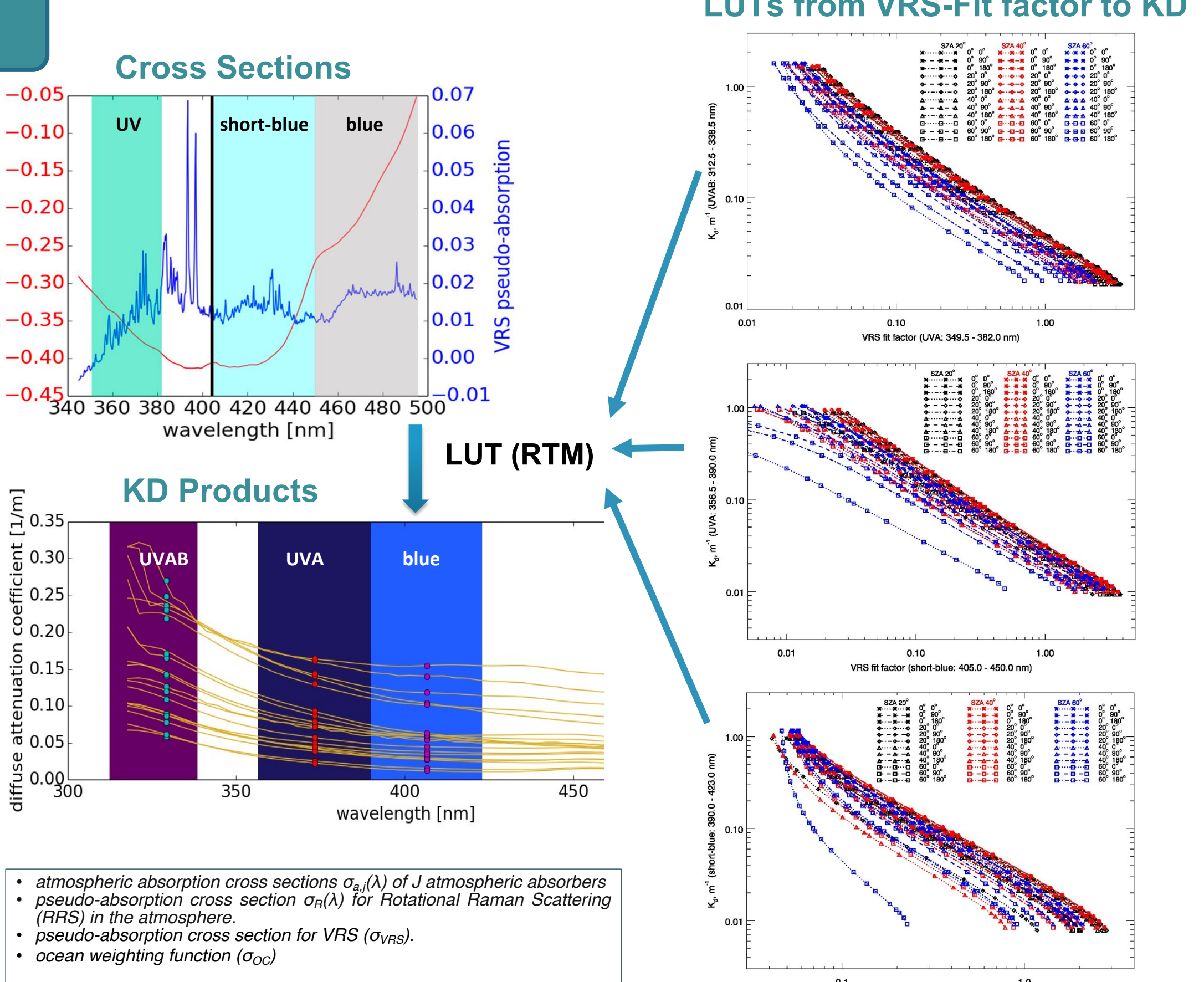
