International Ocean Color Symposium 15 Nov 2023, St. Petersburg, FL, USA


# *Hijacking other thematic satellite sensors for ocean color application*

**Astrid Bracher**

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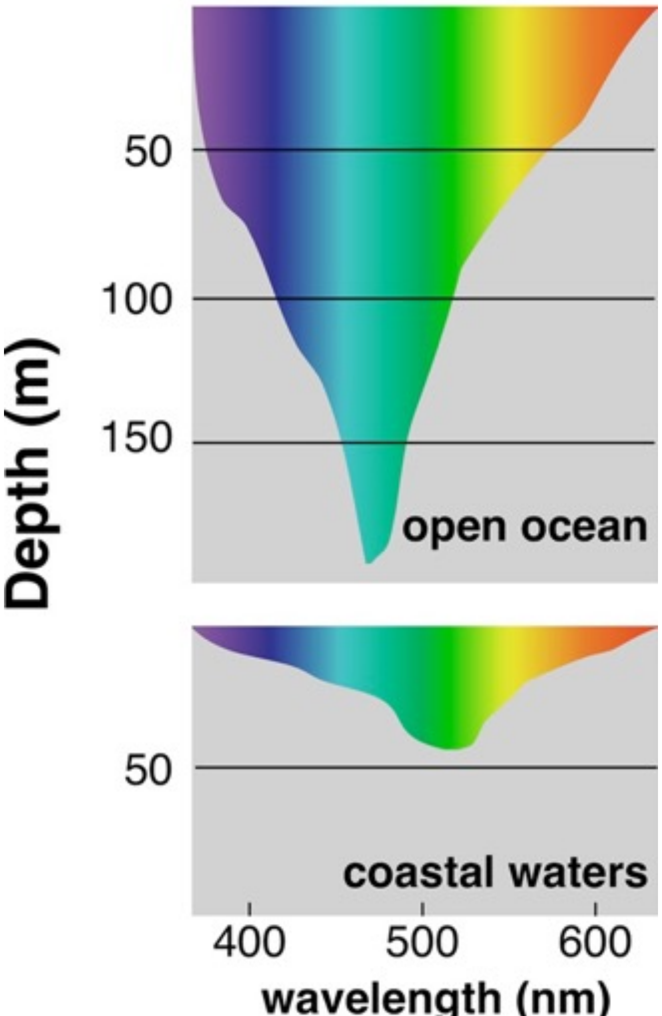
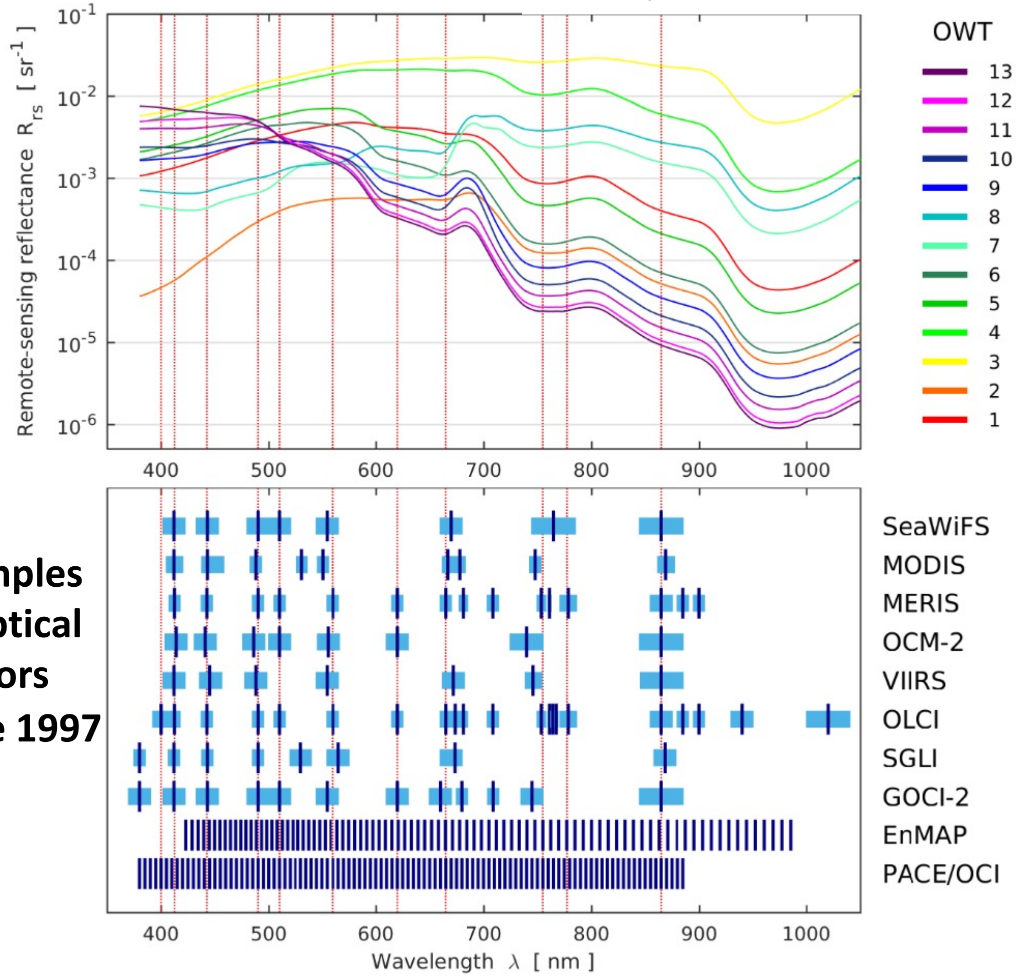
https://www.awi.de/en/science/climate-sciences/physical-oceanography/main-research-focus/ocean-optics

# Common Sensors for Ocean Colour & Products




Pinhassi et al. 2016

Hieronymi et al. 2019




**Examples of optical sensors since 1997**

# Atmospheric Satellite Sensors for Novel Ocean Colour Products

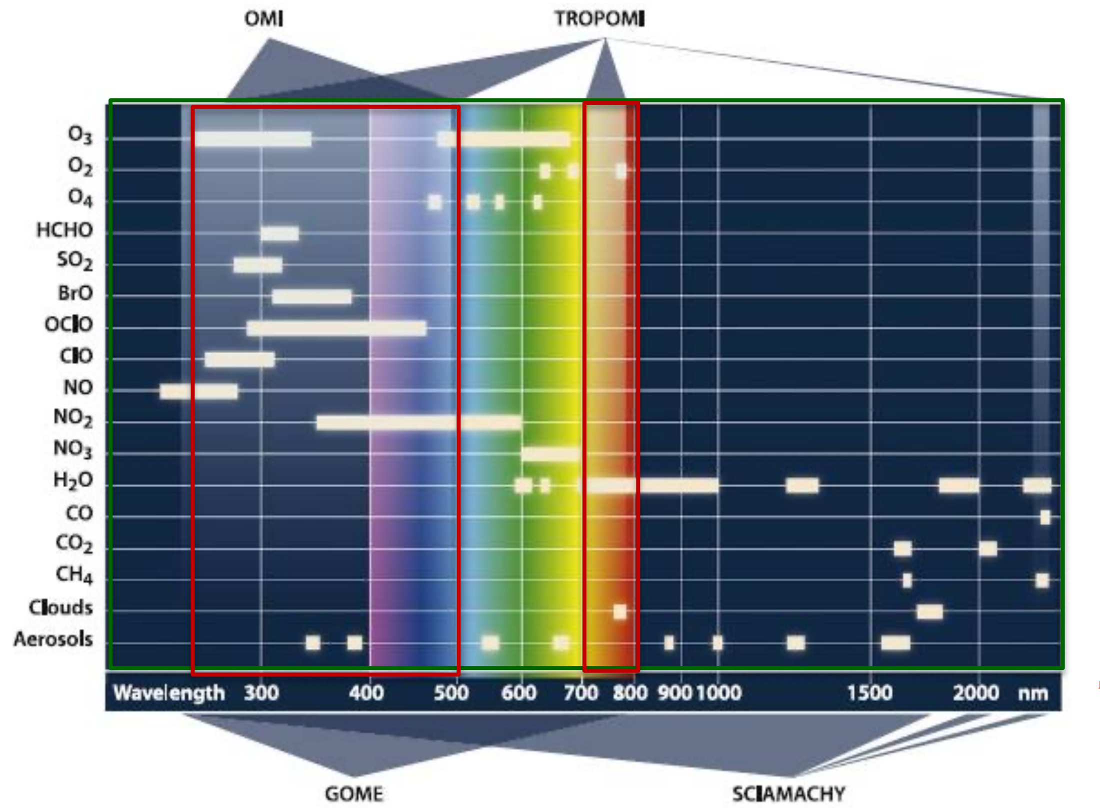
**SCIAMACHY**

(Scanning Imaging Absorption Spectrometer for Atmospheric Chartography)

*ENVISAT*

| | |
|---|---|
| **Operation time** | 2002-2012 |
| **Global coverage** | 6 days |
| **Local overpass time** | 10:00 |
| **Spatial resolution** | 30 km x 60 km |
| **Spectral resolution*** | 0.47 nm |
| **Wavelength window** | 280-2400nm |
| **SNR*** | >2000 |

***for ~450 nm**



# Atmospheric Satellite Sensors for Novel Ocean Colour Products

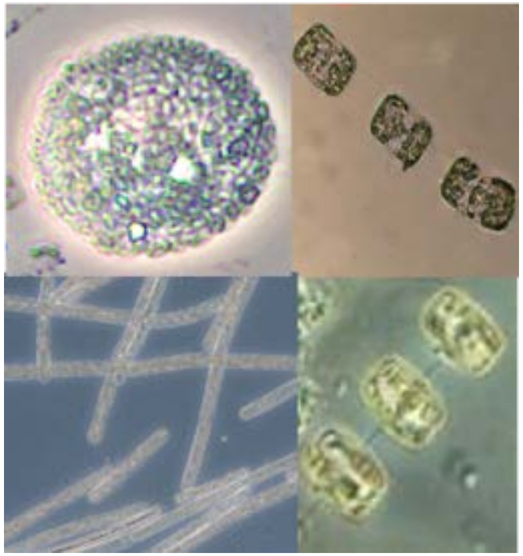
| | SCIAMACHY (Scanning Imaging Absorption Spectrometer for Atmospheric Chartography) *ENVISAT* | OMI (Ozone Monitoring Instrument) *AURA* | GOME-2 (Global Ozone Monitoring Experiment-2) *Metop-A, B, C* | TROPOMI (TROPOspheric Monitoring Instrument) *Sentinel-5P* |
|---|---|---|---|---|
| **Operation time** | 2002-2012 | Since 2004 | Since 2006 | Launch 2017 |
| **Global coverage** | 6 days | daily | ~ 1.5 days | daily |
| **Local overpass time** | 10:00 | 13:30 | 9:30 | 13:30 |
| **Spatial resolution** | 30 km x 60 km | 13 km x 24 km | 40 km x 40/80 km | 3.5 km x 7 km |
| **Spectral resolution*** | 0.47 nm | ~0.63 nm | ~0.51 nm | ~0.54 nm |
| **SNR*** | >2000 | 500 | 1000 | 1000 |
| **Wavelength window** | 280-2400nm | 280-500 nm | 280-800 nm | 270-500 nm & 675-775 nm |

