IDEAS-QA4EO

ADVANCED RETRIEVAL METHODS AND UNCERTAINTIES ESTIMATION FOR OCEAN COLOR PRODUCTS

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CONTEXT OF WP 2120 & 2155

- **R&D activity focusing on Ocean Color Radiometry** (OCR, i.e. water-leaving radiance from blue to NIR)
  - Primary satellite measurement used by oceanographers & modelers to derive bio-geophysical products
  - TOA signal corrected for atmospheric effects (absorption & scattering) and other potential contaminations (sky-dome, residual sun glint, white-caps, reflectance, adjacency effects in vicinity of land, …)

- **Limitations of standard algorithms for MERIS & OLCI, developed for ideal conditions:**
  - Spectral range: Detection of aerosols in 2 NIR spectral bands + extrapolation to VIS bands
  - Spatial range: Processing performed sequentially on a pixel-basis, without accounting for information from surrounding pixels and potential spatial constraints
  - Purely optical: No synergy with other sensor missions (due to operational constraints) or external data (except for meteorology)

OC inverse problem very challenging in actual conditions (complex waters, Sun-glint, absorbing aerosols…) ⇒ Need to investigate more innovative approaches in term of signal processing

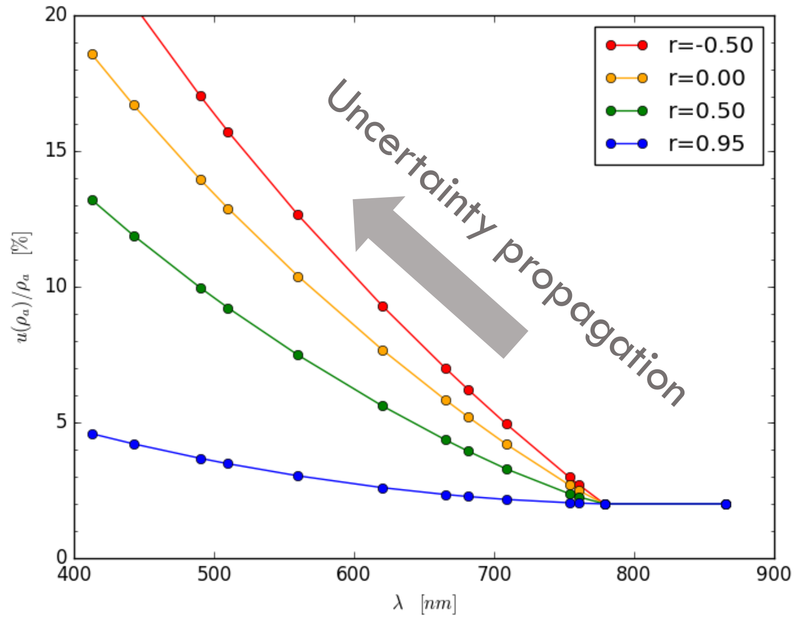
OVERALL ACTIVITY OF WORK-PACKAGE 2120 DURING PHASE 1

- **Multi-spectral inversion from VIS to NIR**
  - New non-linear aerosol spectral shape and inversion, to break ambiguity between aerosol and marine signal
  - Development of a prototype OLCI processor. Further investigations with EUMETSAT "SACSO" project. ATBD v1 released in 2021
- **Multi-pixel inversion**
  - Extension of the Bright Pixel Atmospheric Correction code in multi-pixel. ATBD (v2) under completion for end of April 2022
- **Constraints with external information**
  - Generation of a synthetic DB of atmospheric scattering functions (ASF) with AERONET IOPs and CALIOP vertical profiles
- **Cal/Val platform (with support from Telespazio):** use-case demonstration for Ocean Colour
- **Paper submitted (+ poster at Living Planet 2022):** "*Uncertainty of atmospheric scattering functions relevant for satellite ocean colour radiometry in European Seas*"

MULTI-SPECTRAL INVERSION FROM VIS TO NIR

UNCERTAINTY PROPAGATION: STD VS NON-STD ATM. CORR.

- **Standard Atmospheric Correction (MERIS/OLCI baseline AC)**
  - **Two bands in the NIR** only to detect aerosol, then extrapolate to the VIS
  - **Strong uncertainty propagation** to the VIS: radiometric noise, possibly overcorrection (negative marine signal)…
  - Method **not robust for actual remote-sensing conditions**



- **Alternative: Use a spectral model over the full spectrum for aerosol detection; no extrapolation**
  - Introduce a **coupled ocean-atmosphere** problem, due to non-negligible marine signal in the VIS:

$$\rho_{Rc}^{mod}(\lambda_i, \boldsymbol{x}_a, \boldsymbol{x}_w) = \rho_a^{mod}(\lambda_i, \boldsymbol{x}_a) + t_{Ra}^{mod}(\lambda_i, \boldsymbol{x}_a)\rho_w^{mod}(\lambda_i, \boldsymbol{x}_w)$$ with atmospheric and marine unknowns

  - Non-linear least-square (NLLSQ) minimisation **well adapted to uncertainty formalism**: input/output uncertainties:

$$\chi^2(\boldsymbol{x}_a, \boldsymbol{x}_w) = \frac{1}{n_{obs} - n_x} \sum_{i=1}^{n} \left(\frac{\rho_{Rc}^{mod}(\lambda_i, \boldsymbol{x}_a, \boldsymbol{x}_w) - \rho_{Rc}^{obs}(\lambda_i)}{\sigma(\lambda_i)} \right)^2$$

WHICH SPECTRAL MODEL FOR THE AEROSOL?

- **Standard approach with tabulated models** (Gordon and Wang, 1994): complex modelling to get the aerosol mixing from NIR to VIS, impossibility to detect absorbing aerosols in the NIR, sensitivity to aerosol layer height…
- **POLYMER** (Steinmetz et al., 2011): $\rho_a^{mod}(\lambda) = c_O * T(\lambda) + c_1 * \left(\frac{\lambda}{\lambda_0}\right)^{-1} + c_2 * \left(\frac{\lambda}{\lambda_0}\right)^{-4}$ → linear
- **Simple power law** (BPAC in the NIR): $\rho_a^{mod}(\lambda) = \rho_{a0}\left(\frac{\lambda}{\lambda_0}\right)^{-\alpha}$ → no multiple scattering effect
- **Improved power law** (QA4EO, 2014, tech note ESA/14/QWG/TN1): $\rho_a^{mod}(\lambda) = \rho_{a0}\frac{(1-\tau_R(\lambda))}{(1-\tau_{R0})}\left(\frac{\lambda}{\lambda_0}\right)^{-\alpha}$
- **Multiple Scattering Approximation** (**MSA**) – proposed to QA4EO & to EUMETSAT in recent "SACSO" study:

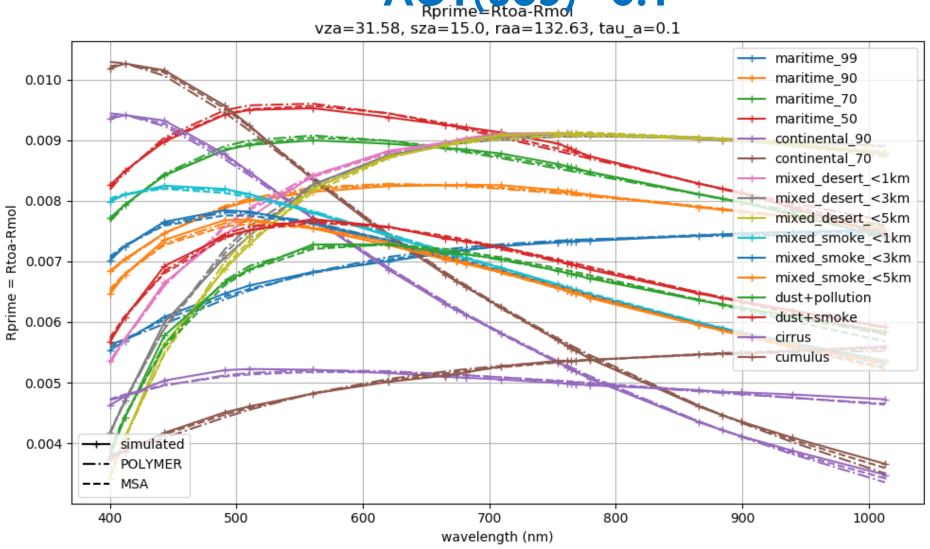
$$\rho_a^{mod} = \rho_{a0} * \left(\frac{\lambda}{\lambda_0}\right)^{-\alpha}\left(\frac{1+k*\left(\frac{\lambda}{\lambda_0}\right)^{-\alpha}}{1+k}\right)$$

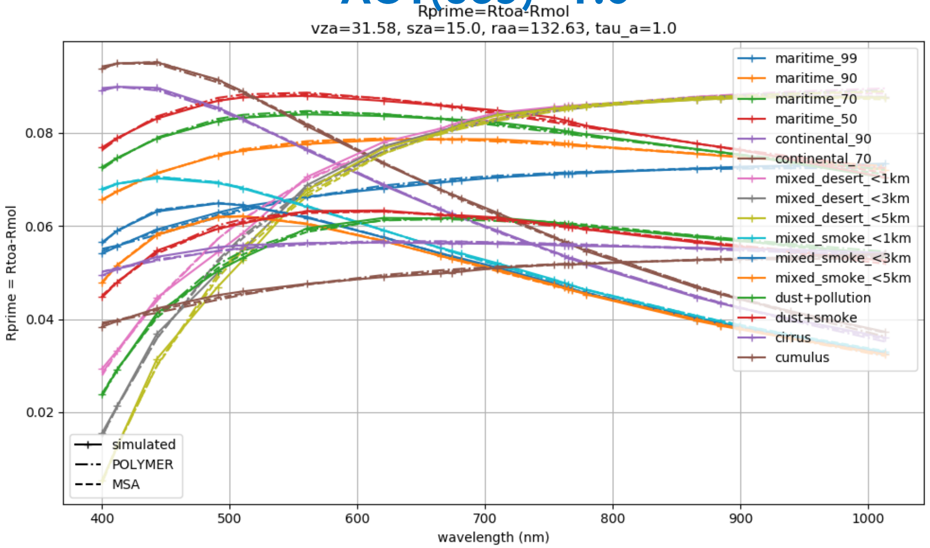
→ non-linear, robust over the whole VIS-NIR spectrum