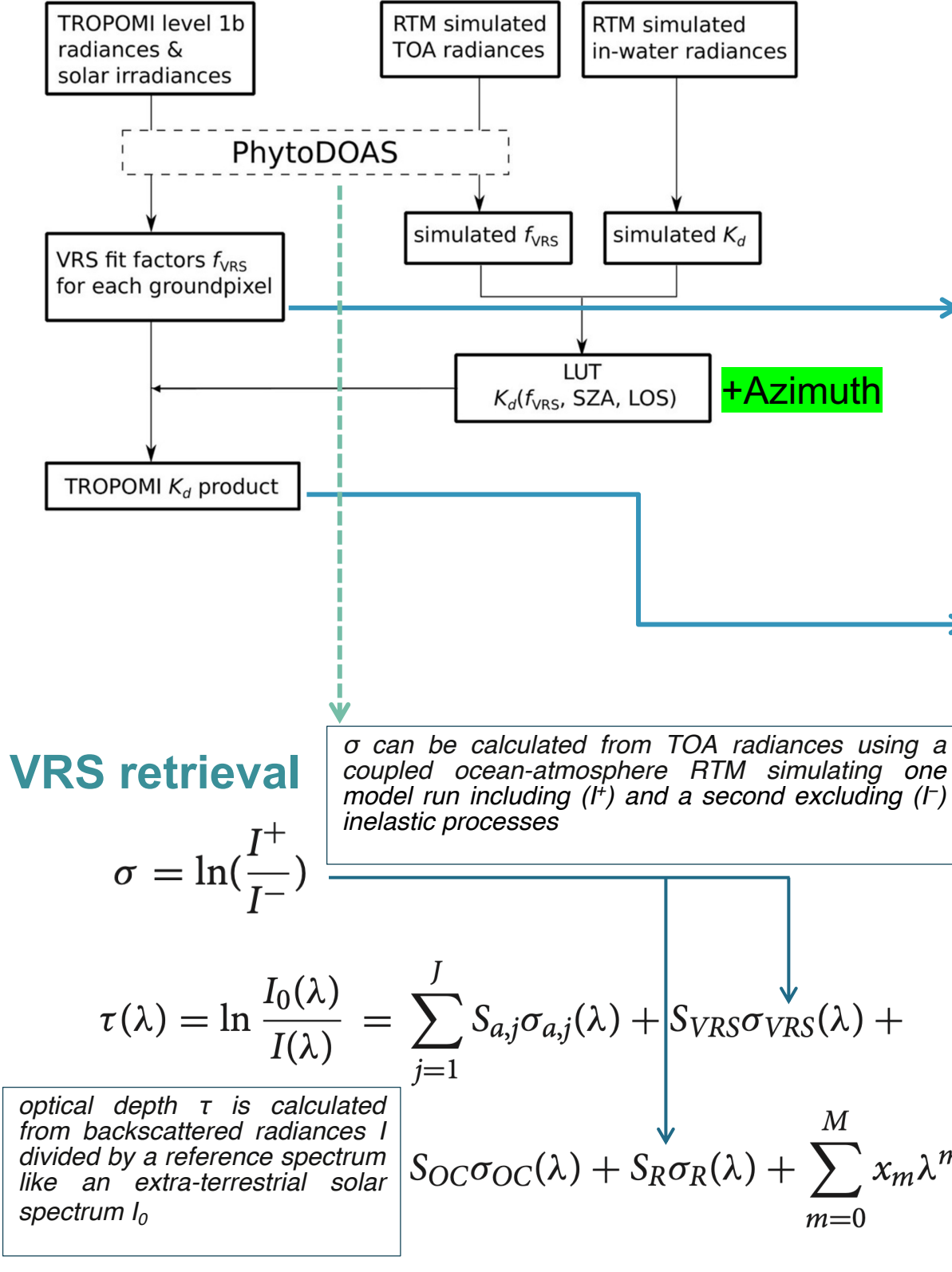
Sentinel-5P TROPOMI