***for ~450 nm**

- ✓ Sources of CDOM, UV-absorbing compounds.
- ✓ Shortwave radiation budget in the ocean
- ✓ Better descriptors of primary production & ocean carbon pool

# Novel Ocean Color Products from Atmospheric Sensors

PFTs: phytoplankton functional types

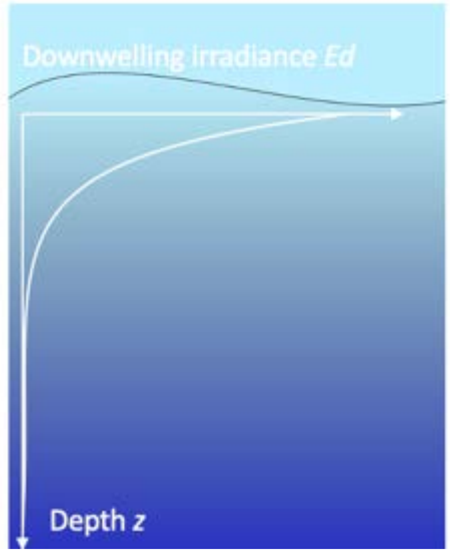



PFT-CHL from spectral inversion

↕

Only empirical multispectral retrievals

Kd(λ): Spectral diffuse attenuation

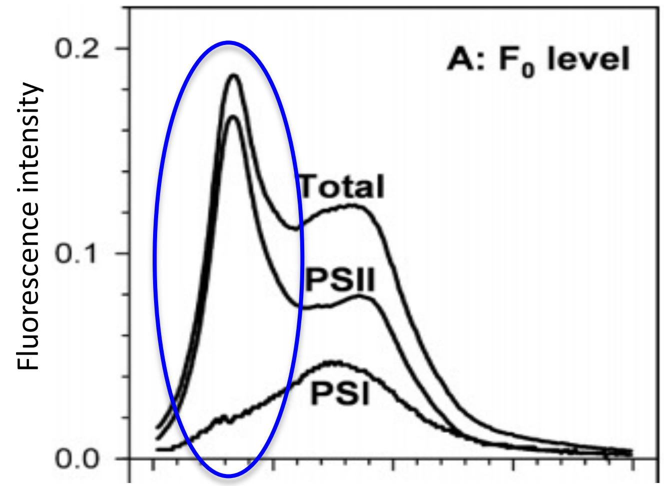



Distribution of underwater radiation in UV and short blue

↕

Only KD490 from multispectral

FLH: Chlorophyll flourescence line height




Spectral signatures of fluorescence in hyperspectral data

↕

FLH multispectral not at peak and not accounting for CHL absorption effect

# Atmospheric Sensors for Ocean Colour: Retrieval

PhytoDOAS (Phytoplankton Differential Optical Absorption Spectroscopy)

Bracher et al. 2009, Sadeghi et al. 2012, Dinter et al. 2015, Losa et al. 2017, Oelker et al. 2019 & 2022

Based on Beer-Lambert law

absorption / scattering cross sections of all constituents

concentration of all constituents

light path

PhytoDOAS equation

Polynomial

Oceanic contribution

Atmospheric contribution

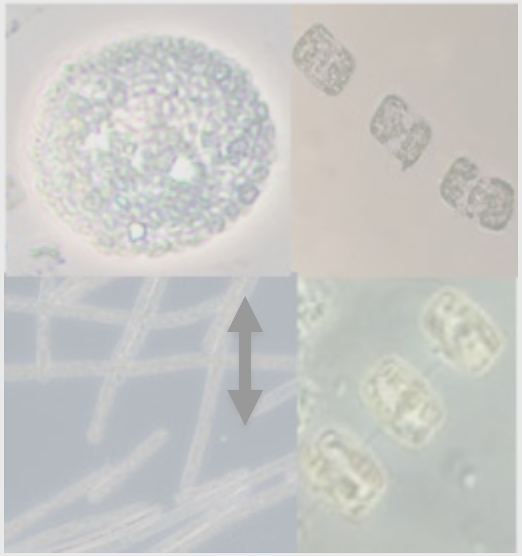
Slant column density (fit factors)

,

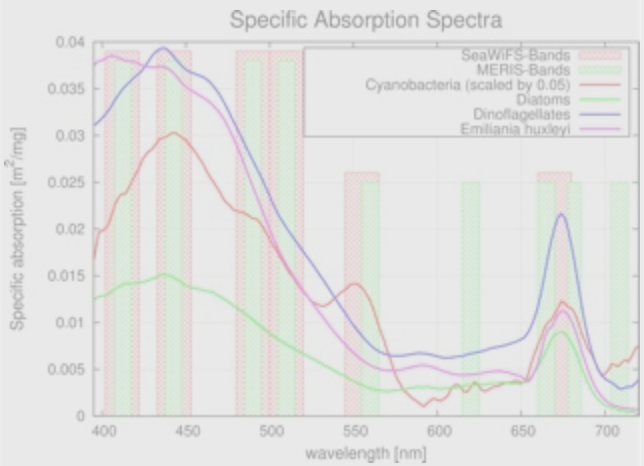
Differential absorption cross sections

# Novel Ocean Color Products from Atmospheric Sensors

PFTs: phytoplankton functional types

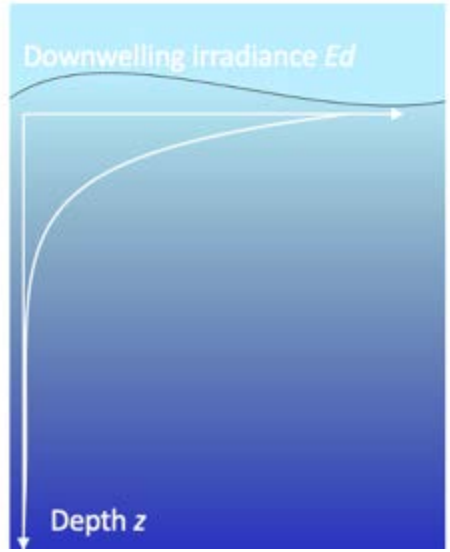


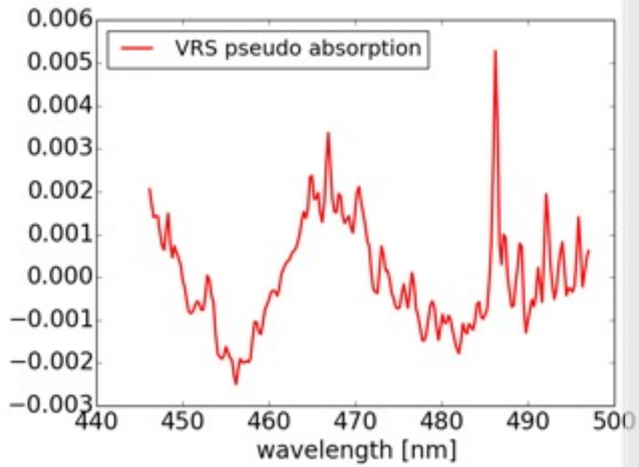
Photos by Sonja Wiegmann - AWI




Bracher et al. 2009, Sadeghi et al. 2012, Losa et al. 2017

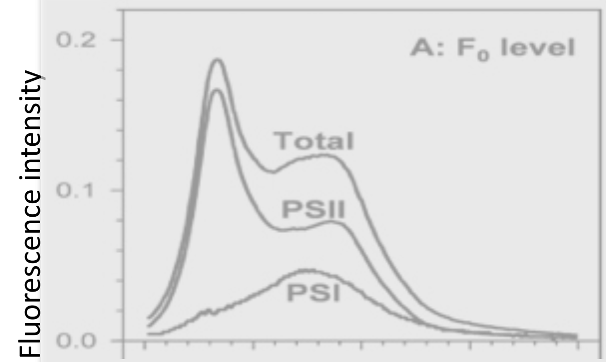
Kd(λ): Spectral diffuse attenuation

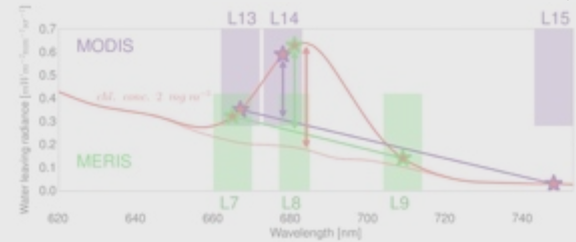


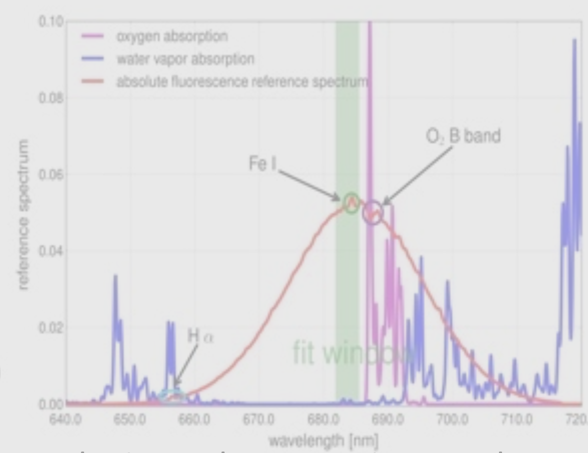




Dinter et al. 2015, Oelker et al. 2019, Oelker et al. 2022

FLH: Chlorophyll flourescence line height



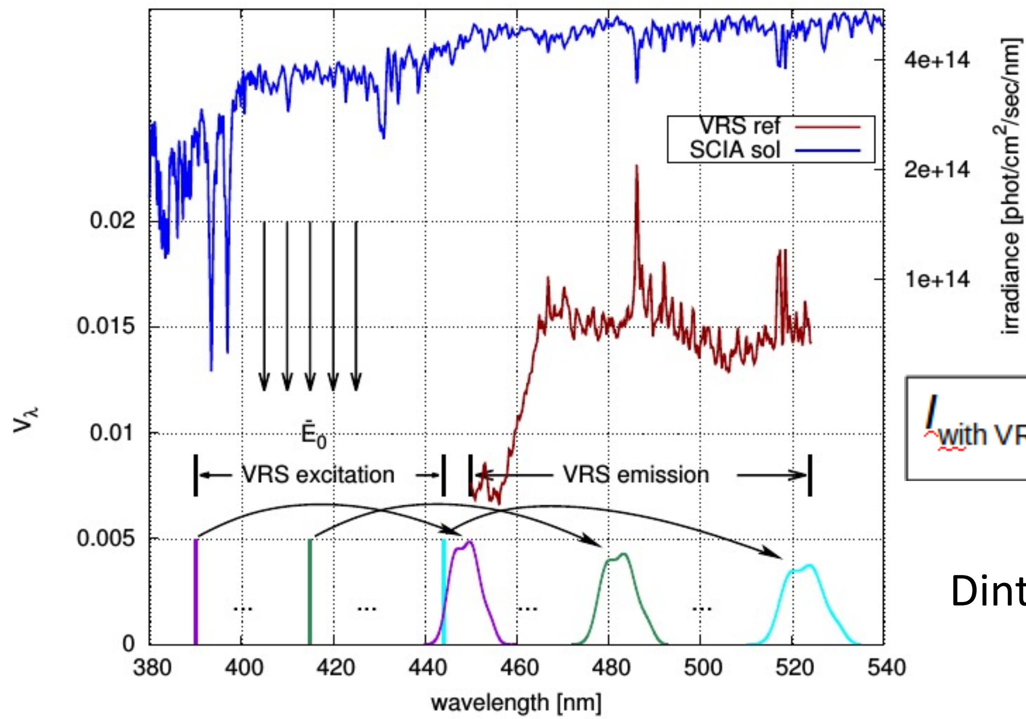




in PhD thesis 2015

Wolanin et al. 2015, Joiner et al. 2016, Köhler et al. 2020

# Ocean light attenuation (Kd) utilizing Vibrational Raman Scattering (VRS) identified in hyperspectral data




Derived VRS fit-factor used to calculate

- diffuse attenuation (Kd)
- PFT Chla (= PFT-fit factor / VRS-fit factor * X)