PERFORMANCE OF MSA

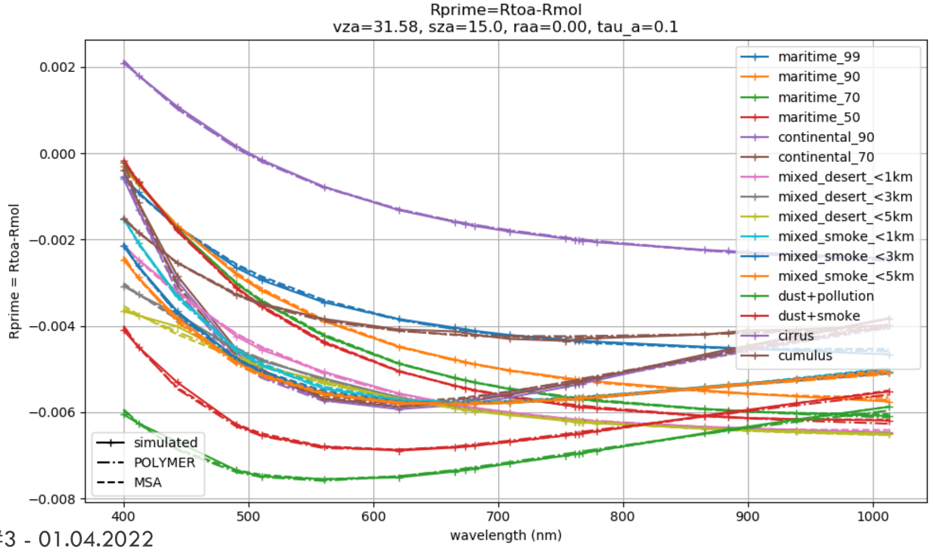
AOT(865)=0.1 | AOT(865)=1.0

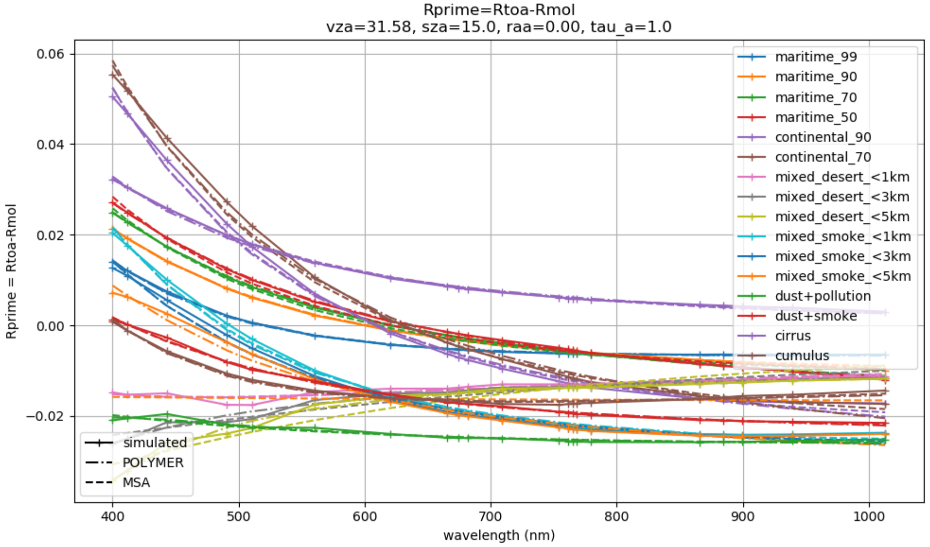
No Sun glint





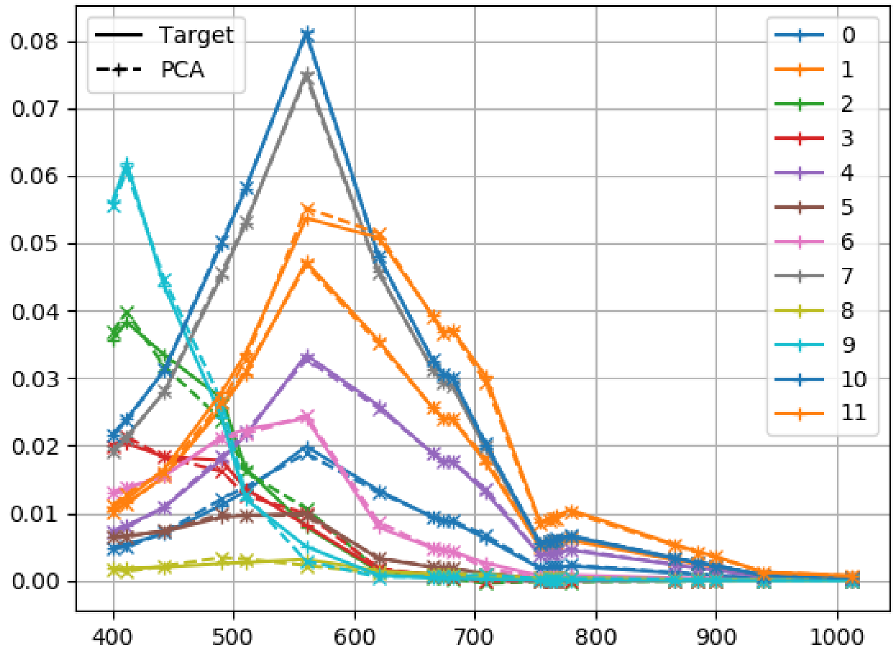
Sun glint residual

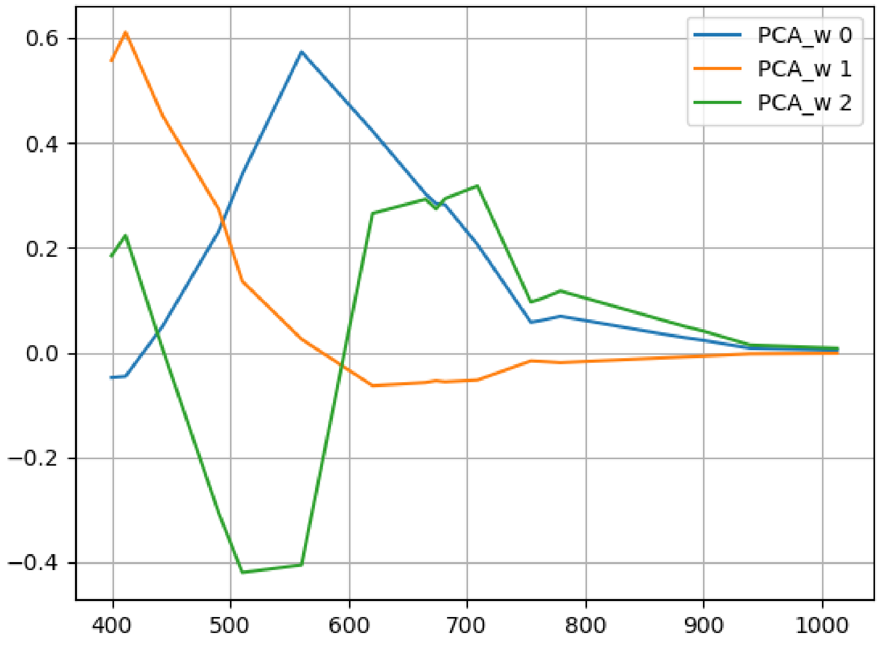




AMBIGUITY BETWEEN "LINEAR" ATM. MODEL AND OCEAN

- **Principal Component Analysis on marine spectra**
  - Three linear components allow to construct very well the various marine spectra





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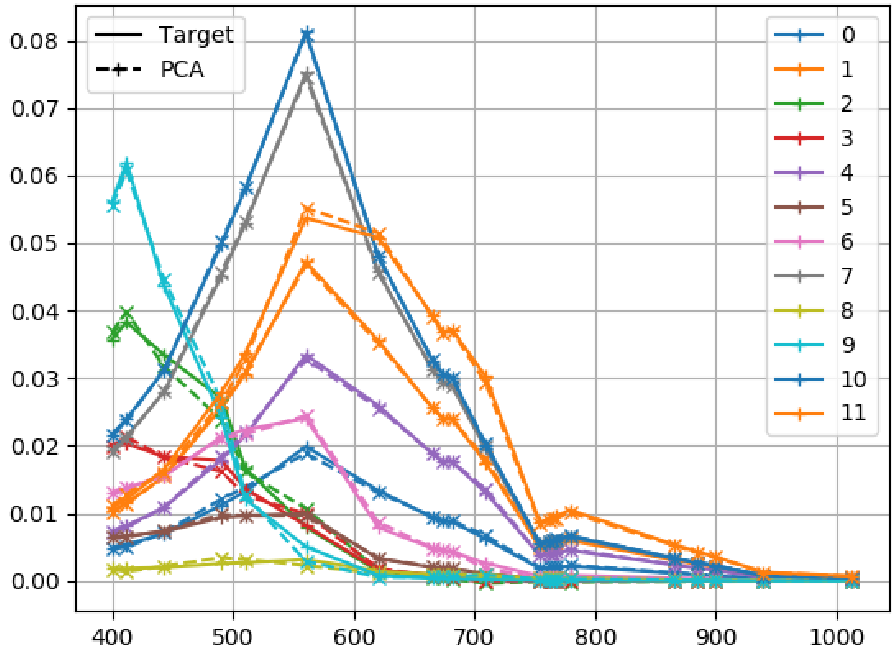

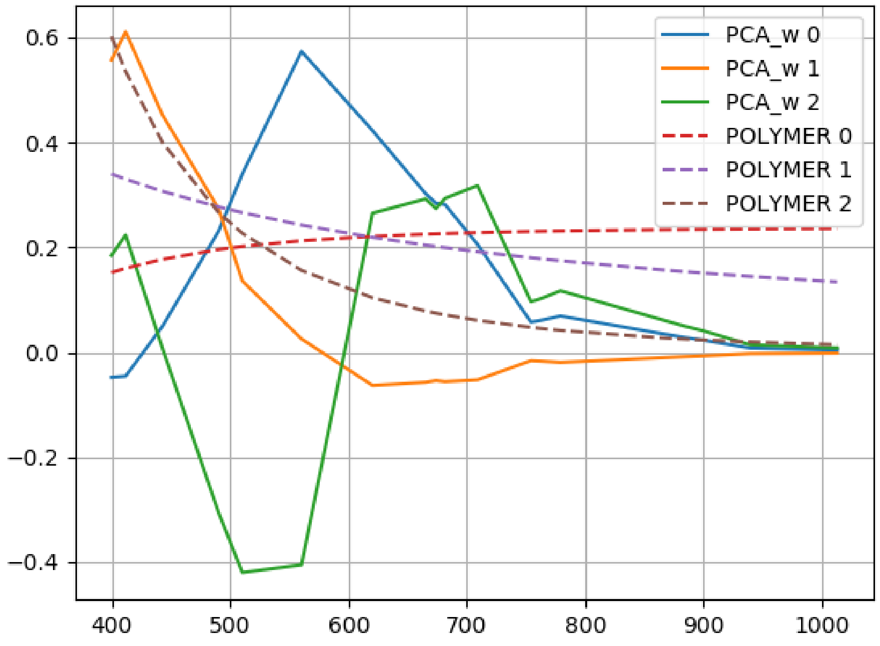

- **2nd component of the marine signal is very close to POLYMER λ^{-4} term**
  - "Linear" atmospheric model may absorb some marine components → ambiguity
  - Ideally, the eigenvectors of atmospheric and ocean linear decompositions should be orthogonal

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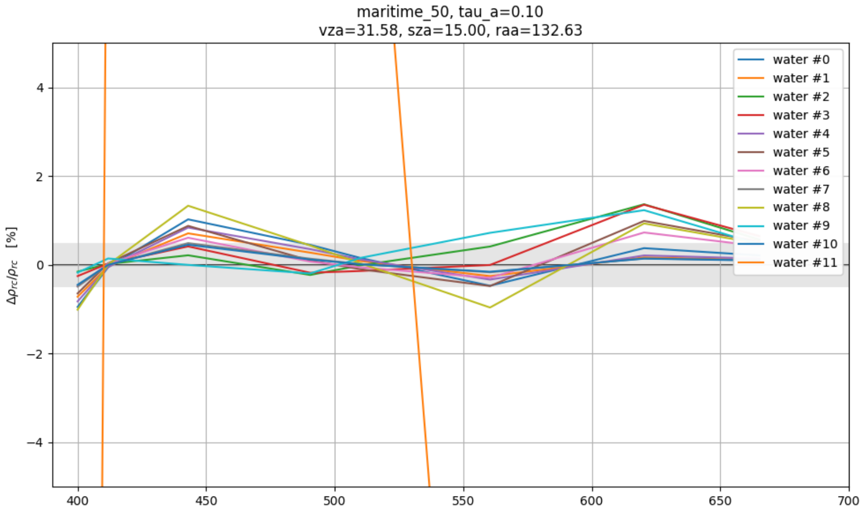
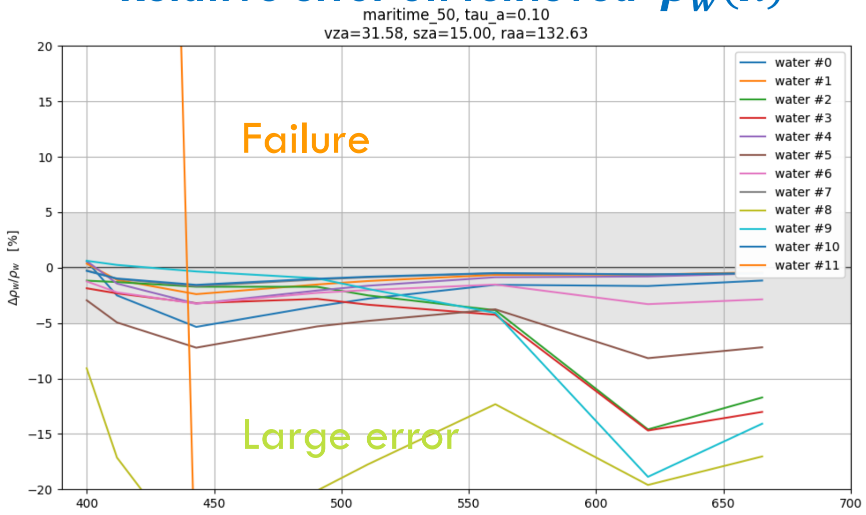
INVERSION ERROR: LINEAR VS MSA MODEL

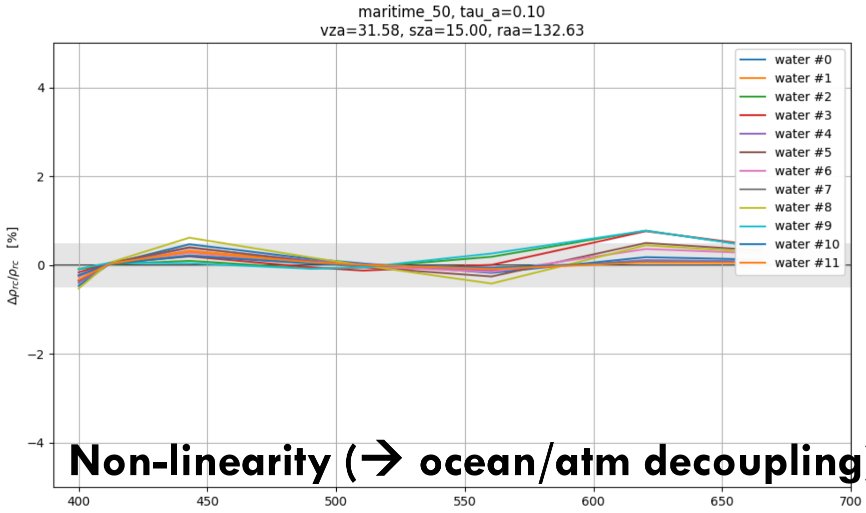
Relative error on re-constructed TOA signal $\rho_{RC}(\lambda)$

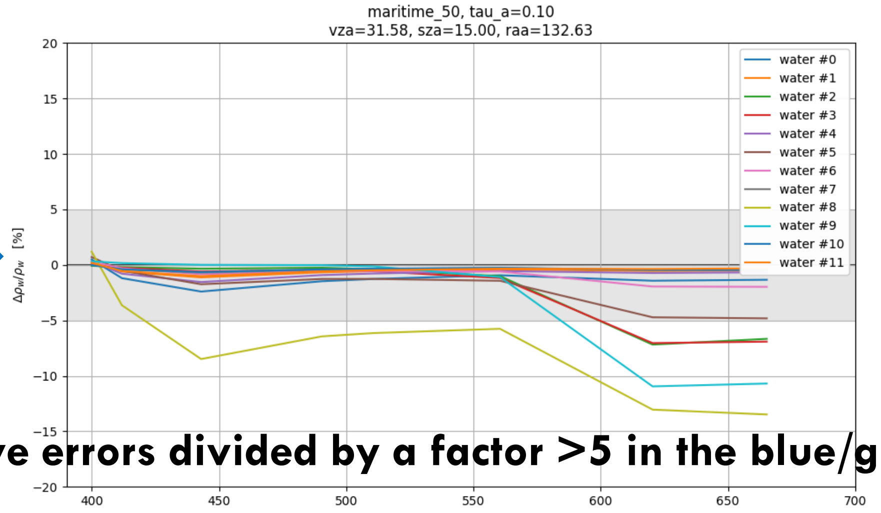
Relative error on retrieved $\rho_w(\lambda)$