- Spectral Resolution:** 0.25–0.5 nm
- Pixel Resolution:** 3.5 km × 5.5 km
- Swath Width:** ~2,600 km (~1 day) coverage
- Input Data:** L1B (Channels 3 and 4)



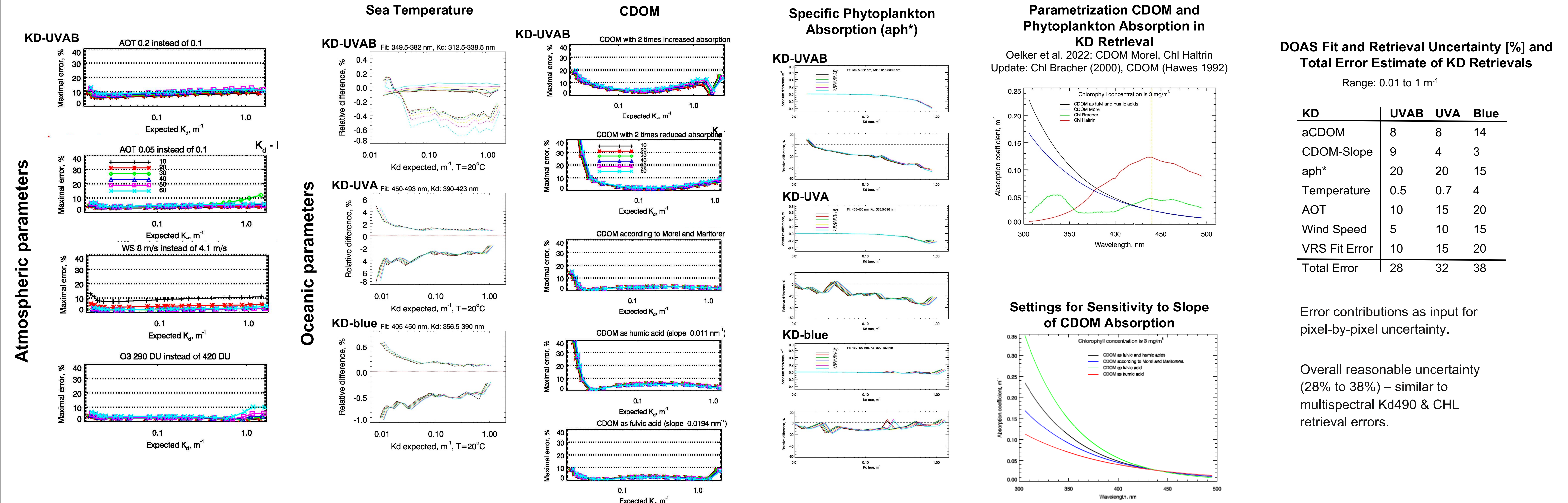
In-situ Data for Validation:
Irradiance data were obtained from BGC-Argo floats; see data processing DOI 10.13155/51541, quality control DOI 10.13155/62466 .