$I_{\text{with VRS}} / I_{\text{without VRS}}$

Dinter et al. (2015)

- Inelastic scattering process: photons ↔ water molecules
- The more photons, the more inelastic scattering events
- Causes filling in of Fraunhofer lines in top-of-atmosphere (TOA) radiances
- VRS in atmosphere is negligible

➡ Spectral signature of VRS in TOA radiances ↔ **amount of photons in the ocean**

seen in GOME: Vasilkov et al. 2002, Vountas et al 2003;

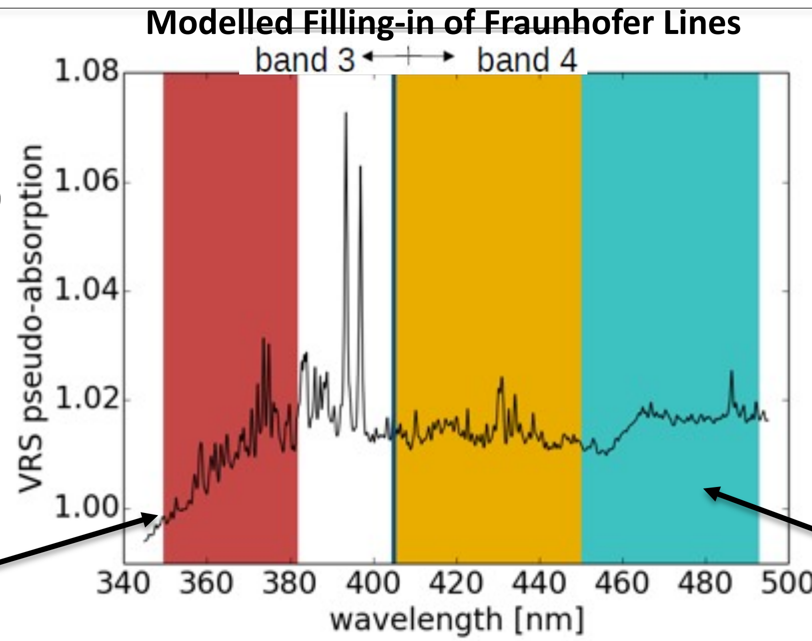
SCIAMACHY: Vountas et al. 2007, Dinter et al. 2015, Oelker et al. 2019

OMI and TROPOMI: Oelker et al. 2019, Oelker et al. 2022

# Diffuse Attenuation (Kd) Products

## (derived from VRS via LUT) from hyperspectral atmospheric sensors

Via **PhytoDOAS** to derive inelastic scattering (VRS, RRS) based on their simulated **pseudo-absorption** using coupled Ocean-Atmoshere **RTM SCIATRAN**.




All three Kd in *Oelker et al. FMARS 2022*

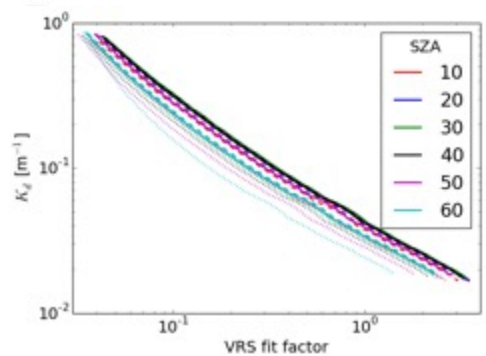
*Vountas et al. OS 2007*

*Dinter et al. OS 2015*
*Oelker et al. OE 2019*

| | UV | short-blue | blue |
|---|---|---|---|
| VRS fit: | 349.5 – 382 nm | 405 – 450 nm | 450 – 493 nm |

LUT ↓

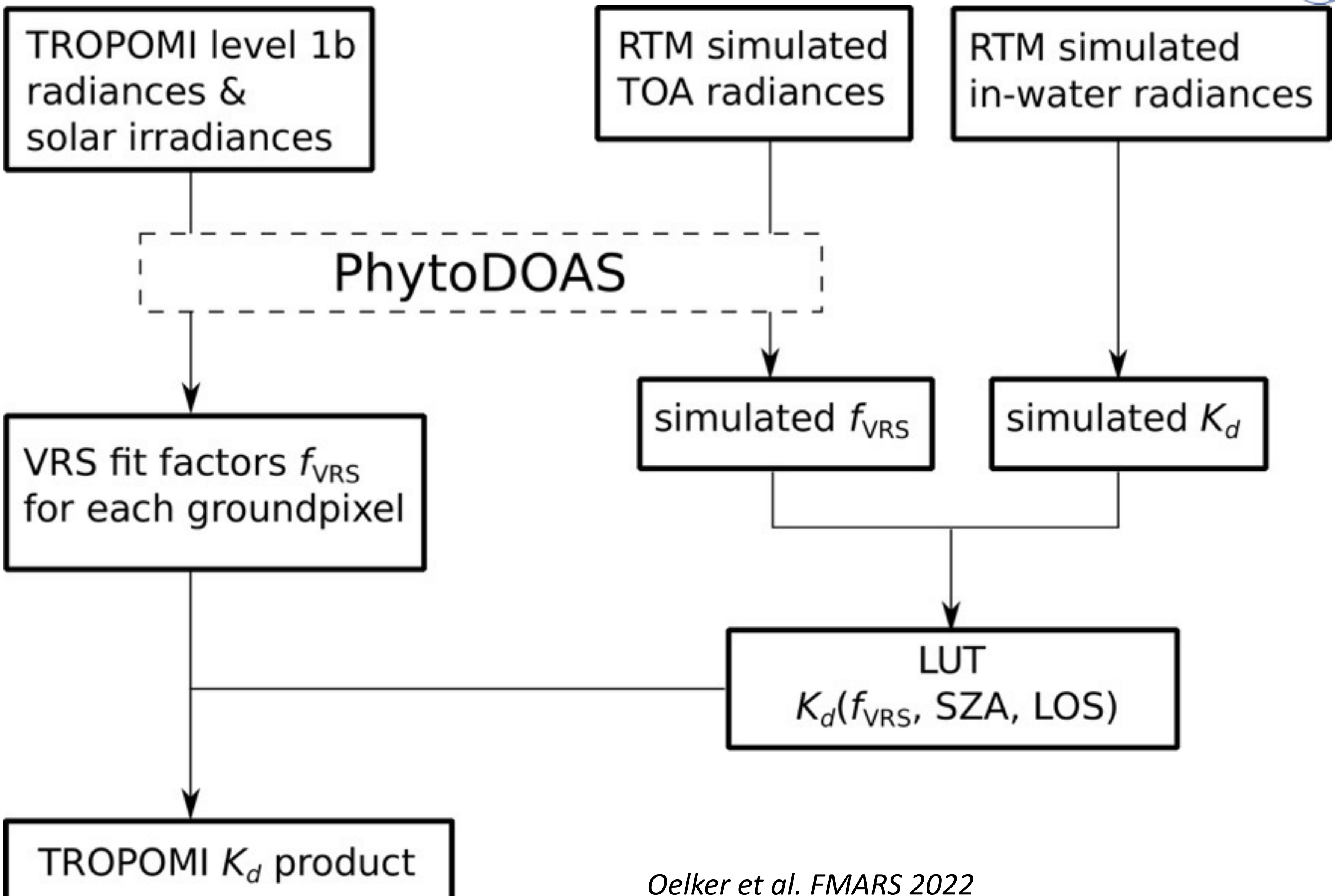
| | UVAB | UVA | short-blue |
|---|---|---|---|
| Kd product: | 312.5 – 338.5 nm | 356.5–390 nm | 390 – 423 nm |




**LUT** (Look-Up Table) from coupled O-A RTM links VRS-Fit factor in spectral retrieval range to Kd accounting for **solar zenith and viewing angle** geometry.

# Diffuse Attenuation (Kd) Products

## (derived from VRS via LUT) from hyperspectral atmospheric sensors




*Oelker et al. FMARS 2022*

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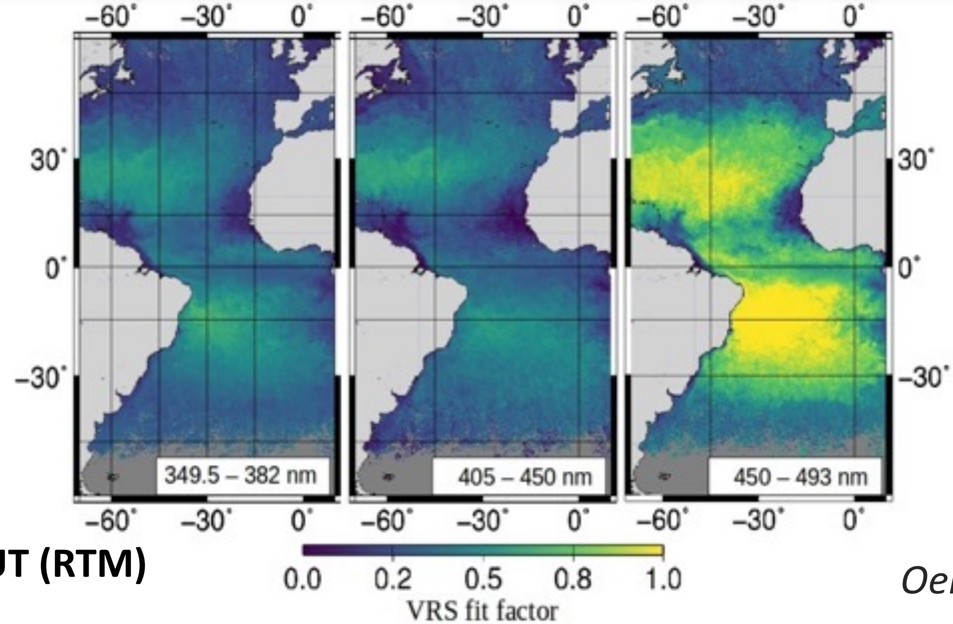
# Diffuse attenuation (Kd) in UVAB, UVA and short-blue from S5P's instrument TROPOMI