Linear model





MSA

Non-linearity (→ ocean/atm decoupling) + constraint: relative errors divided by a factor >5 in the blue/green

FROM IDEAS-QA4EO TOWARDS OPERATION

IDEAS+ IDEAS-QA4EO

$$\rho_a^{mod}(\lambda) = \rho_{a0}\frac{(1-\tau_R(\lambda))}{(1-\tau_{R0})}\left(\frac{\lambda}{\lambda_0}\right)^{-\alpha}$$

Modelling investigations

$$\rho_a^{mod} = \rho_{a0} * \left(\frac{\lambda}{\lambda_0}\right)^{-\alpha}\left(\frac{1+k*\left(\frac{\lambda}{\lambda_0}\right)^{-\alpha}}{1+k}\right)$$

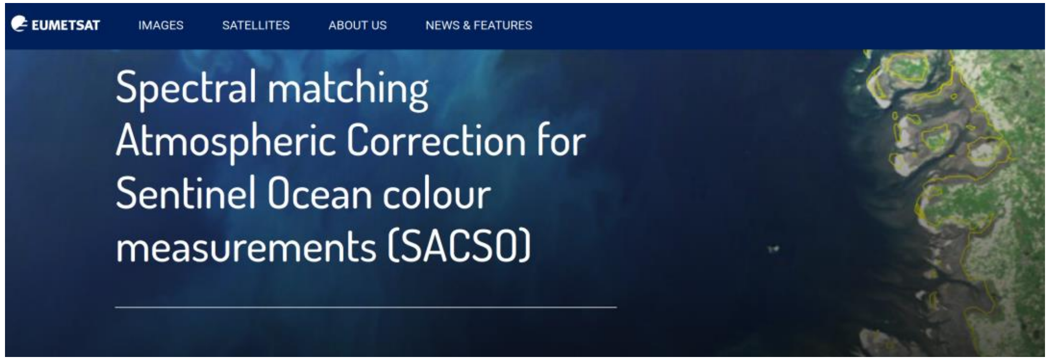
Coding & validation in nearly operational context

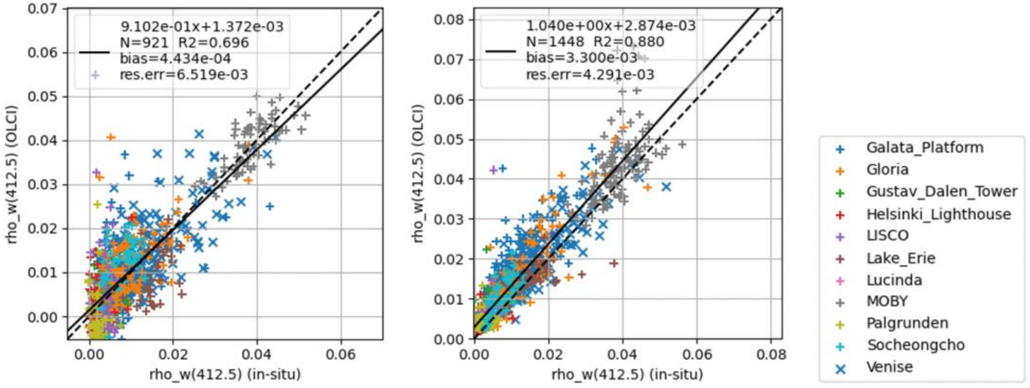
Further developments *not* in SACSO

- **Dimensionality reduction:** inversion of only one parameter, α, with analytic solution of the NLLSQ for ρ_{a0} and k → speed-up time and more robust minimization
- **Input uncertainties:** assess uncertainty of the marine model (at first guess) → spectral weights

EUMETSAT SACSO study, lead by HYGEOS

https://www.eumetsat.int/SACSO





Left: OLCI std processor. Right: SACSO with MSA

MULTI-PIXEL INVERSION

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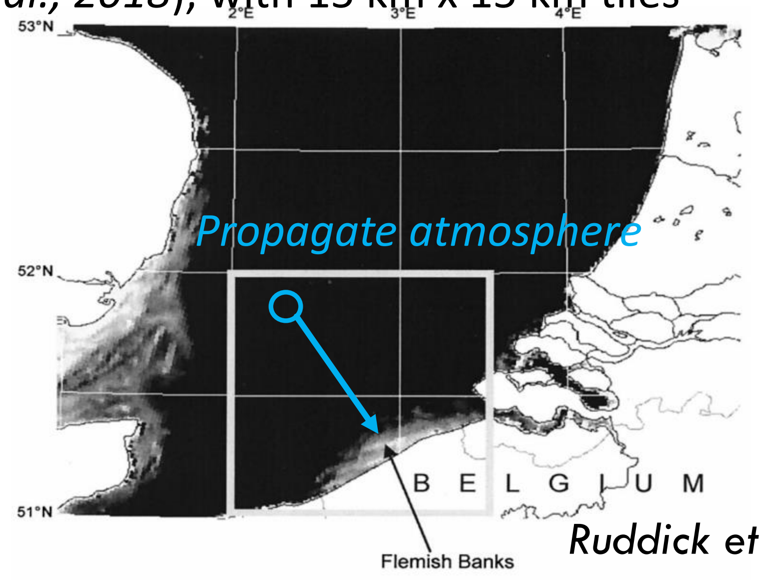
STATE OF THE ART OF "MULTI-PIXEL" OC PROCESSOR

- All OC operational processors are single pixel based (true also for most of R&D processors)
- Principle: constrain the aerosol detection, with assumption on spatial smoothness

"Image base" approach

- Black water assumption: *Ruddick et al. (2000), Vanhellemont and Ruddick (2016), Vanhellemont and Ruddick (2018)*
- Dark land assumption: iCOR processor (*De Keukelaere et al., 2018*), with 15 km x 15 km tiles



Ruddick et al. (2000)

Inter-pixel smoothness

- Dubovik (2004) and Dubovik et al. (2011) → GRASP
- Degree of spatial smoothness → $\partial^m / \partial p^m = 0$
- Example for 2nd order derivative computed over a 1D regular grid of n pixels of step Δp:

$$\frac{\partial^2 x_i}{\partial p^2} \approx \frac{x_{i-1} - 2x_i + x_{i+1}}{\Delta p^2}, \qquad 2 \leq i \leq n-1$$

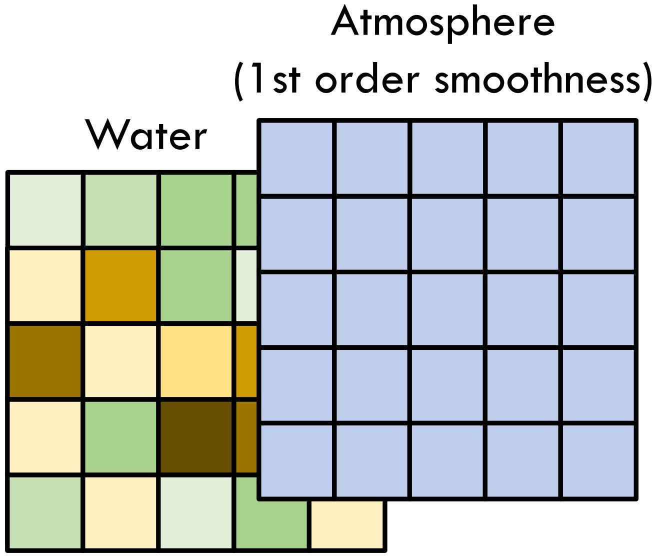
Constraint on the unknown $\boldsymbol{x} = (x_1 \dots x_n)$ writes $\boldsymbol{x}^T \boldsymbol{S}^T \boldsymbol{S} \boldsymbol{x} \approx 0$

$$\mathbf{S} = \begin{pmatrix} 1 & -2 & 1 & 0 & & \cdots & 0 \\ 0 & 1 & -2 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & -2 & 1 & \cdots & 0 \\ \vdots & & & & & \ddots & \vdots \\ 0 & & \cdots & 0 & 1 & -2 & 1 \end{pmatrix}$$

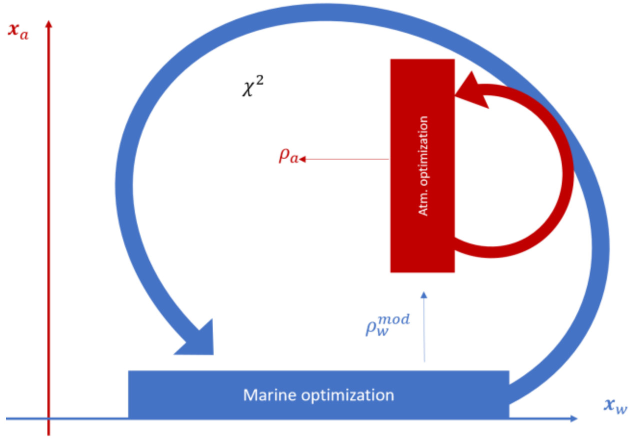
2nd order smoothing matrix of size $(n-2, n)$

- General NLLSQ problem extended to multi-pixel with constraint: $\chi^2_{mult}(\boldsymbol{x}) = \sum_{i=1}^{n} \chi_i^2(\boldsymbol{x}_i) + \gamma_\Delta \boldsymbol{x}^T \mathbf{S}_\Delta^T \mathbf{S}_\Delta \boldsymbol{x} + \dots$
- Applied to PARASOL for Chlorophyll-a retrieval (*Frouin et al., 2019*)

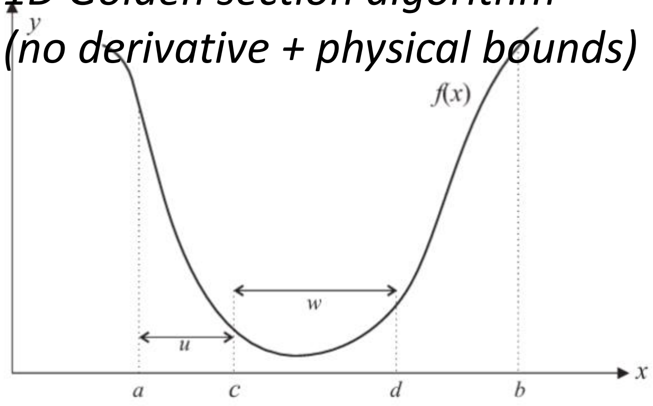
PROPOSED MULTI-PIXEL STRATEGY



- Rely on existing OC inverse algorithm → experience, robustness
- Keep a local multi-pixel inversion (~ few km for OLCI)
- Keep bio-optical variability at pixel level & force spatial smoothness on aerosol
- Application to the Bright Pixel Correction (operational, new OLCI Collection 3)
  - Two atmospheric unknowns and one marine unknown: $\rho_{Rc}^{mod}(\lambda_i, \boldsymbol{x}_a, b_{bp0}) = \rho_a(\lambda_0)\left(\frac{\lambda}{\lambda_0}\right)^{\varepsilon} + t_R^{mod}(\lambda_i)\rho_w^{mod}(\lambda_i, b_{bp0})$
  - Chi-square minimization over n bands : $\sum_{pix}\chi^2(\boldsymbol{x}_a, b_{bp0}) = \sum_{pix}\frac{1}{n-n_x}\left(\boldsymbol{\rho}_{Rc}^{mod}(\boldsymbol{x}_a, b_{bp0}) - \boldsymbol{\rho}_{Rc}^{obs}\right)^T \boldsymbol{W}\left(\boldsymbol{\rho}_{Rc}^{mod}(\boldsymbol{x}_a, b_{bp0}) - \boldsymbol{\rho}_{Rc}^{obs}\right)$