TROPOMI Algorithm

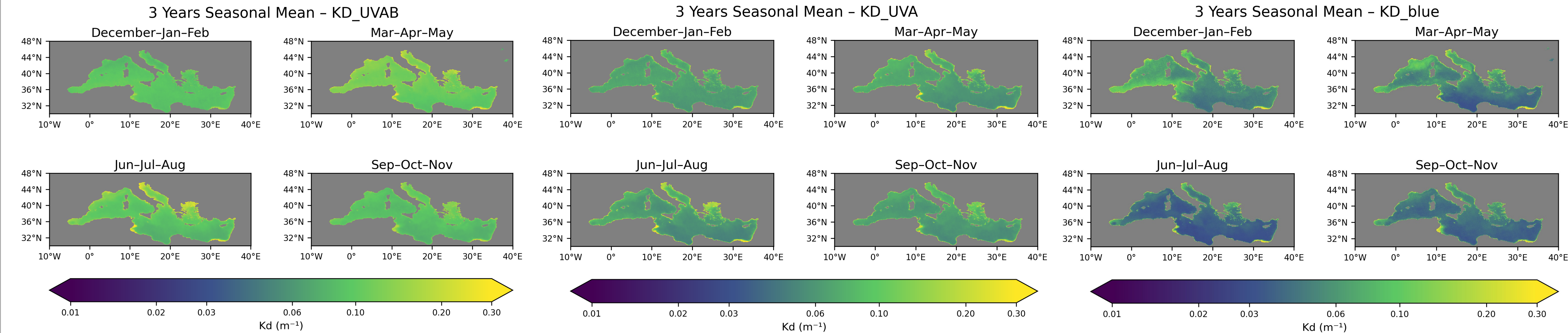


Retrieval Sensitivity with Coupled Ocean-Atmosphere RTM* and Theoretical Error Budget

* SCIATRAN [Rozanov et al. 2014, 2017]



Application to the MedSea: UV and Blue Underwater Radiation, Biogeography and Validation



Conclusions

Enhanced Retrieval Accuracy
By updating phytoplankton and CDOM absorption parametrizations and extending VRS-KD LUTs to encompass all relevant geometry angles, the optimized TROPOMI retrievals derived from RTM-based sensitivity analysis and VRS-Fit factor achieve robust estimates with overall reasonable uncertainty (~ 28%-38%) – similar to multispectral Kd490 & CHL retrieval errors and slightly improved to the former version of the retrieval (Oelker et al. 2022).

Extend Validation to Mediterranean Sea
Comparison with MedSea BGC-Argo multispectral Kd data confirms that TROPOMI UVA and blue Kd products are valid also for this basin. Unfortunately no Kd-UVAB data are available for this basin.

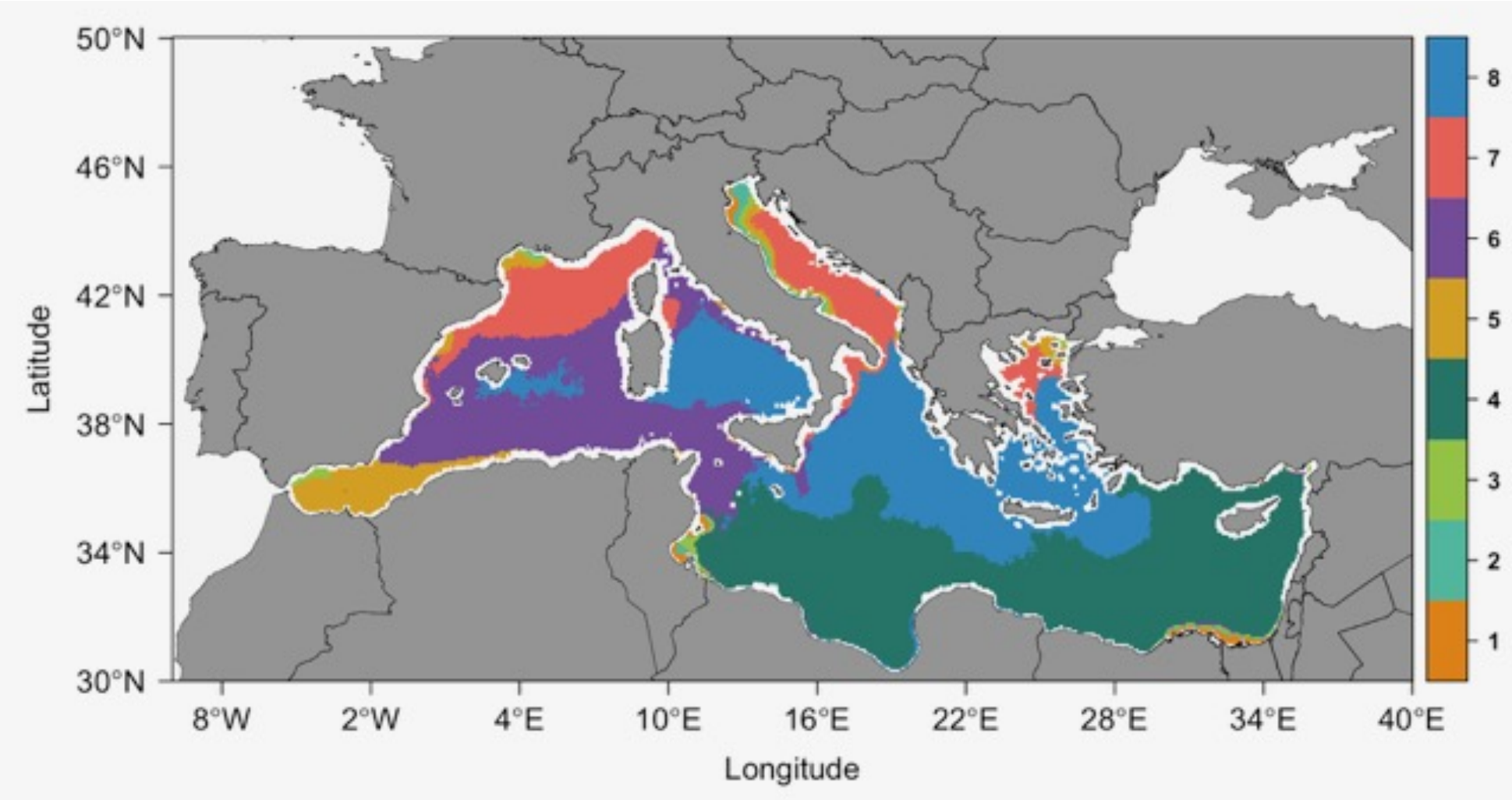
Mediterranean Ecoregionalization
Incorporating Kd products into analysing Mediterranean Sea dynamics enables a finer separation of CDOM sources, facilitating improved ecoregion classification when combined with phytoplankton group chlorophyll-a concentration (PFT), SST and SSS.