**Inelastic Scattering (VRS) in Ocean from TROPOMI**

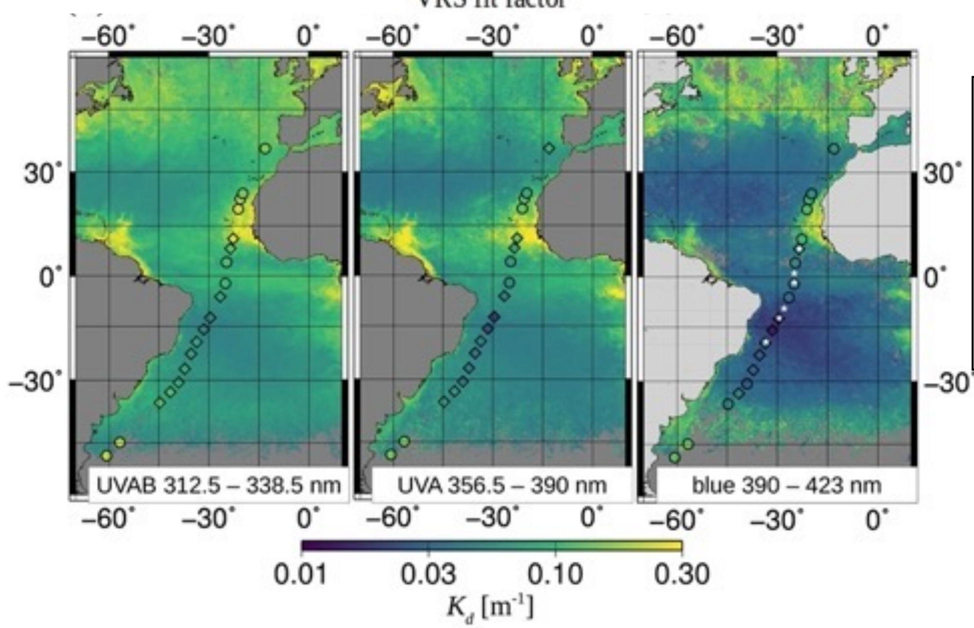



**Mean 10 May-9 June 2018**

**LUT (RTM)**

*Oelker et al. FMARS 2022*

**Diffuse Attenuation in Ocean from TROPOMI and matching in situ data**

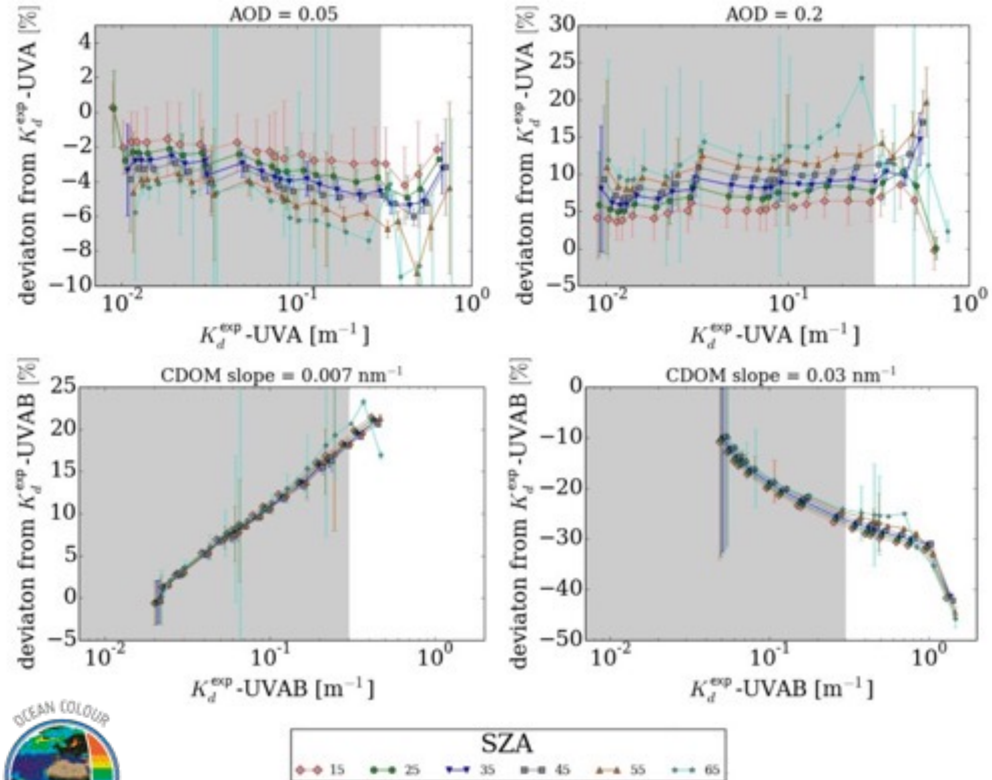



First time Kd retrievals in UV-AB & UV-A from satellite UV data (globally, via inversion).

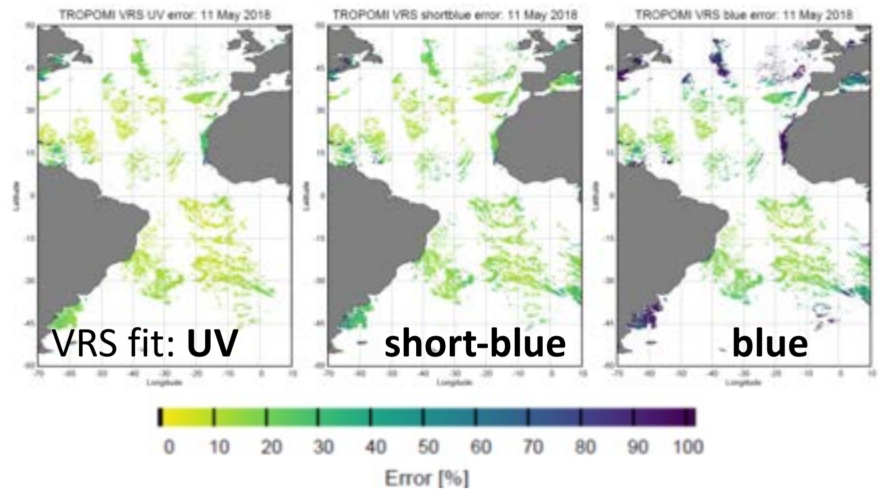
**Data at:**
https://doi.org/10.1594/PANGAEA.940352

# TROPOMI Diffuse Attenuation (Kd) in UVAB, UVA and short blue: uncertainties

## Retrieval sensitivities to parametrizations of Look-Up-Table




## Specific fit factor error [%]




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

Overall uncertainty (max. 35%-45%) ~ multispectral Kd490 & CHL retrieval errors.

**Max. fit and model error [%] of TROPOMI Kd (<0.3 m$^{-1}$)**

| Kd | 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 |

*Oelker et al. FMARS 2022*

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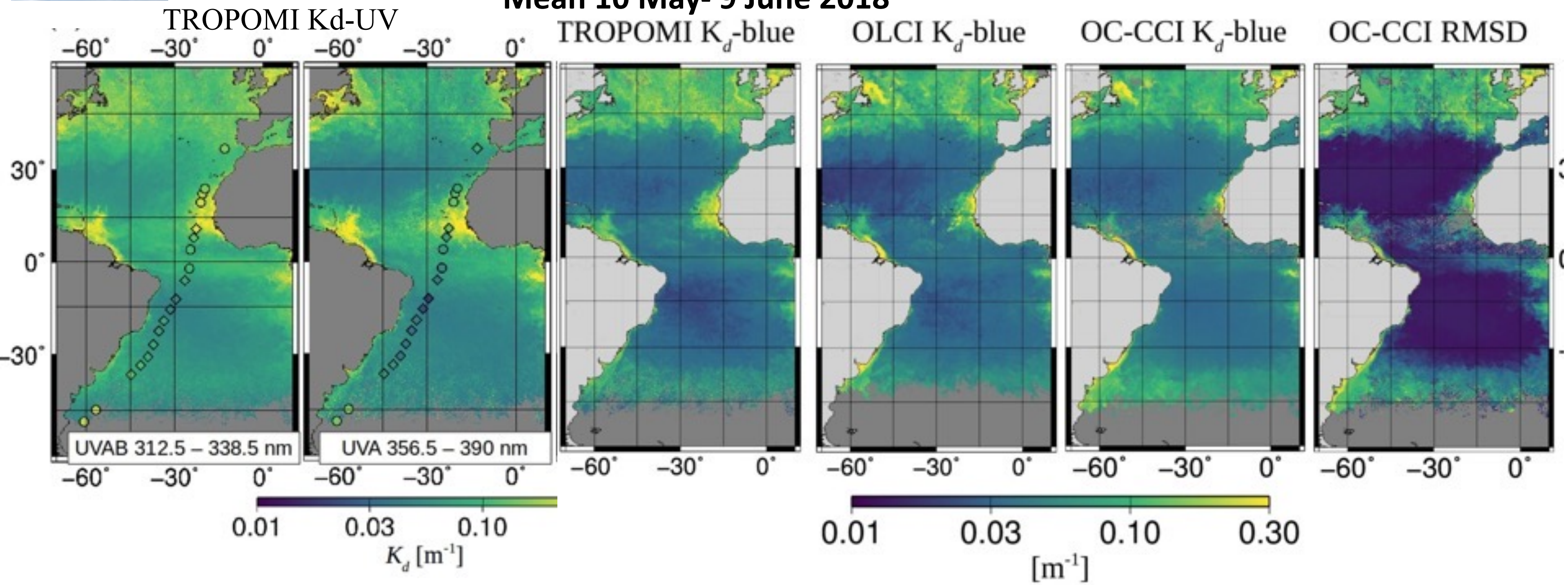
# TROPOMI Kd comparison to in-situ and OLCI & OC-CCI KD490

*Oelker et al. FMARS 2022*

**Mean 10 May- 9 June 2018**




**TROPOMI Kd against in situ [n=42]**

| Criteria | Kd-UVAB | Kd-UVA | Kd-blues |
|---|---|---|---|
| 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 |

**TROPOMI (TRP) vs OLCI (OL) vs OC-CCI (OC)**

| Criteria | TRP vs OC | TRP vs OC | OL vs OC |
|---|---|---|---|
| r | 0.65 | 0.58 | 0.80 |
| Bias (m$^{-1}$) | -0.00 | -0.01 | -0.01 |
| MAE (m$^{-1}$) | 0.03 | 0.03 | 0.02 |
| RMSD (m$^{-1}$) | 0.07 | 0.08 | 0.06 |

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# Short-blue light attenuation derived from different atmospheric hyper-spectral sensors