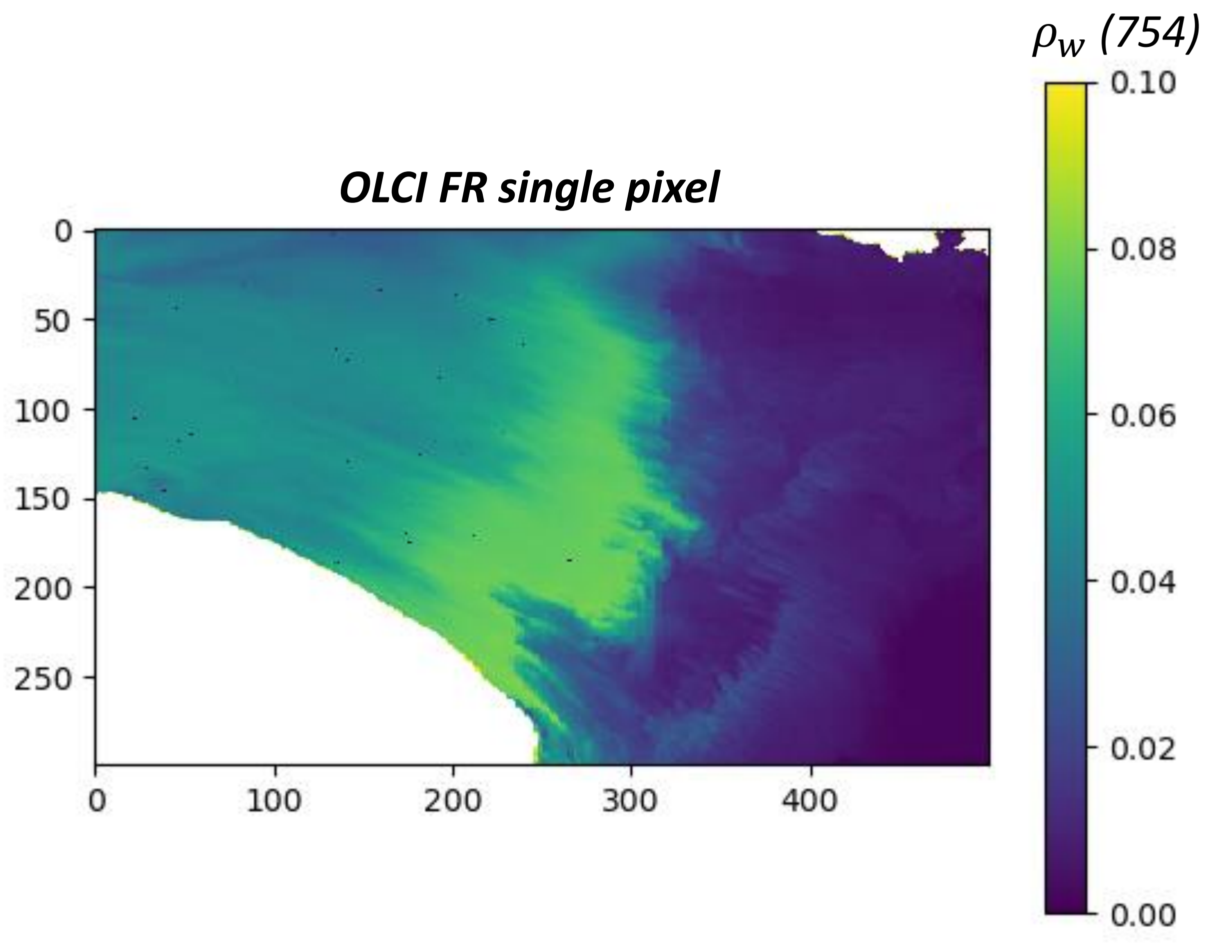
1D Golden section algorithm
(no derivative + physical bounds)

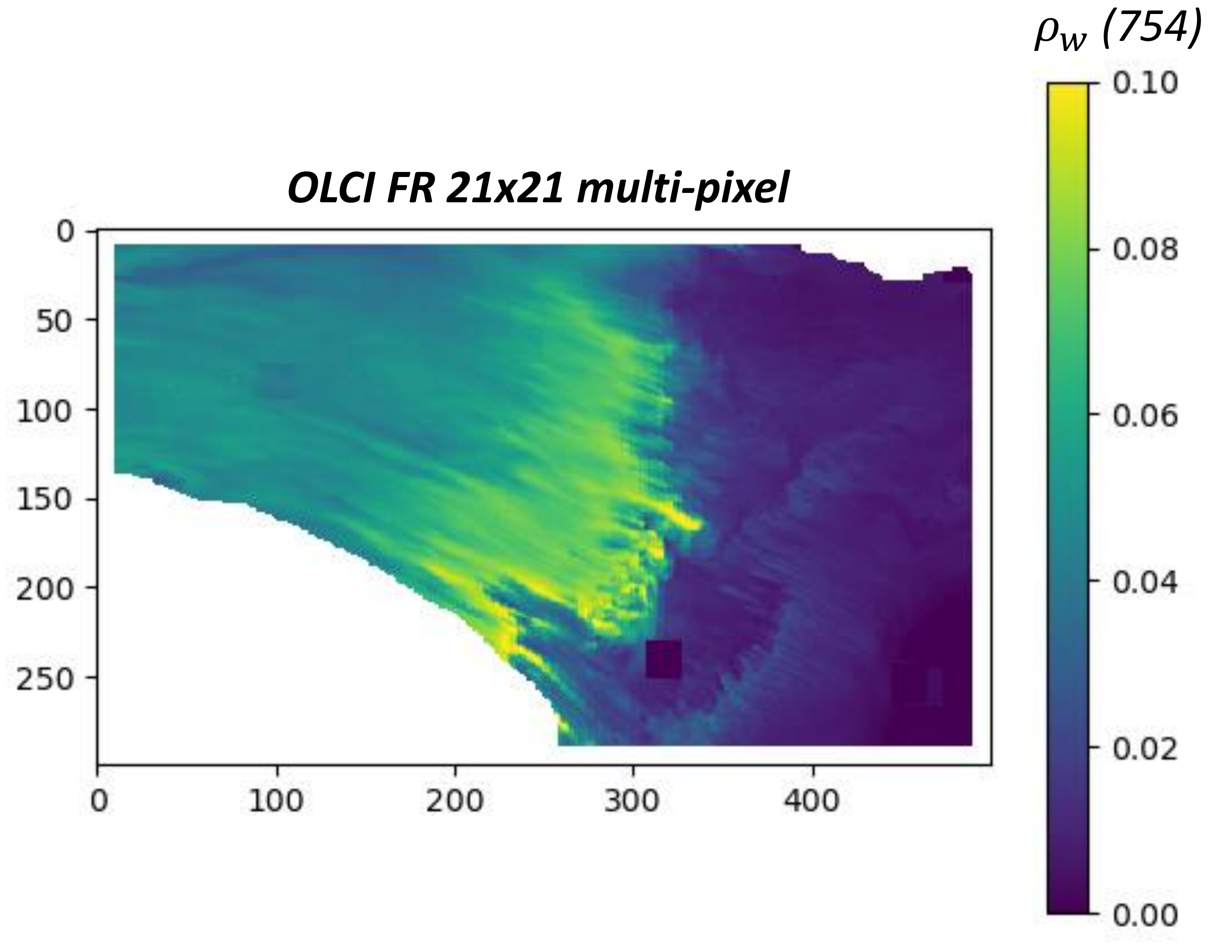


2-step inversion well adapted for multi-pixel:

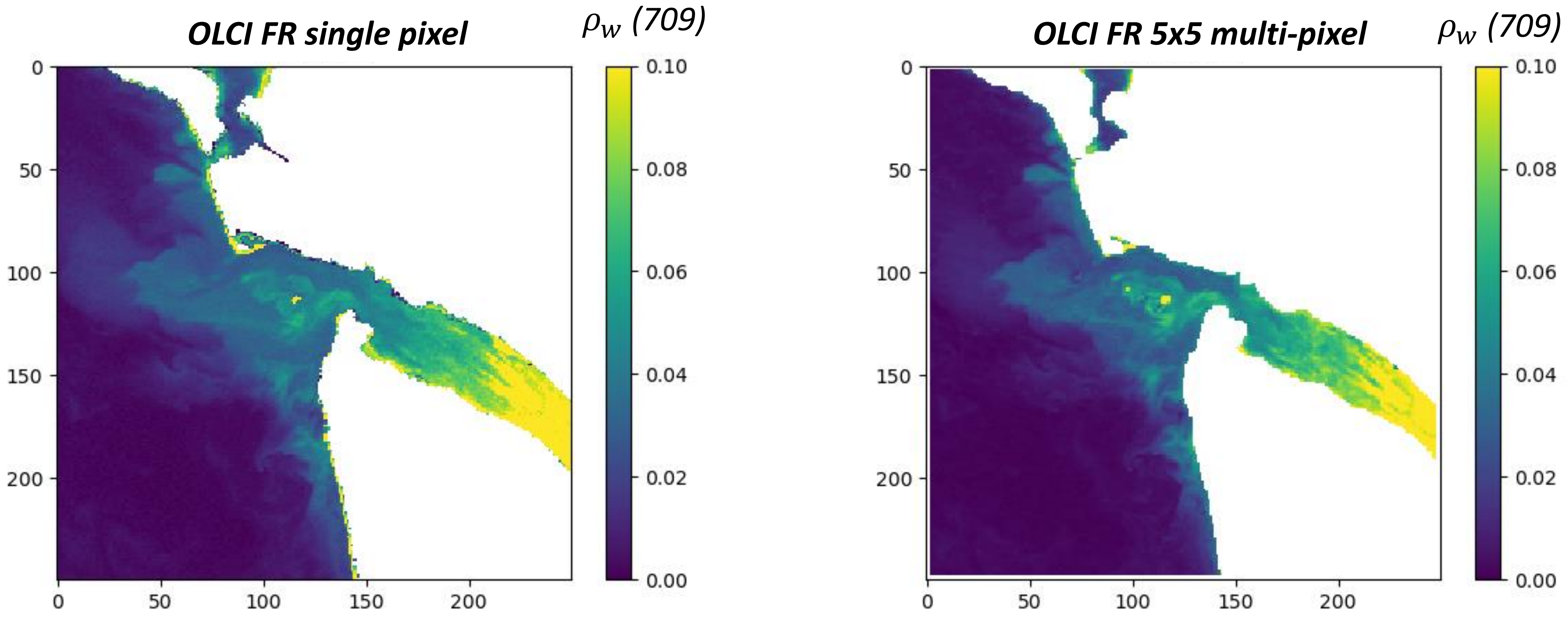
- Given b_{bp0} for all pixels, compute one unique set of $\rho_a(\lambda_0), \varepsilon$
- Minimize globally over b_{bp0}

RESULTS OF MULTI-PIXEL BPC – RIO DE LA PLATA





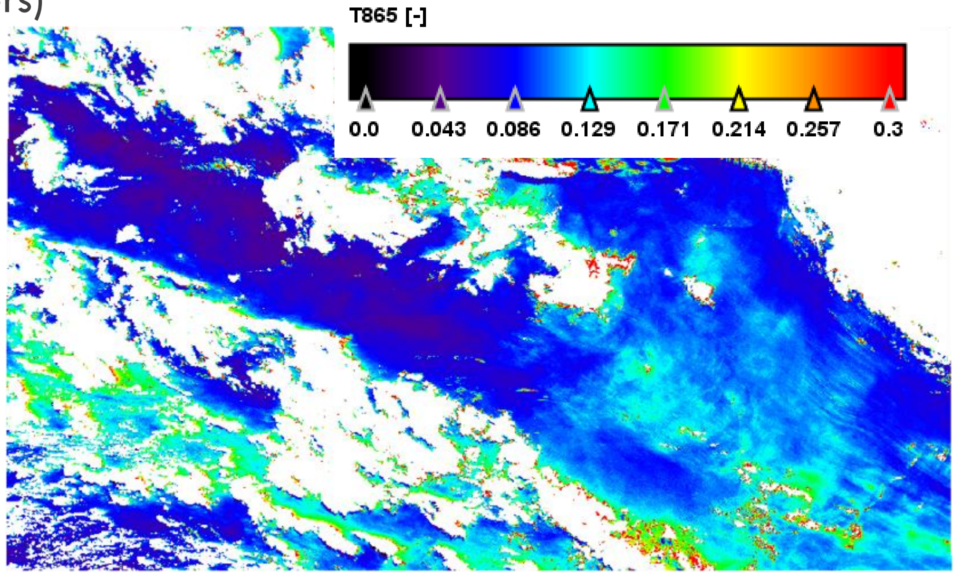
RESULTS OF MULTI-PIXEL BPC – GIRONDE ESTUARY



SOME CONCLUSIONS ON MULTI-PIXEL INVERSION

- **New framework for traditional OC algorithms**
- **Various assumptions can be easily implemented:**
  - Fixed AOT and epsilon, AOT varying by pixel and fixed epsilon, AOT varying by pixel and smooth epsilon ….
- **Need to carefully screen the macro-pixel:** clouds, coastline, cosmic rays (South Atlantic Anomaly) …
- **Not totally conclusive for BPC, which is already very robust**
  - Sharpening effect on heterogeneous area (front with complex waters)
  - Obviously not impacting homogeneous area
  - Care also about OLCI duplicated pixels!
- **To be investigated for the full Clear Water AC**
- **To be assessed on match-ups**

CWAC when fixing aerosol model



CONSTRAINT WITH CALIOP VERTICAL PROFILE

OVERALL PRINCIPLE

- **Main motivations: aerosol vertical distribution impacts the coupling with Rayleigh**
    1. Assess uncertainty at a potential "OC System Vicarious Calibration" site at Lampedusa → EURYBIA* proposal to EUMETSAT
    2. More generally, assess uncertainty of the current AC & improve performance with more constraints
- **Principle:** compare MERIS path reflectance and transmittance with reference data built from better aerosol knowledge + RTM
- **AERONET data:** $AOT(\lambda) + SSA(\lambda) + P_{aer}(\Theta, \lambda)$ at $\lambda = \{440, 675, 870\}\ nm$
- **CALIOP data:** Vertical profiles of extinction coefficient profiles derived from total backscatter measurements at 532 & 1064 nm from a near-nadir-viewing geometry during both day and night phases of CALIPSO orbit
- **CALIOP seasonal statistics:** computed by CNR over 10 years (12/2006-11/2016) at Lampedusa

(*) Liberti, G.L., D'Alimonte, D., di Sarra, A., Mazeran, C., Voss, K., Yarbrough, M., Bozzano, R., Cavaleri, L., Colella, S., Cesarini, C., Kajiyama, T., Meloni, D., Pomaro, A., Volpe, G., Yang, C., Zagolski, F., Santoleri, R. (2020). **European Radiometry Buoy and Infrastructure (EURYBIA): A Contribution to the Design of the European Copernicus Infrastructure for Ocean Colour System Vicarious Calibration**. *Remote Sens.*, 12, 1178.