Insights to Basin-scale Carbon Pool
This study pioneers the integration of TROPOMI Kd retrievals into assessments of the ocean's carbon reservoir, supporting enhanced modelling of phytoplankton fluxes, particulate export, and dissolved organic carbon dynamics. This enhances the ability to resolve mesoscale ocean dynamics.

References

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- Ocean Colour (ST-AWI-S5P-PAL-WO-012)
- TROPOMI L1b processing: (S&T) S5P PAL (Product Algorithm Laboratory)
- Sentinel-5P mission support: ESA and the European Copernicus Programme
- for PFT satellite products: Copernicus Marine Service.
- for PP, SST & SSS: 4DMED-sea
- In-situ underwater irradiance data from MedSea: BGC-Argo programme
- In-situ data for validation: were collected and made freely available by the International Argo Program and the national programs that contribute to it. (https://argo.ucsd.edu, https://www.ocean-ops.org). The Argo Program is part of the Global Ocean Observing System. https://doi.org/10.17882/42182
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Ecoregion clustering of the Med Sea using self-organising mapping (SOM) (2019-2021)



Kd: <https://data-portal.s5p-pal.com/products/kd.html>
Diatoms, Prokaryotes: [10.48670/moi-00280](https://doi.org/10.48670/moi-00280)
PP, SST and SSS: <http://ricerca.ismar.cnr.it/4DMED/Products.html>

The Mediterranean seascape is complex and underlines regions characterized by different interplay between phytoplankton groups and dissolved organic matter. Cluster 1 is only present in front of Po and Nile rivers. While the most productive regions are described by Cluster 7, Clusters 4, 6, 8 are widespread across the basin within well-known oligotrophic regions.

Validation with Kd380 and Kd412 products from Bio-ARGO programme Ed Sensors from the Mediterranean Sea (2018-2024)
Match up criterion:
• Within 1×1 pixel match (using Haversine distance) and same day
• Value filter: Only matchups with Kd < 0.3 m⁻¹ included
• Residual filter: Applied linear fit with residual threshold ≤ 0.05