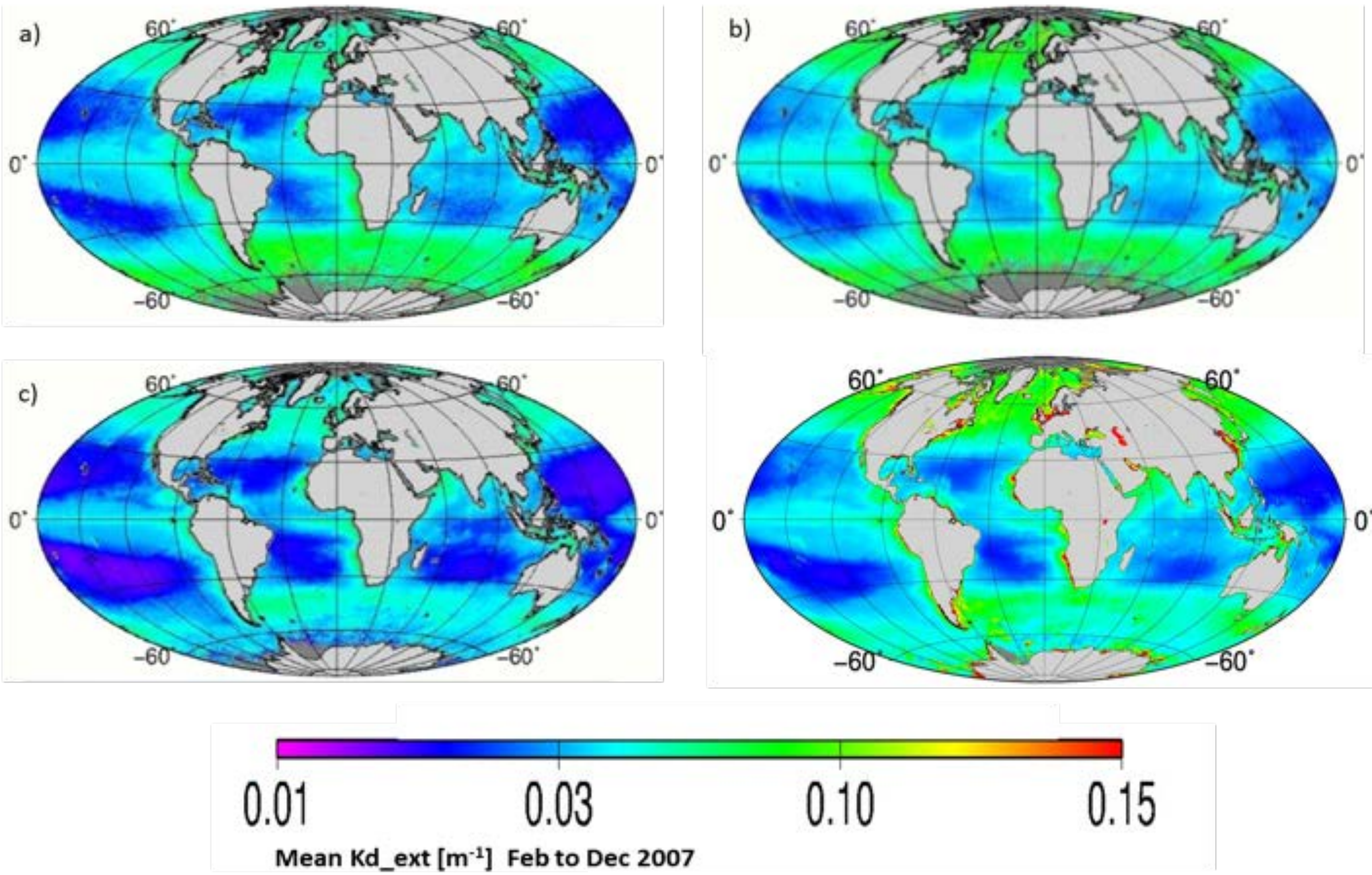
Important for understanding **biogeochemical processes and heat budget** of global ocean

**SCIAMACHY**

**GOME-2**

**OMI**

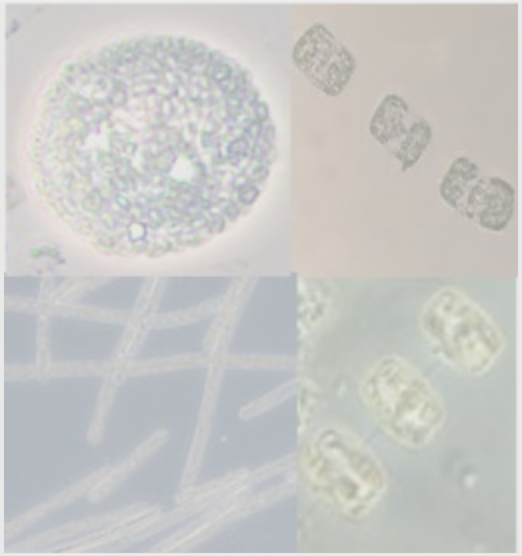
**OC-CCI product** (merged SeaWiFS-MODIS-MERIS)



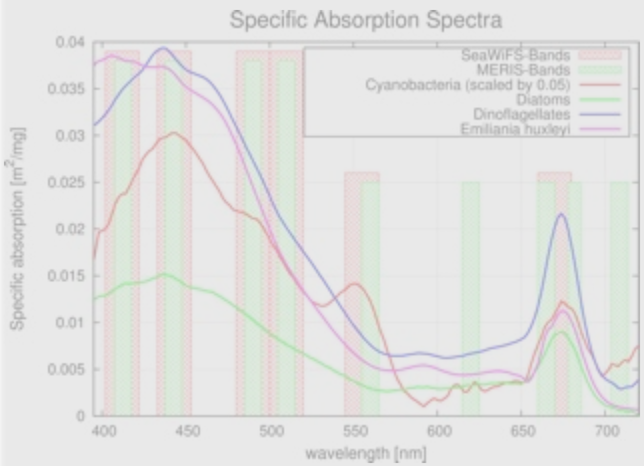

Oelker et al. 2019. Optics Express

# Novel Ocean Color Products from Atmospheric Sensors

## PFTs: phytoplankton functional types

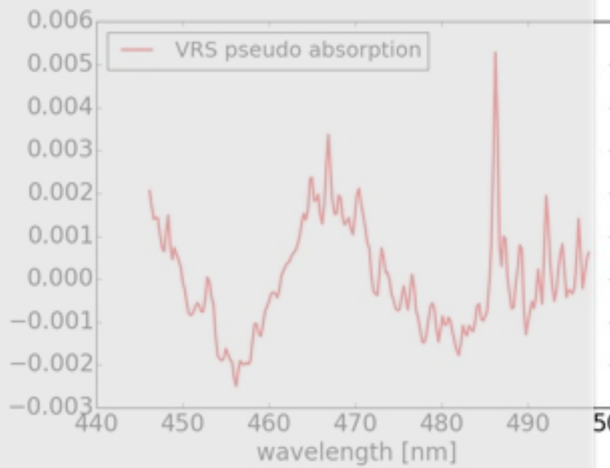


Photos by Sonja Wiegmann - AWI



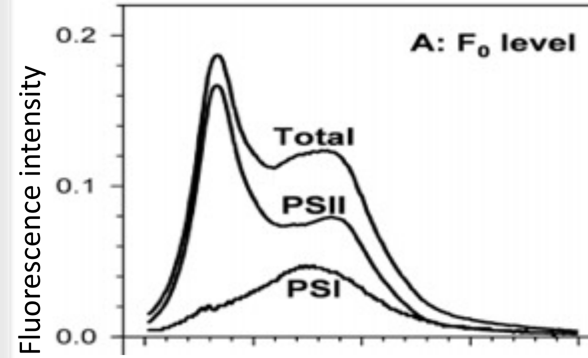

Bracher et al. 2009, Sadeghi et al. 2012, Losa et al. 2017

## Kd(λ): Spectral diffuse attenuation (Kd

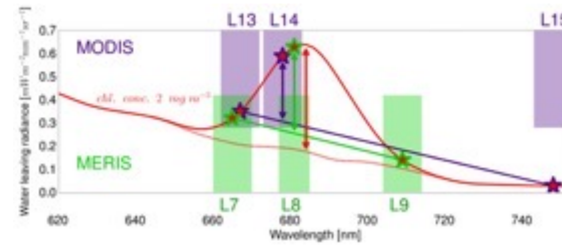



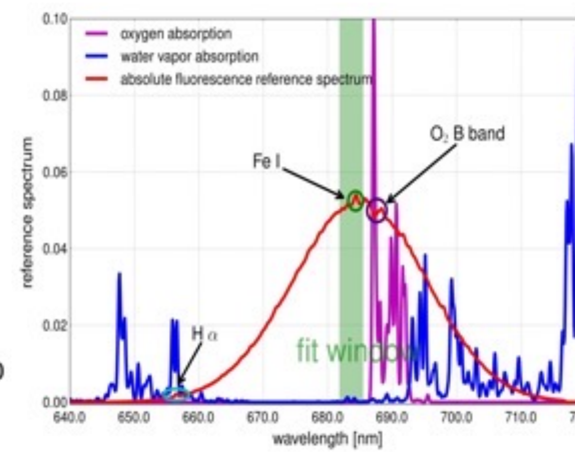

Dinter et al. 2015, Oelker et al. 2019, Oelker et al. 2022

## FLH: Chlorophyll flourescence line height




Wolanin PhD thesis 2015

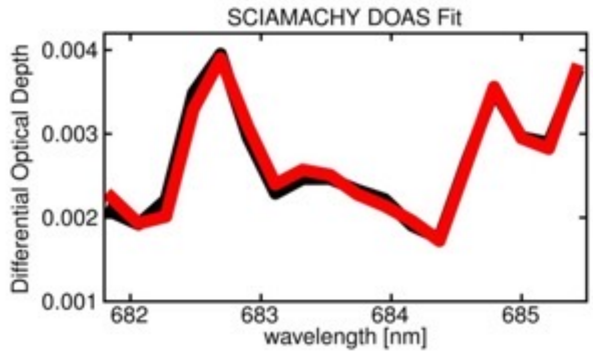


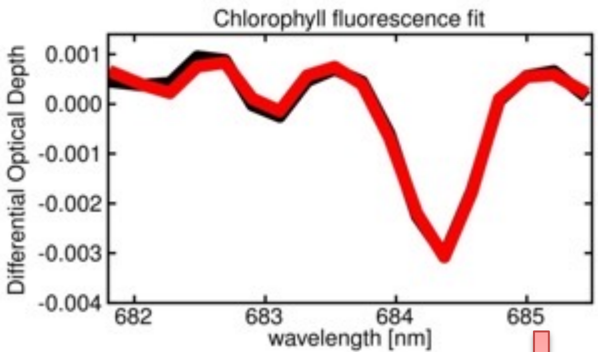

Wolanin et al. 2015, Joiner et al. 2016, Köhler et al. 2020

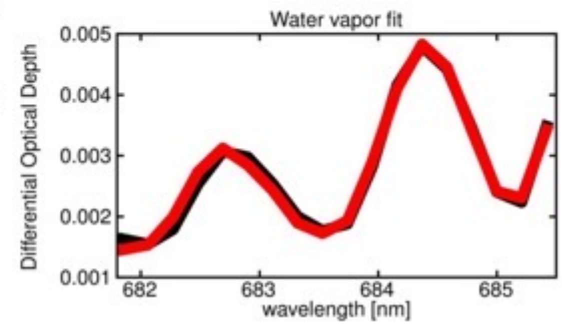
# Chl fluorescence from SCIAMACHY

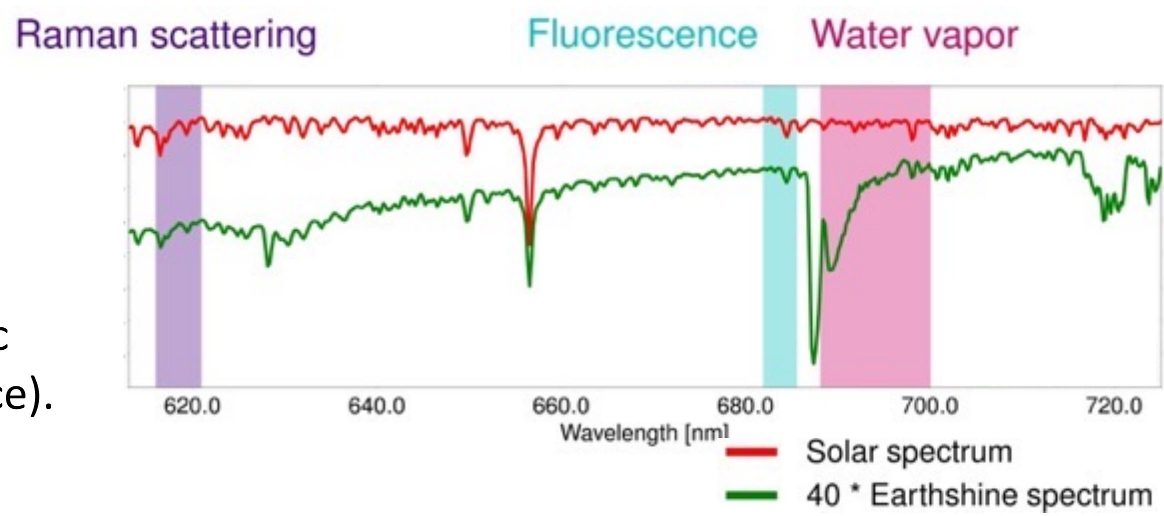
Wolanin et al. Remote Sensing of Environment 2015