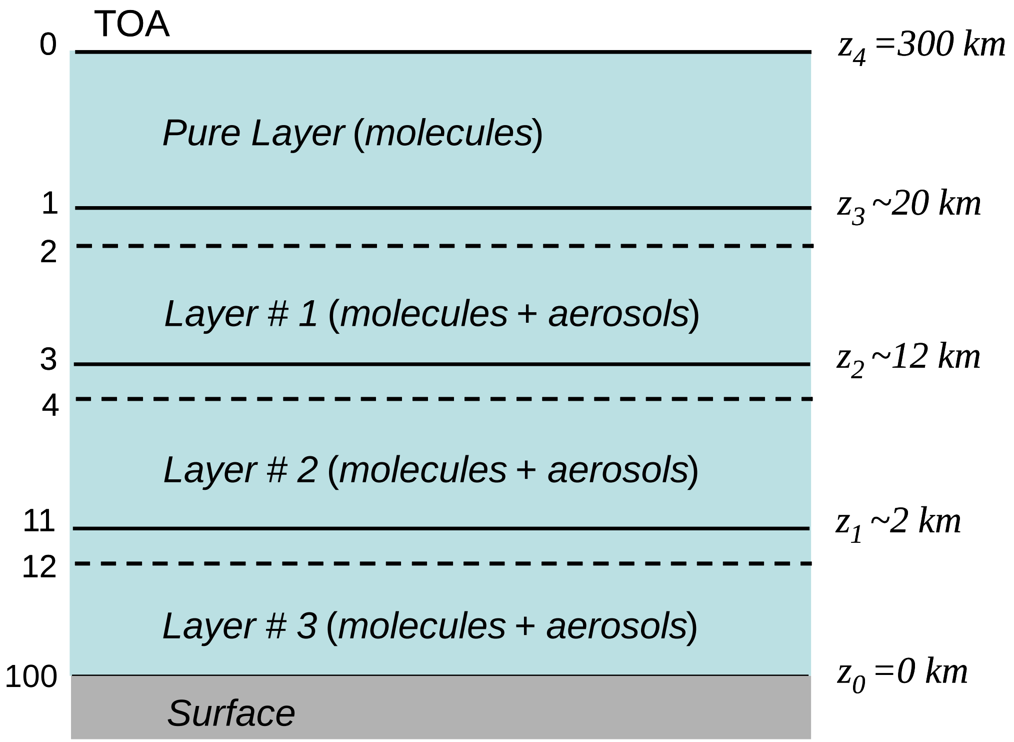
MERIS & OLCI STANDARD AEROSOL MODELS

⇨ 12 SAMs (Shettle & Fenn, 1979): Maritime, Coastal & Rural (RH=50, 70, 90, 99%)

⇨ 1 aerosol model spectrally white

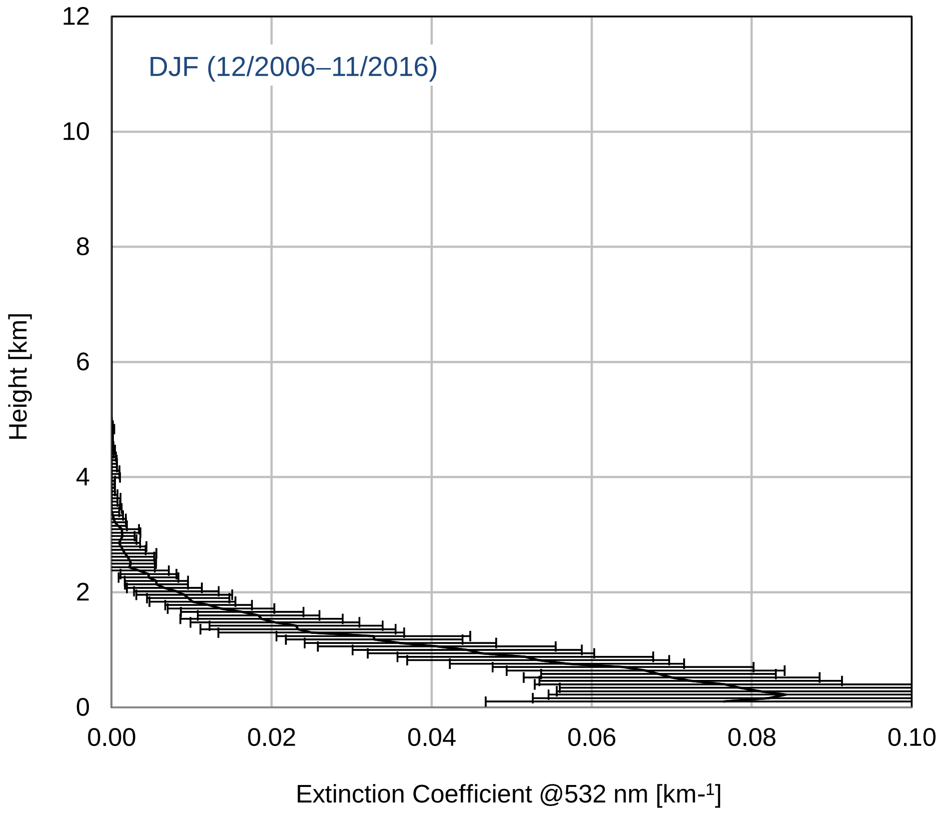
⇨ 3 blue aerosol models including a spectral dependence extracted from an approach combining micro-physical properties of small particles with IOP's derived from CIMEL radiometric measurements (Zagolski & Santer, 2010)

- Above 20 km: free aerosol layer
- Stratosphere [12–20]km: (optically fixed layer)
- Troposphere [2–12]km: Continental (optically fixed layer)
- **Boundary layer [0–2]km: MAR, RUR, COA, BLUE (optically variable layer)**

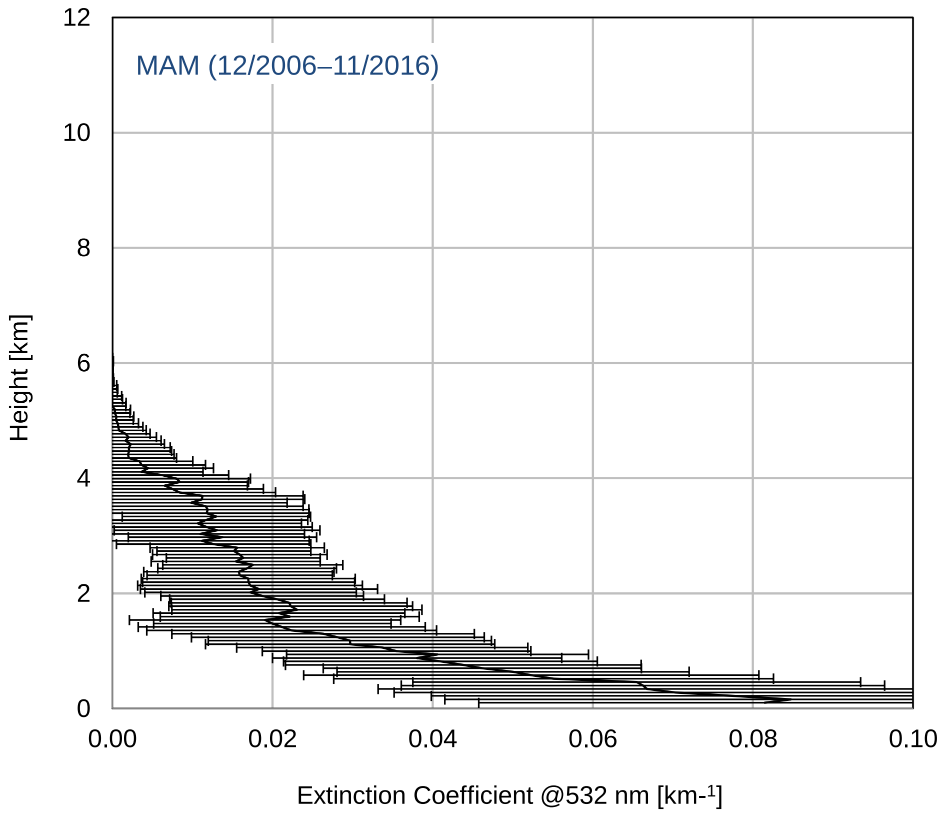


CALIOP VERTICAL PROFILE OF EXTINCTION COEFFICIENT @532 NM

Dec./Jan./Feb.



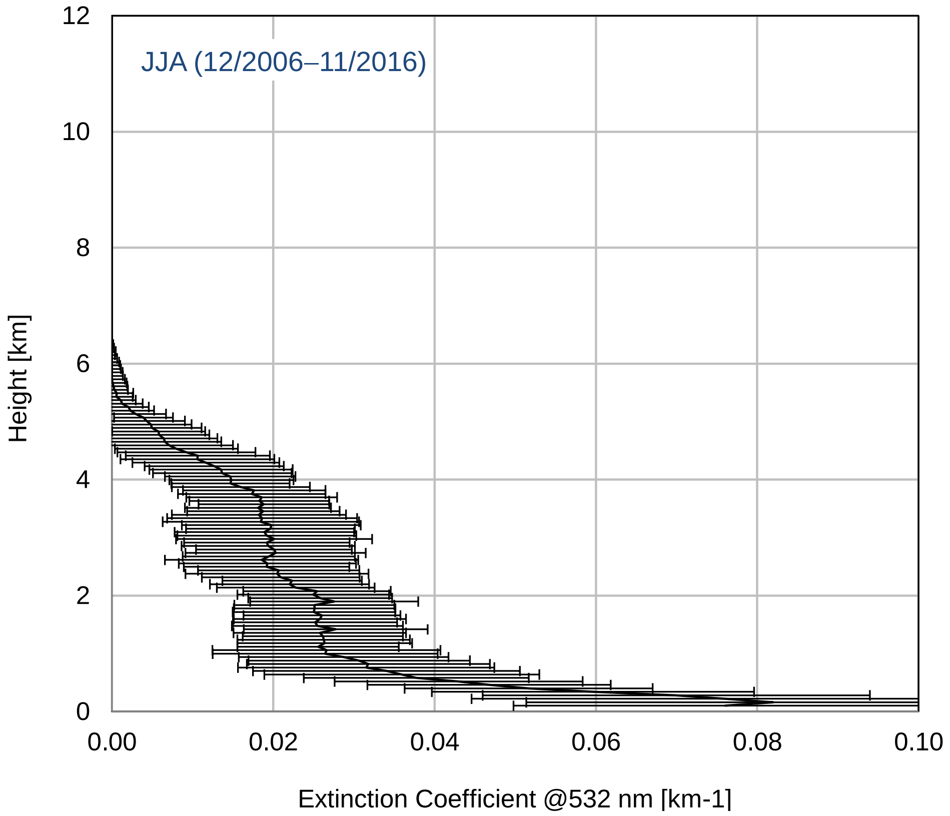
Mar./Apr./May



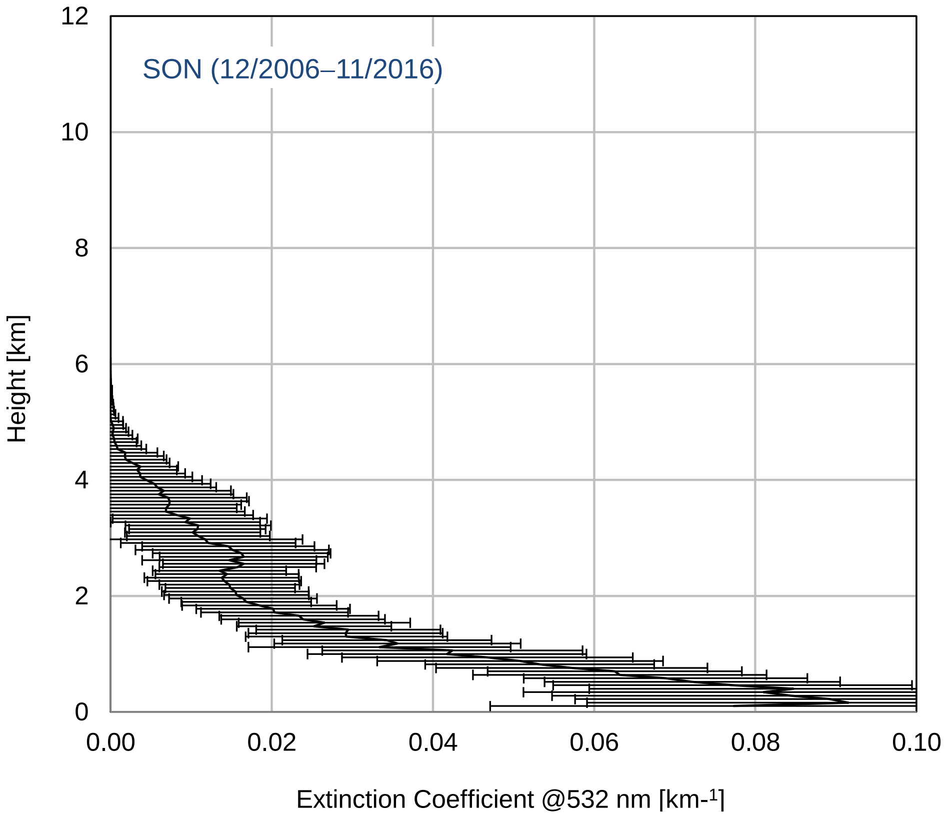
Seasonal variation of vertical distribution of extinction coefficient @ 532nm collected with the CALIOP instrument for a period of 10 years (i.e., from December 2006 to November 2016) over Lampedusa.