Chl fluorescence
DOAS Fit window
681.8 nm – 685.5 nm



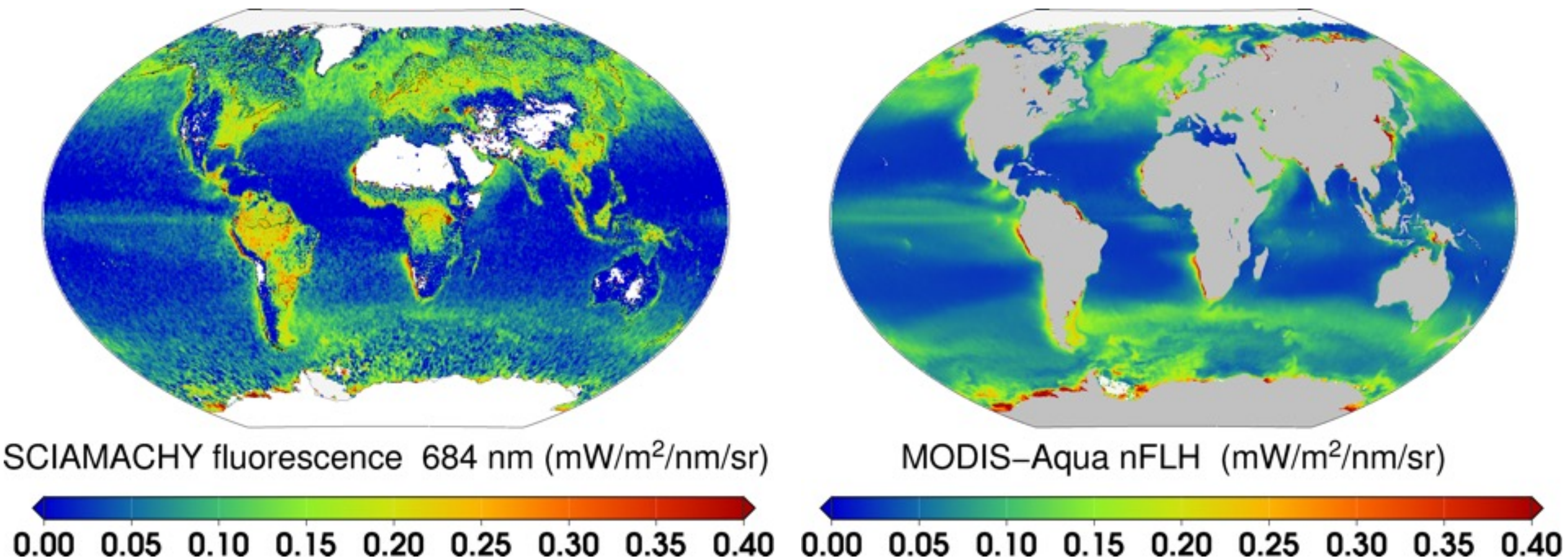




Account for:

- water vapor,
- inelastic scattering (rotational and vibrational Raman scattering),
- background radiance (atmospheric transmittance & surface reflectance).

# Fluorescence 2003-2011 SCIAMACHY & MODIS

Wolanin et al. RSE 2015

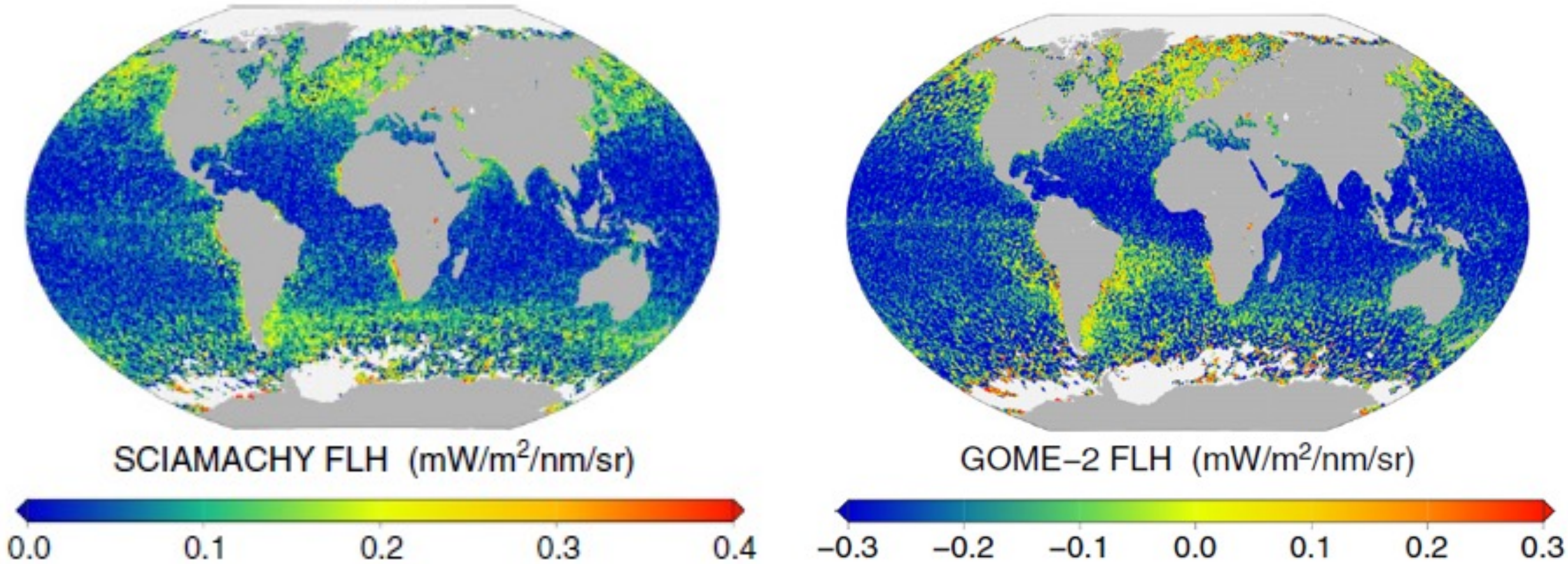



Wolanin et al. 2019: SCIAMACHY 2003-2011 data
https://doi.org/10.1594/PANGAEA.897169.

FCHL: Generally representative of the **photophysiological state of phytoplankton** and linked to primary production.

# Fluorescence 2009 SCIAMACHY & GOME-2

Wolanin et al. RSE 2015




Similar methods to retrieve red fluorescence in ocean waters:

1) **Joiner et al. AMT 2016** with GOME-2 data (data set at avdc.gsfc.nasa.gov)

2) **Köhler et al. GRL 2020** https://doi.org/10.1029/2020GL087541 with TROPOMI data ( ftp://fluo.gps.caltech.edu/data/tropomi/ )

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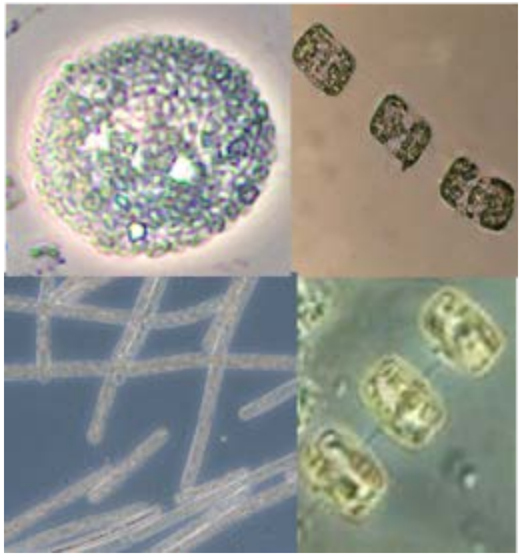
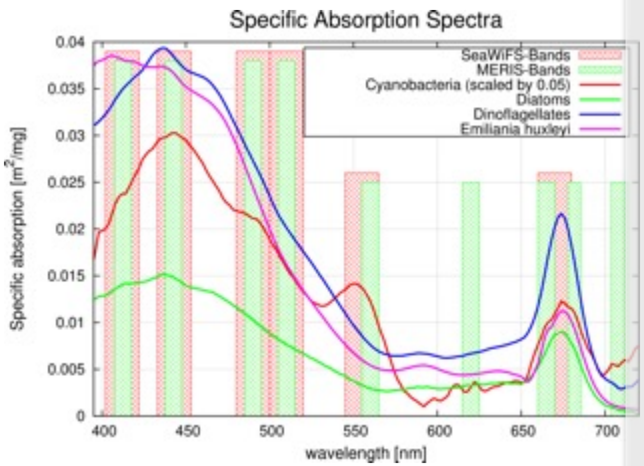
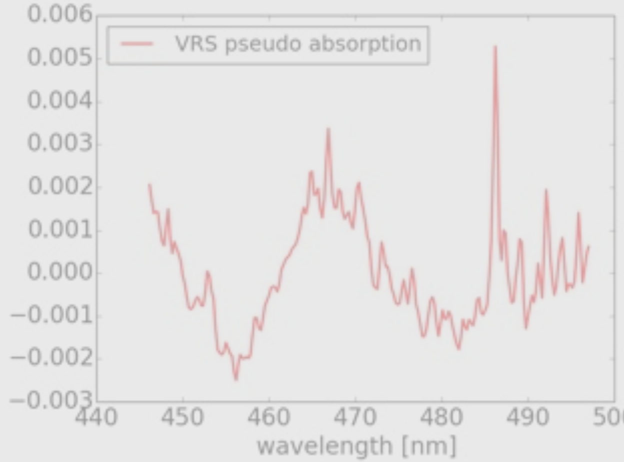


Photos by Sonja Wiegmann - AWI



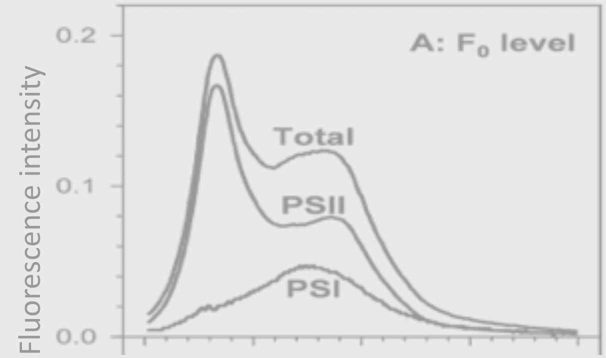

Bracher et al. 2009, Sadeghi et al. 2012, Losa et al. 2017

## Kd(λ): Spectral diffuse attenuation (Kd

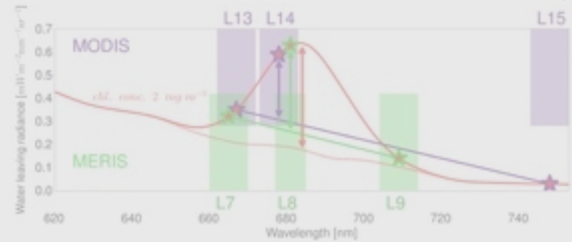



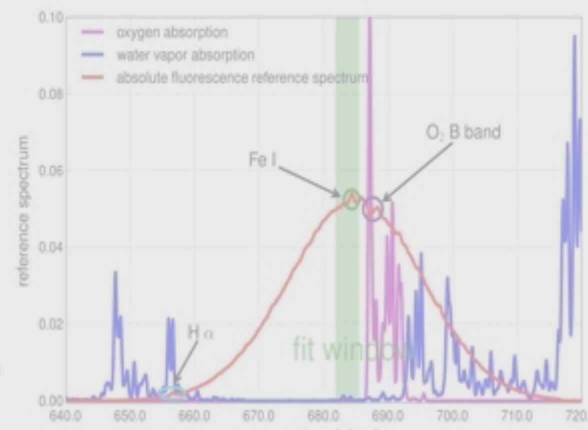

Dinter et al. 2015, Oelker et al. 2019, Oelker et al. 2022

## FLH: Chlorophyll flourescence line height




Wolanin PhD thesis 2015




Wolanin et al. 2015 , Joiner et al. 2016, Köhler et al. 2020

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# PhytoDOAS Retrieval for deriving Chl-a conc. of Phytoplankton Groups (PFT-CHL)

Pl

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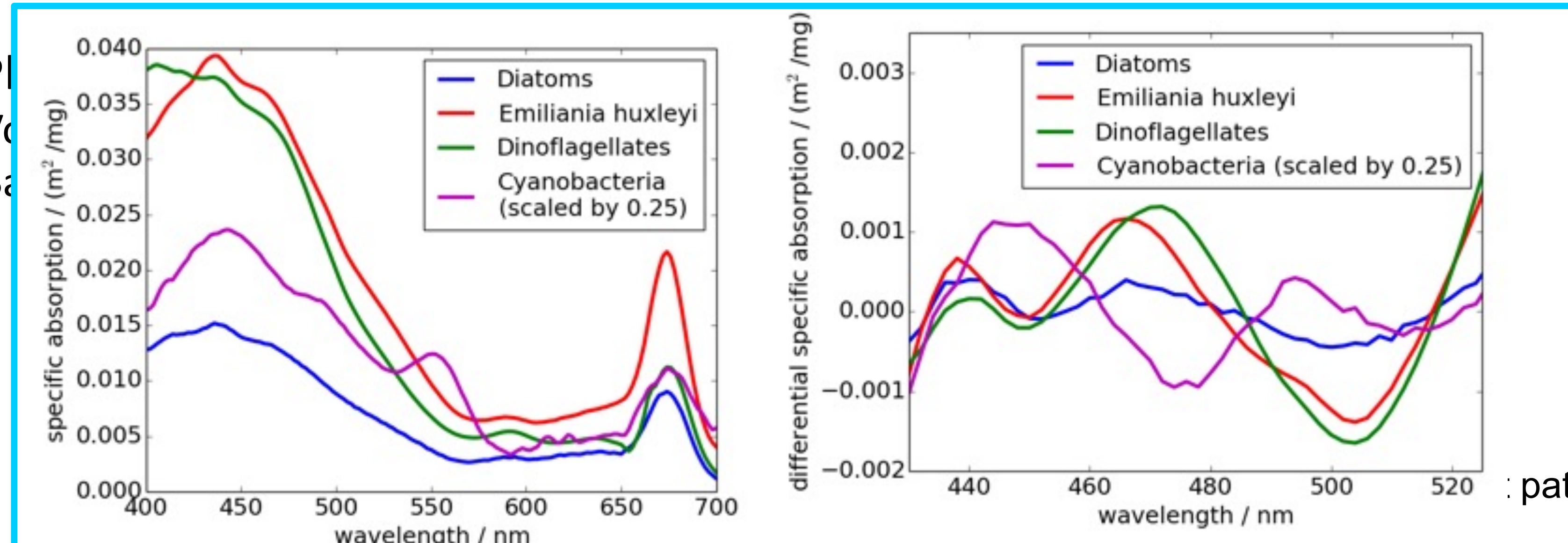
Ba




: path

PhytoDOAS equation

Polynomial

Oceanic contribution

Atmospheric contribution

Slant column density (fit factors)

,

Differential absorption cross sections

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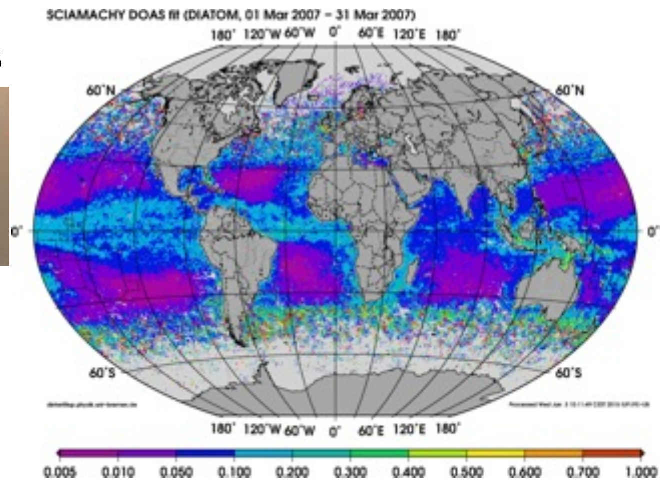
# Phytoplankton Groups Chla conc. (PFT-CHL) from SCIAMACHY

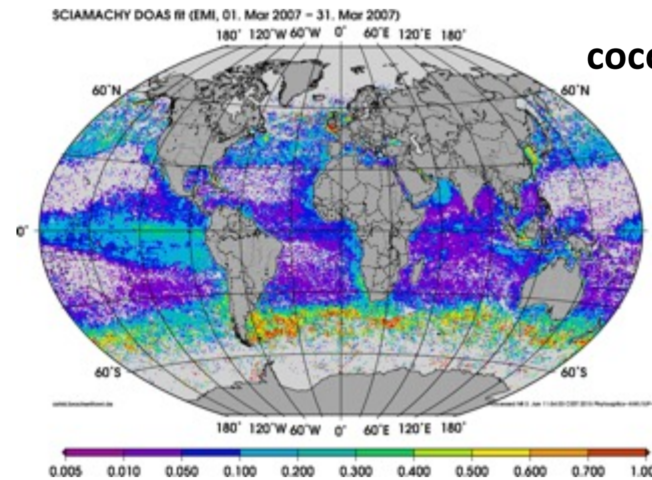
**Different PFTs** play **different roles in the biogeochemical cycles** of the ocean and **food web**.

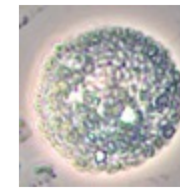
Monthly Concentration (mg m$^{-3}$) – March 2007

**diatoms**

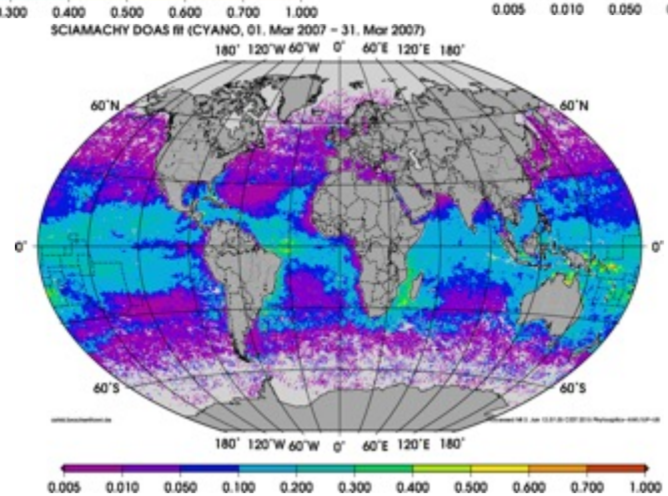



**coccolithophores**



**cyanobacteria**




Drawback:
Spatial resolution ~60 km x 30 km, monthly coverage

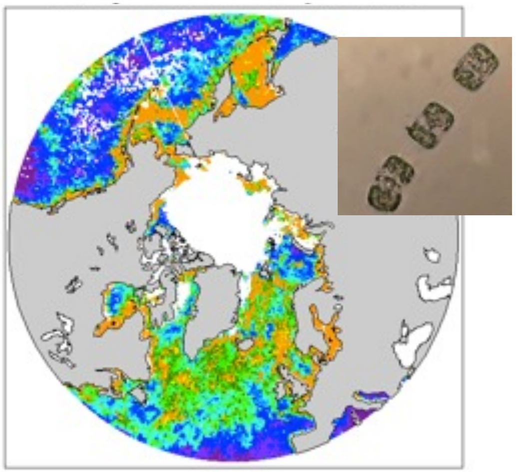
Bracher et al. BG 2009
Sadeghi et al. OS 2012

SCIAMACHY global longterm data set (2002-2012)
https://doi.pangaea.de/10.1594/PANGAEA.870486

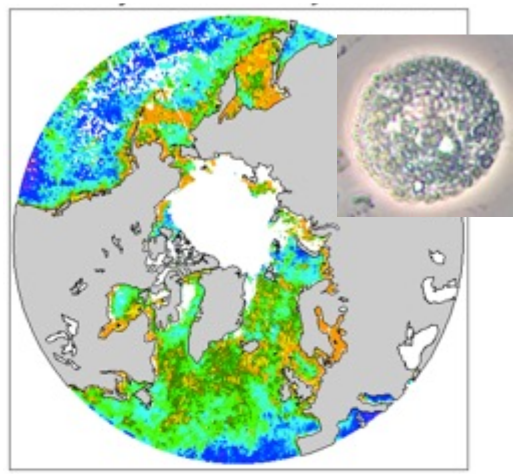
# High temporal & spatial resolution data set on three major phytoplankton groups

Losa S., Soppa M. A., Dinter T., et al. Bracher A. (2017) Synergistic exploitation of hyper- and multispectral precursor Sentinel measurements to determine Phytoplankton Functional Types (SynSenPFT). Frontiers in Marine Science 4: 203, doi: 10.3389/fmars.2017.00203

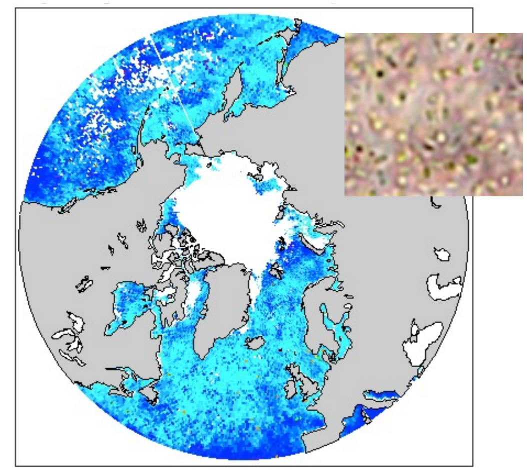
**diatom chl-a**



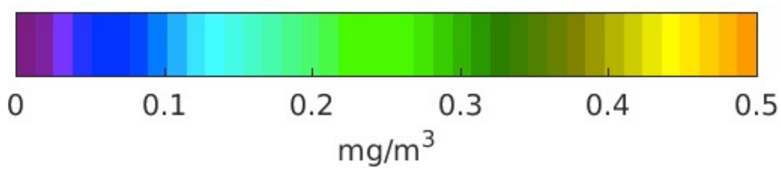
**coccolithophore chl-a**



**cyanobacteria chl-a**



Mean June 2010 Mean June 2010




available global 2002-2012
daily at 4 km pixel resolution

https://doi.org/10.1594/PANGAEA.873210

Obtained by synergistic use of hyper- (SCIAMACHY/ PhytoDOAS) and multi-spectral (OC-CCI (merged MERIS-MODIS-SeaWiFS)/ OC-PFT) data.