CALIOP VERTICAL PROFILE OF EXTINCTION COEFFICIENT @532 NM

Jun./Jul./Aug.



Sep./Oct./Nov.



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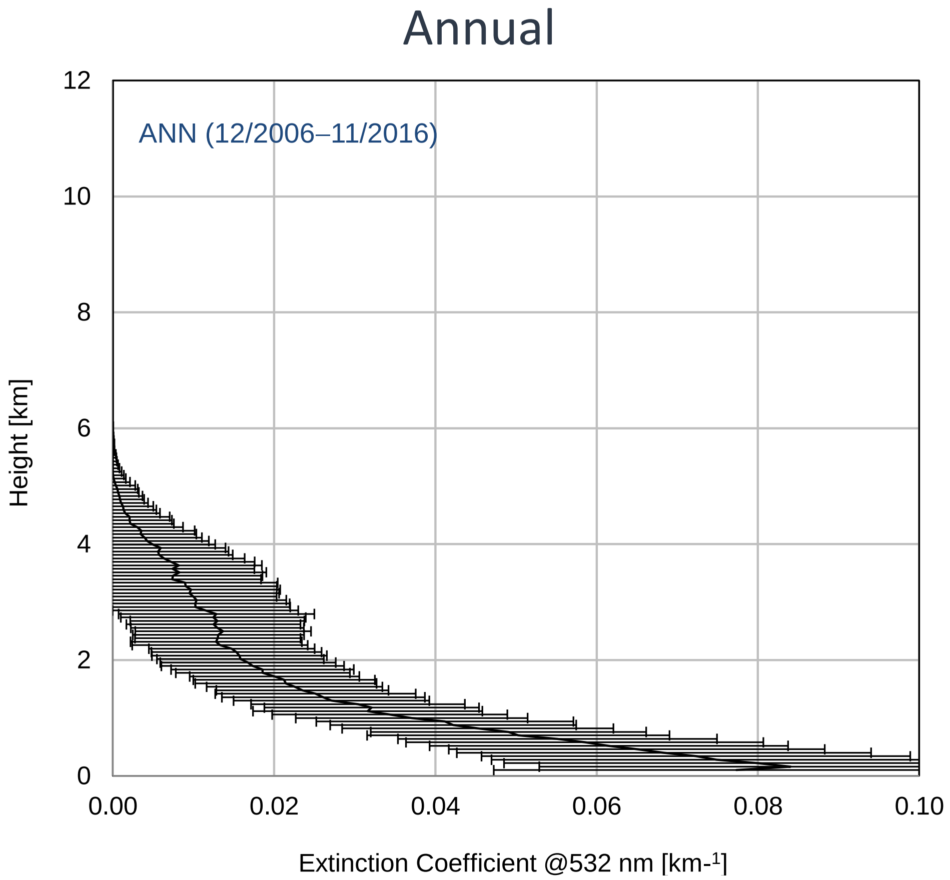

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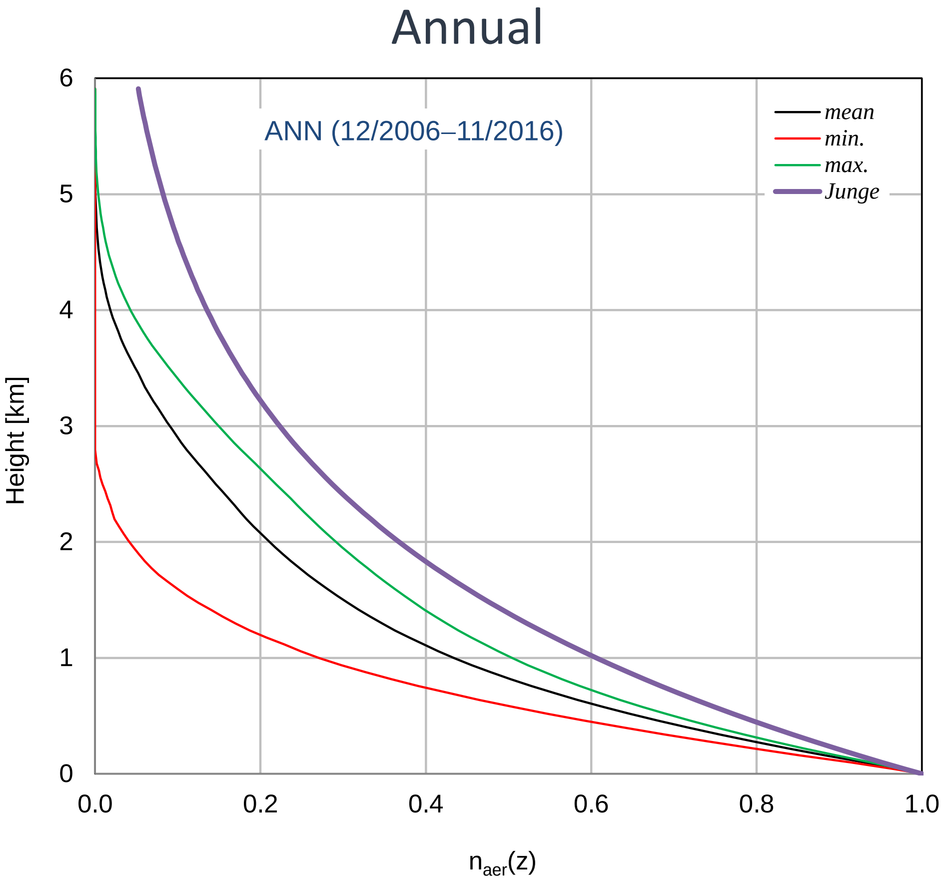
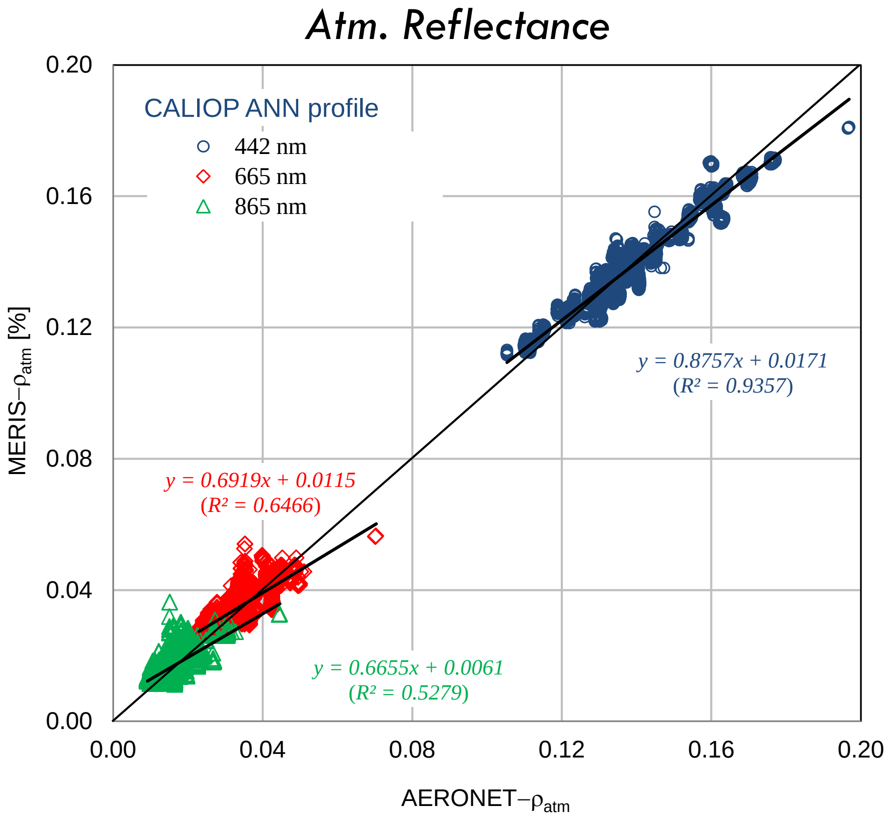
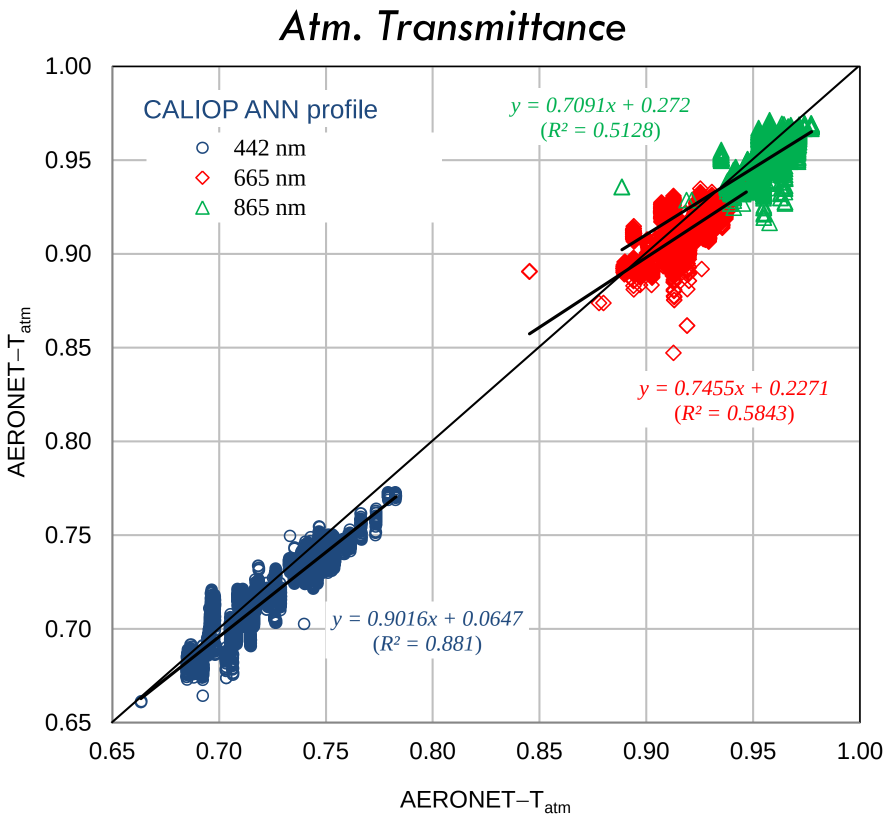


Comparison between CALIOP vertical size distribution and a classical Junge's power model with exponential distribution (Ha=2km) over the Lampedusa site.