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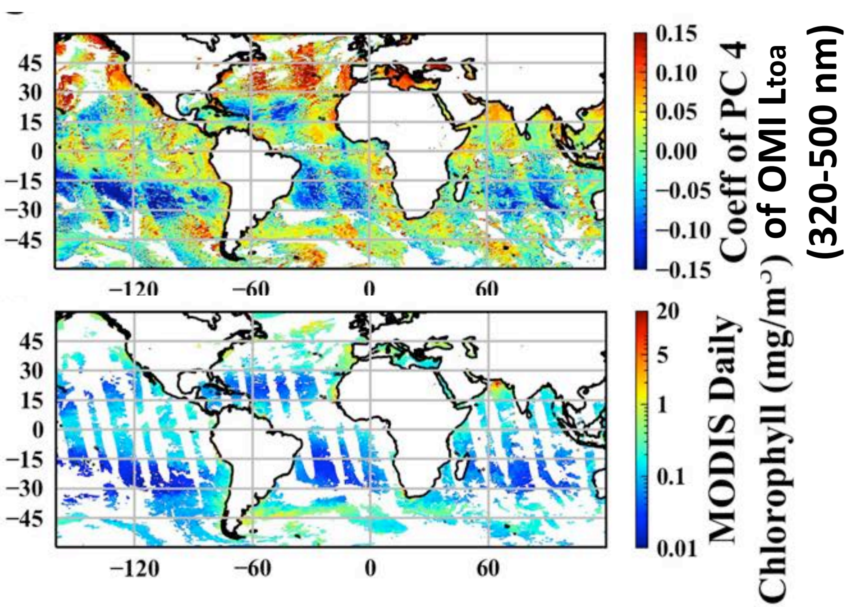
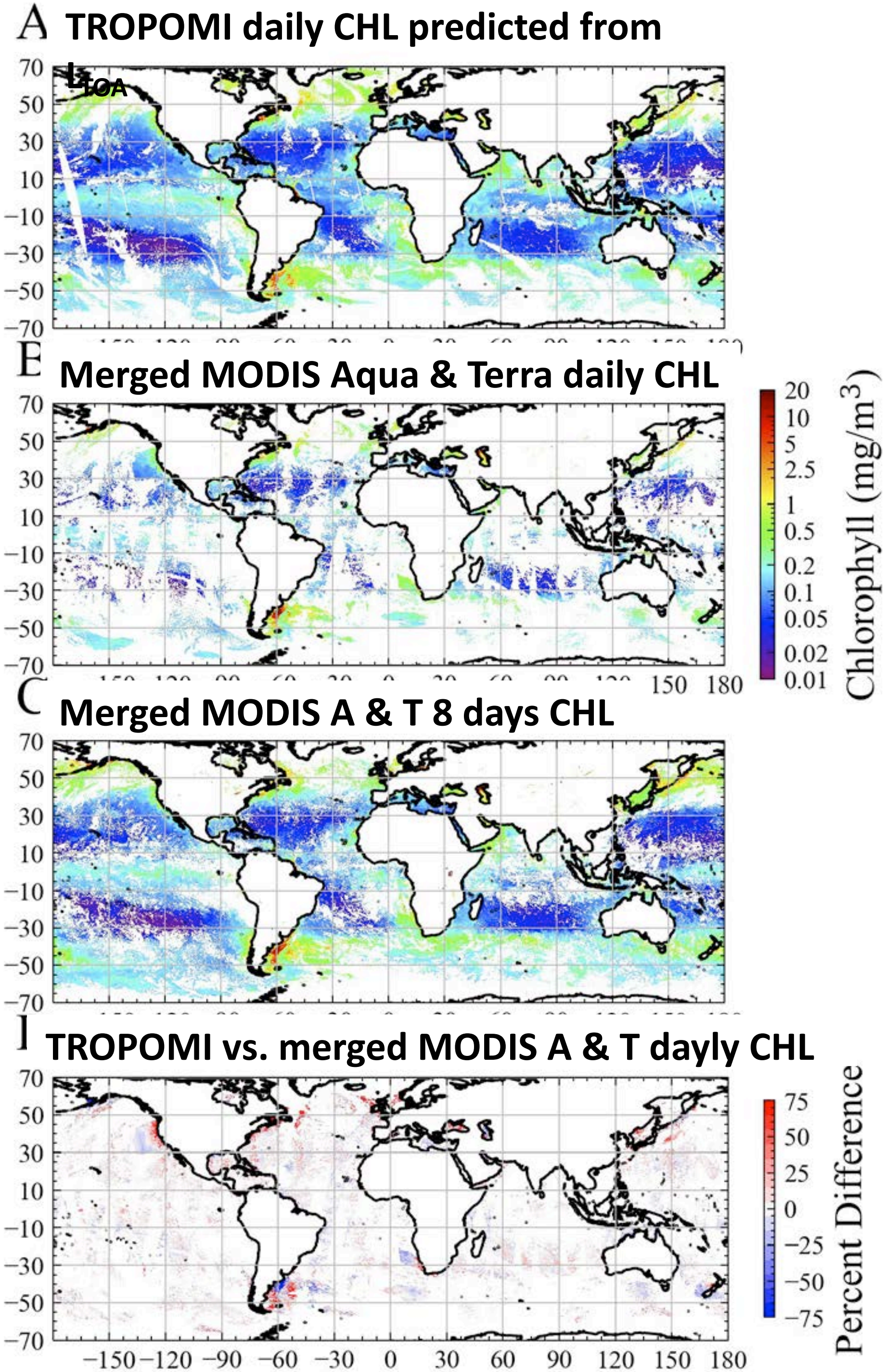
# OMI/TROPOMI TOA hyper-spectral radiances ($L_{TOA}$) for predictions of Chla under thin clouds

Via PCA decomposition, matchups with MODIS Chla (+ blue bands) and ML-models




**Fasnacht et al. (2022)** Using Machine Learning for Timely Estimates of Ocean Color Information From Hyperspectral Satellite Measurements in the Presence of Clouds, Aerosols, and Sunglint. Frontiers in Remote Sensing. https://doi.org/10.3389/frsen.2022.846174

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# Conclusions for atmospheric sensors’ OC products

High spectral resolution of the optical atmospheric sensors SCIAMACHY, GOME-2, OMI and TROPOMI enables analytical retrievals of innovative products: PFT-CHL, FLH, Kd-short blue and recently Kd in UVAB & in UVA.

TROPOMI’s products with much higher spatial resolution and daily global coverage than SCIA, OMI, …

- show less retrieval uncertainty and enable a better assessment of their quality with much more matchups to in-situ;
- enhance their application for understanding global processes (e.g. carbon cycling, primary production, radiative SW budget).

Using ML-based prediction methods with high spectral resolution LTOA data from TROPOMI enables gap filling of operational (multispectral) OC-products leading to quasi global daily coverage.

The similar OC products from the atmospheric sensors serve as alternative evaluation of multispectral (mostly empirical / statistical retrievals) sensor products, and serve as test-beds and demonstration for algorithm development and comparisons to recently launched (PRISMA; EnMAP, …) and soon upcoming hyperspectral (PACE, SBG, CHIME, …) sensors.

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# Outlook for atmospheric sensors' OC products

<u>Next 5 years:</u>

Combining TROPOMI retrievals with OLCI (and similar data) to obtain

- Kd(λ) at ≥9-bands from 325-700 nm (325, 373, 405 , 412, 443, 490, 510, 560, 665)
- Synergy of PFT-products
- Alternative evaluation of common sensors' products (FCHL, PFT)

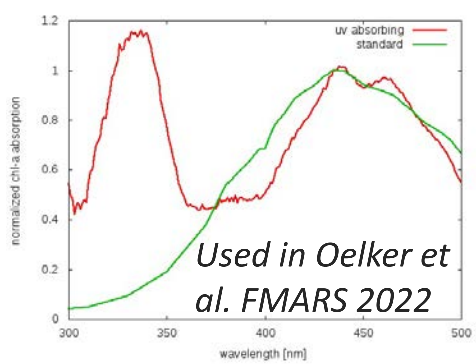
Developing new TROPOMI products: MAAs, CDOM sources, photobleaching

Transfering Know-How: TROPOMI-OC to UVN on S4 (GEO) & S5 – PACE, EnMAP, DESIS, PRISMA

<u>10 years:</u>

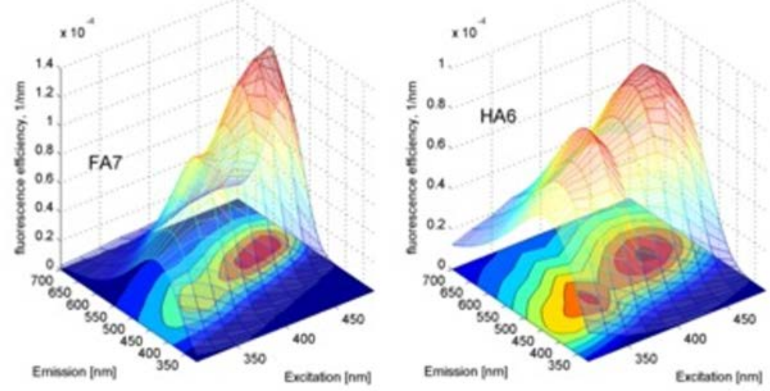
Long term data sets at best spatial and temporal coverage including pixel uncertainty from synergy of historic, current and upcoming sensors for Kd(λ), PFTs, photobleaching, type of CDOM,… for many applications (climate/ecosystem/bgc ocean modelling, etc.)

**Phytoplankton absorption 300-500 nm**




*Used in Oelker et al. FMARS 2022*

**Exciation-Emission-Spectra for Fulvic (FA7) and Humic (HA6) Acids**




*Hawes (1992) master thesis at USF*

# Thank you!

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- **Our Collaborators** Ilka Peeken (AWI), Rüdiger Röttgers (Hereon), Robert J. Brewin (then PML), Annick Bricaud (LOV), Bernard Gentili (LOV)
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