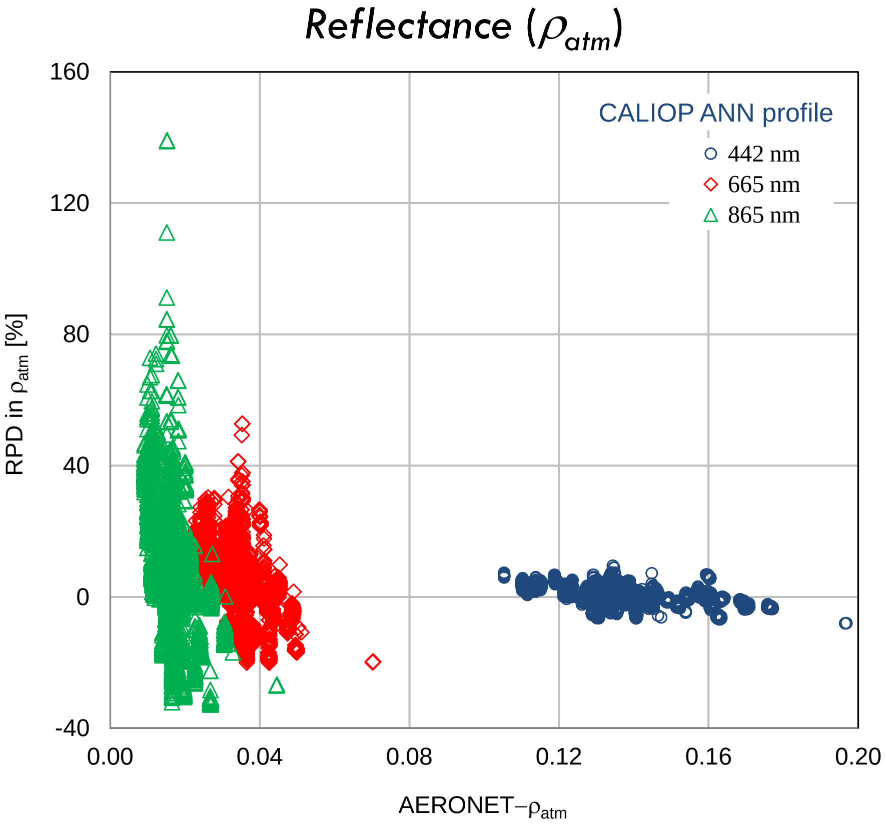
MERIS VS AERONET+CALIOP_ANN

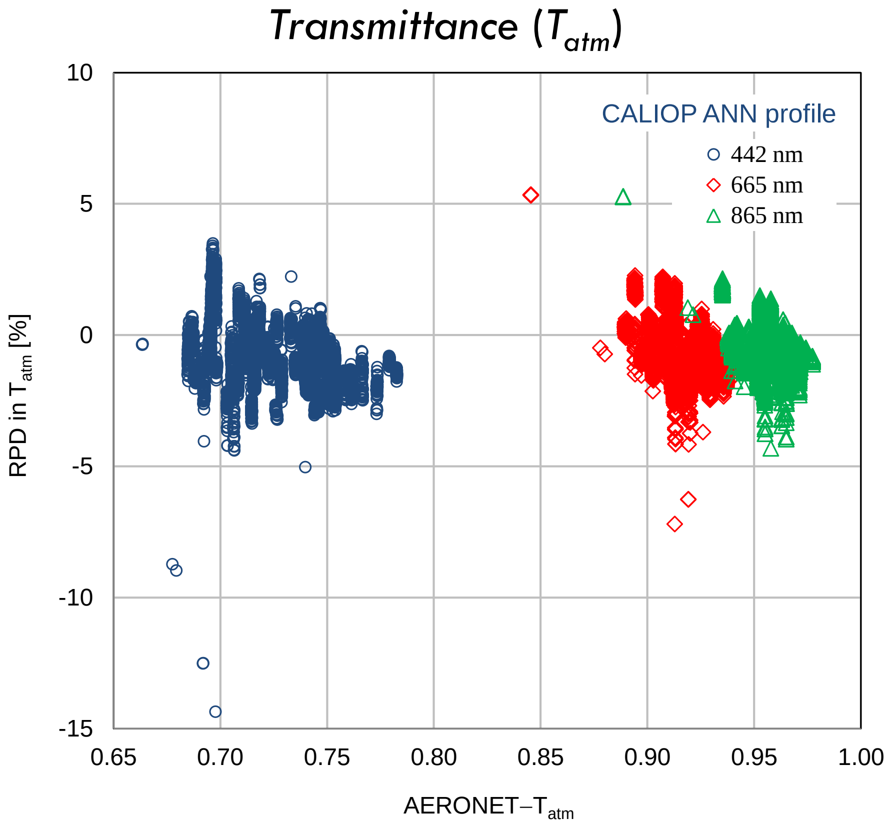




Comparison between MERIS and computed ASFs with AERONET and 'ANN_mean' profile (CALIOP) over Lampedusa. MERIS L2 extractions are achieved for a window of (9 x 9) pixels in RR mode and filtered by 2 flags ('PCD_13' flag and AOT_865 < 0.15).

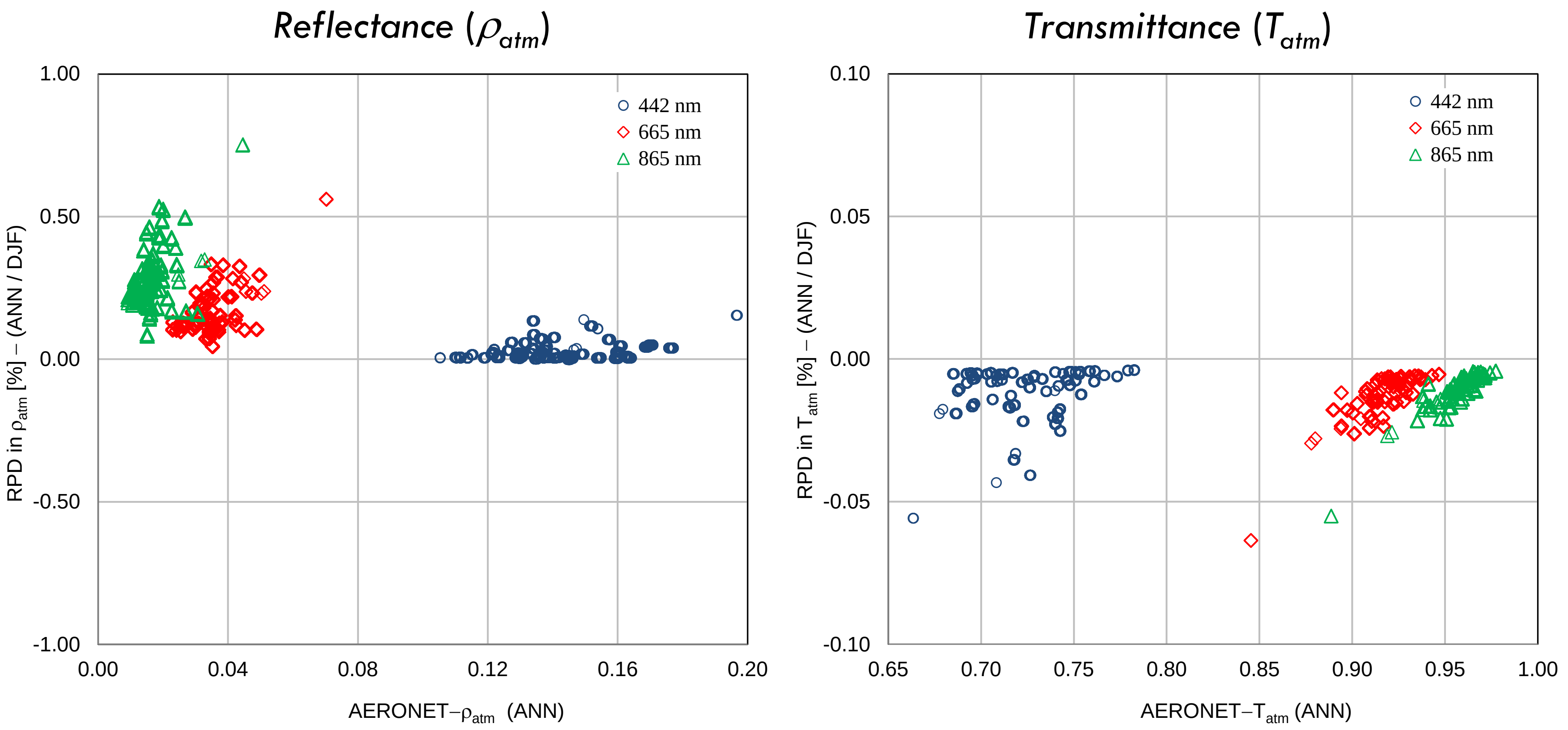
MERIS VS AERONET+CALIOP_ANN





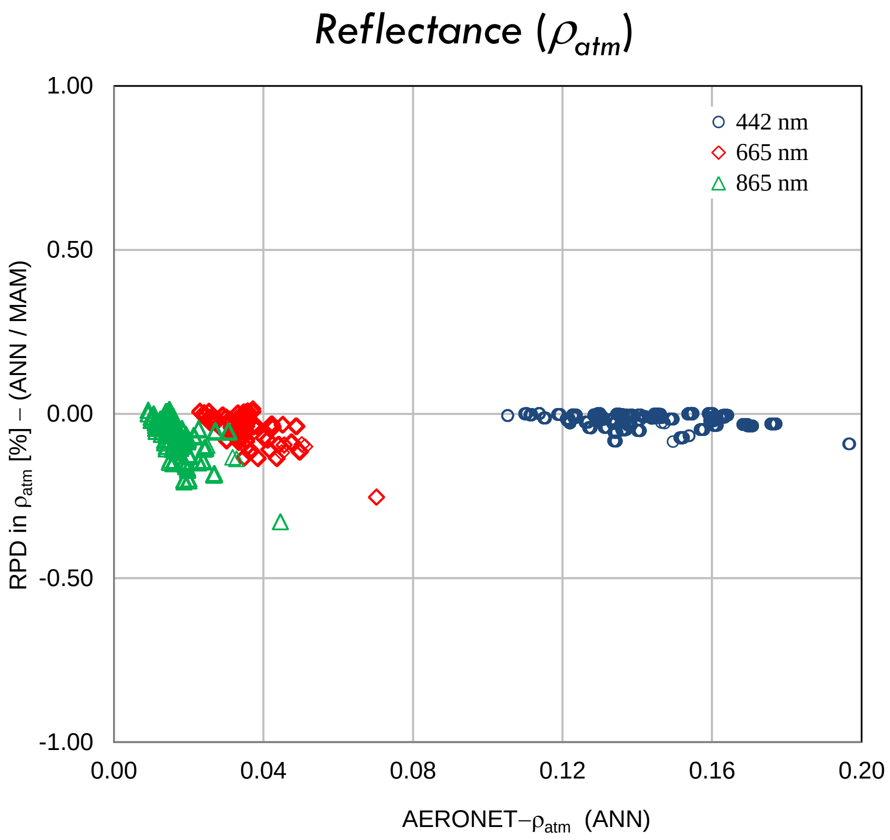
RPD is computed between MERIS and computed ASFs with AERONET and 'ANN_mean' profile (CALIOP) over Lampedusa. MERIS L2 extractions are achieved for a window of (9 x 9) pixels in RR mode and filtered by 2 flags ('PCD_13' flag and AOT_865 < 0.15).

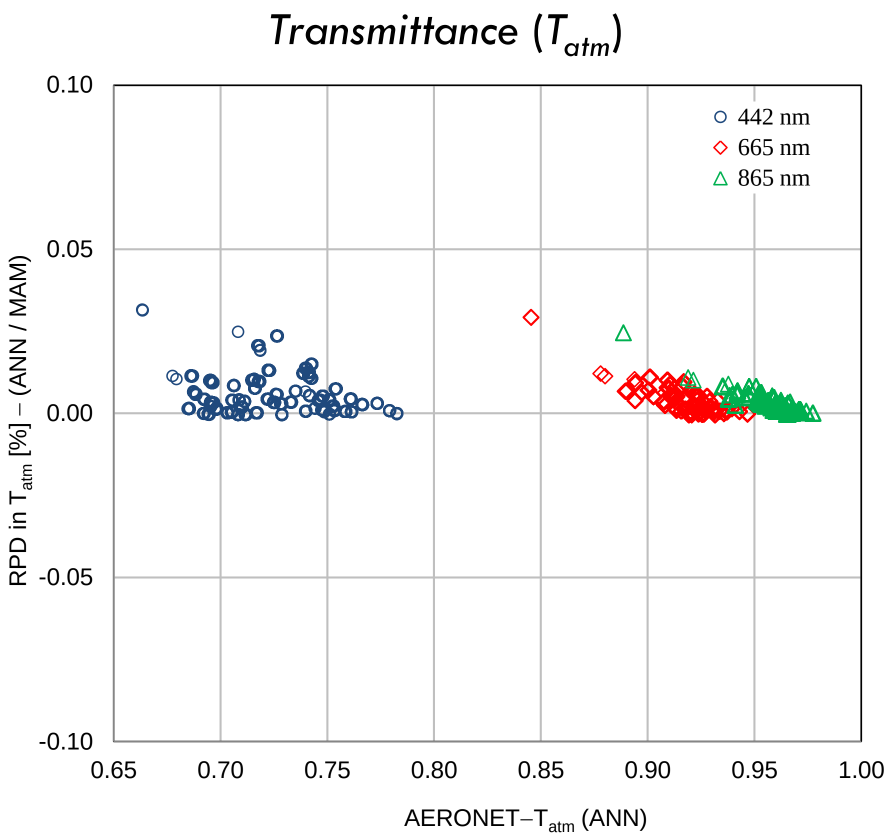
AERONET+CALIOP_ANN VS AERONET+CALIOP_DJF



RPD is computed between AERONET - ASFs calculated with 'ANN_mean' and 'DJF_mean' profiles (CALIOP) over Lampedusa. MERIS L2 extractions are achieved for a window of (9 x 9) pixels in RR mode and filtered by 2 flags ('PCD_13' flag and AOT_865 < 0.15).

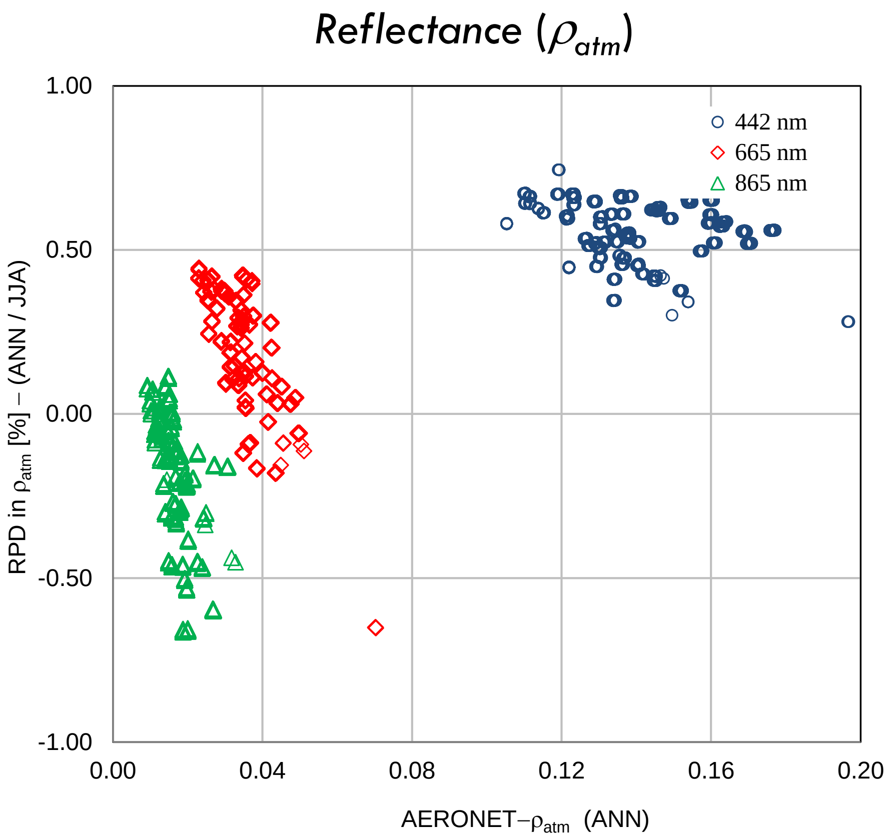
AERONET+CALIOP_ANN VS AERONET+CALIOP_MAM

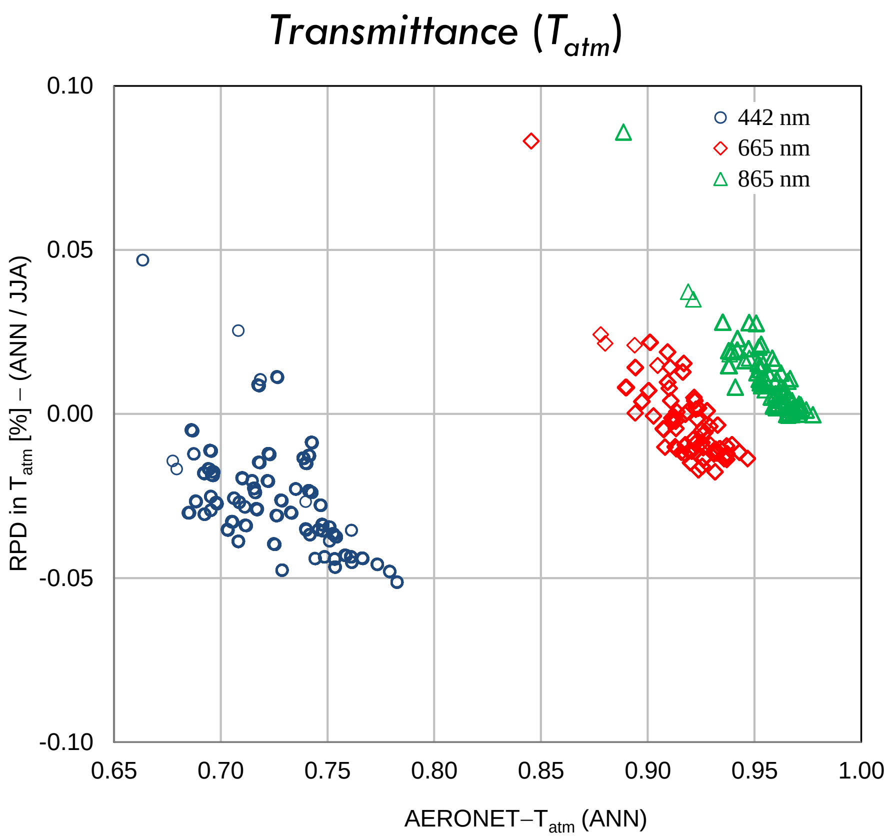




RPD is computed between AERONET - ASFs calculated with 'ANN_mean' and 'MAM_mean' profiles (CALIOP) over Lampedusa. MERIS L2 extractions are achieved for a window of (9 x 9) pixels in RR mode and filtered by 2 flags ('PCD_13' flag and AOT_865 < 0.15).

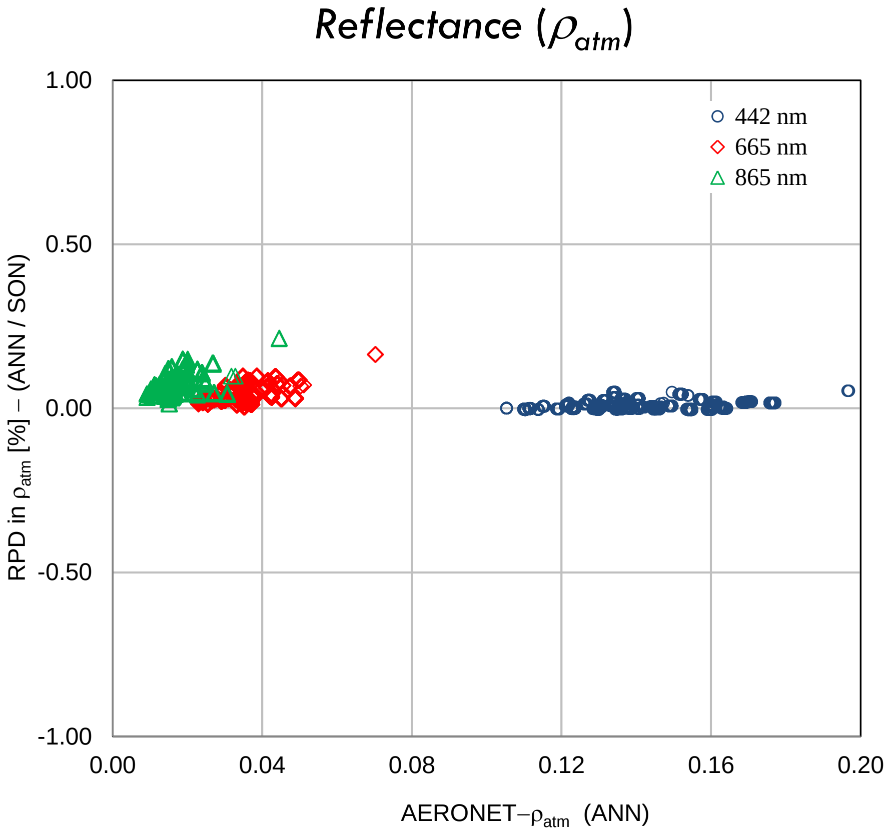
AERONET+CALIOP_ANN VS AERONET+CALIOP_JJA

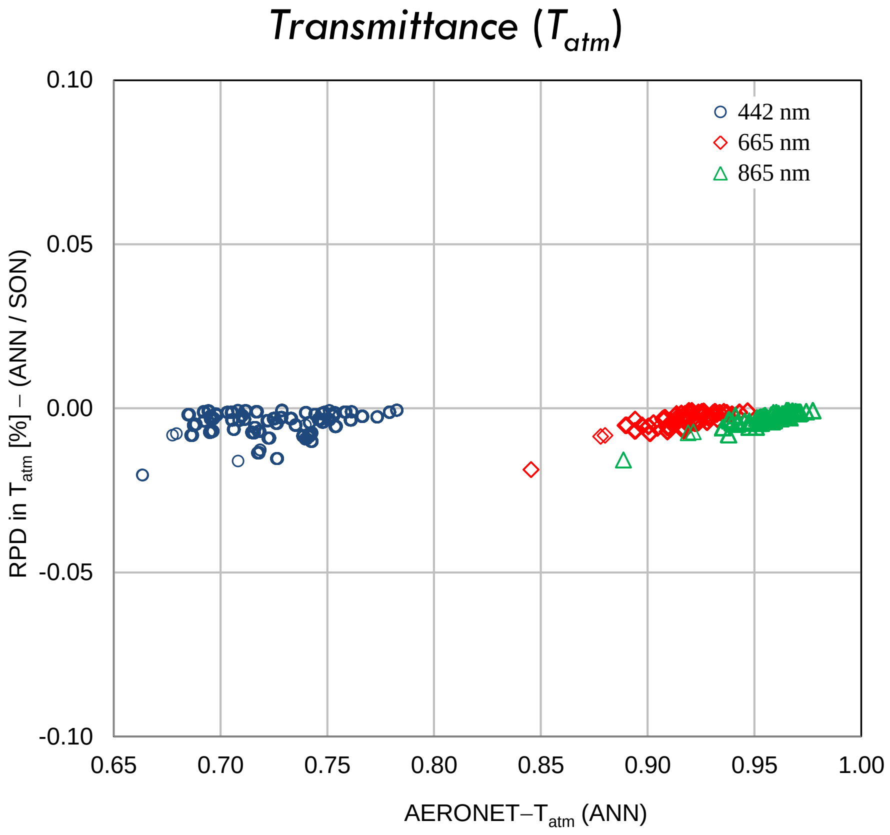




RPD is computed between AERONET - ASFs calculated with 'ANN_mean' and 'JJA_mean' profiles (CALIOP) over Lampedusa. MERIS L2 extractions are achieved for a window of (9 x 9) pixels in RR mode and filtered by 2 flags ('PCD_13' flag and AOT_865 < 0.15).

AERONET+CALIOP_ANN VS AERONET+CALIOP_SON





RPD is computed between AERONET - ASFs calculated with 'ANN_mean' and 'SON_mean' profiles (CALIOP) over Lampedusa. MERIS L2 extractions are achieved for a window of (9 x 9) pixels in RR mode and filtered by 2 flags ('PCD_13' flag and AOT_865 < 0.15).

CONCLUSIONS ON AEROSOL PROFILE CONSTRAINT

- **Not accounting for the real vertical distribution of aerosol in the lower atmospheric layers yields very large absolute relative errors in ASFs (beyond OC requirements of 5% at sea level):**
  - Errors on ρ_{atm} : up to ~10 % (blue), ~30% (red), and ~80% (NIR)
  - Errors on T_{atm} : up to ~5 % (blue, red and NIR)

- **Seasonal variability of aerosol vertical profile could be neglected:**
  - Errors on ρ_{atm} : < 0.5% whatever the wavelength
  - Errors on T_{atm} : < 0.05% whatever for blue, red and NIR bands

⇨ **The CALIOP annual profile can be used as a first approximation**

PLAN FOR PHASE 2

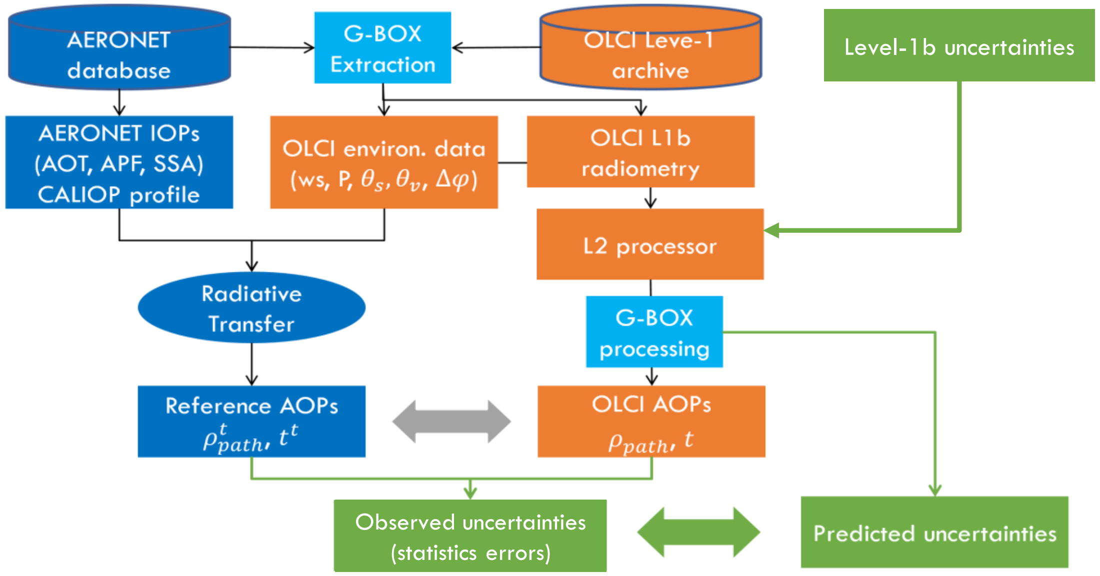
PLAN FOR IDEAS-QA4EO PHASE2 (WP 2120, 2155)

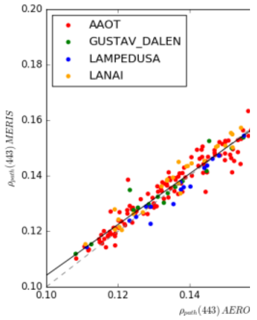
I. OCR processor consolidation

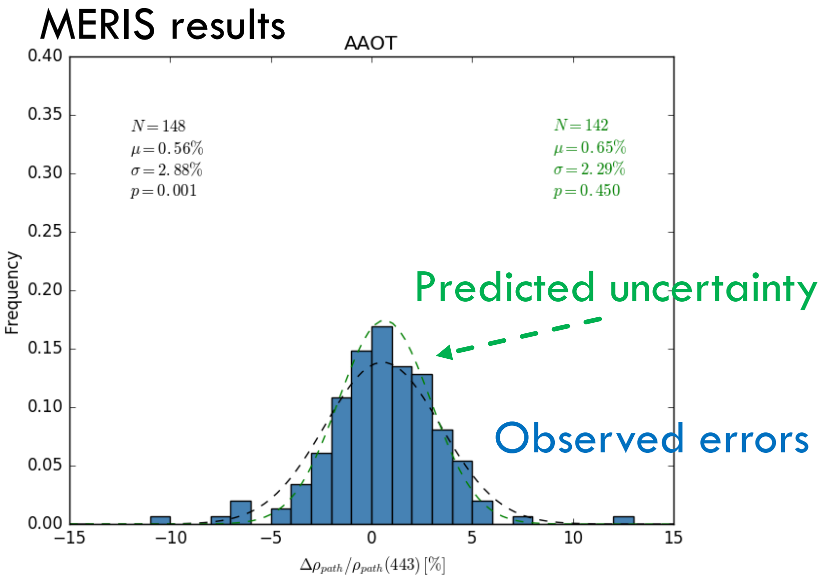
- i. Extend the MSA analytical approach to the aerosol transmittance, currently oversimplified (← uncertainties)
- ii. Further investigate the multi-pixel approach (full Atmospheric Correction chain, until the VIS)
- iii. Implement CALIOP climatology in standard AC, assess performance

II. Validation of OLCI AC and AC uncertainties: prototype tool using the IDEAS-QA4EO Cal/Val platform

- Start from OLCI Level-1b uncertainties characterization (← ESA)







THANK YOU

esa

IDEAS-QA4EO