

# Ocean Colour Standard Atmospheric Correction

## Algorithm Theoretical Basis

### Deliverable D-4

**Version v5.2**

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solvo



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## 1 INTRODUCTION

### 1.1 SCOPE OF THE DOCUMENT

This document is the Algorithm Theoretical Basis Document (ATBD) of the EUMETSAT Ocean Colour Standard Atmospheric Correction (OC-SAC) study and constitutes the study deliverable D-4 (version v5.2). It describes in details the physics of the problem, the mathematical formulation of the inversion, the algorithm implemented in the OLCI Level-2 ground segment and its performance.

This ATBD strongly relies on the OC-SAC Requirement Baseline (RB) document ([AD-1]). More detailed validation is available in the OC-SAC Product Validation Report (PVR, [AD-2]).

### 1.2 STRUCTURE OF THE DOCUMENT

Present ATBD is structured as follows:

- Section 1 gives hereafter applicable documents, scientific references and notations used throughout the document.
- Section 2 provides an overview of the core delivered products: the marine reflectance, aerosol by-products and flags. It also summarises the OC-SAC requirements and state-of-the art from [AD-1].
- Section 3 describes briefly the specificity of the OLCI instrument, relevant for current OC-SAC algorithm.
- Section 4 is the detailed description of the algorithm, comprising the processing outline, inputs and outputs, physical and mathematical description, performance estimate, practical considerations and validation. The validation in this ATBD refers to algorithmic checks, sensitivity studies and components validations, while validation of OLCI Level-2 data is part of the PVR [AD-2].
- Section 4.6.7 lists the assumptions and limitations of the OC-SAC algorithm, with potential improvements for future developments.
- Section 6 is an appendix giving details on the LUT grid optimization.
- Section 7 is an appendix giving details about the SVC gains specifically generated for OC-SAC.

### 1.3 APPLICABLE DOCUMENT

|        |                                                                                                                                                                                         |
|--------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| [AD-1] | OC-SAC Requirement Baseline Document. EUMETSAT deliverable ref. EUM/21/SAC/RB                                                                                                           |
| [AD-2] | OC-SAC Product Validation Report. EUMETSAT deliverable ref. EUM/21/SAC/PVP, version 4.1.                                                                                                |
| [AD-3] | OC-SAC Detailed Processing Model. EUMETSAT deliverable ref. EUM/21/SAC/DMP, version 1.0                                                                                                 |
| [AD-4] | SACSO Algorithm Theoretical Baseline Document. EUMETSAT deliverable ref. EUM/19/SACSO/ATBD, available from: <a href="https://www.eumetsat.int/SACSO">https://www.eumetsat.int/SACSO</a> |

|        |                                                                                                                                                                                                                                   |
|--------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| [AD-5] | Sentinel-3 OLCI Marine User Handbook. EUMETSAT, available from:<br><a href="https://www.eumetsat.int/media/45743">https://www.eumetsat.int/media/45743</a>                                                                        |
| [AD-6] | OC-BPC (Ocean Colour Bright Pixel Correction) Algorithm Theoretical Baseline Document. EUMETSAT deliverable ref. EUM/18/BPC/ATBD, available from<br><a href="https://www.eumetsat.int/OC-BPC">https://www.eumetsat.int/OC-BPC</a> |

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## 1.5 ACRONYMS AND ABBREVIATIONS

|            |                                                                         |
|------------|-------------------------------------------------------------------------|
| 3MI        | Multi-viewing, Multi-channel, Multi-polarisation Imager                 |
| AC         | Atmospheric Correction                                                  |
| AD         | Applicable Document                                                     |
| ADF        | Auxiliary Data File                                                     |
| AERONET    | AERosol RObotic NETwork                                                 |
| AERONET-OC | Ocean Color component of the Aerosol Robotic Network                    |
| AOD        | Aerosol Optical Depth (similar to AOT)                                  |
| AOT        | Aerosol Optical Thickness                                               |
| APF        | Aerosol Phase Function                                                  |
| ATBD       | Algorithm Theoretical Basis Document                                    |
| BOUSSOLE   | Buoy for the acquisition of a long-term optical series                  |
| BOA        | Bottom of atmosphere                                                    |
| BPC        | Bright Pixel Correction                                                 |
| BRDF       | Bidirectional Reflectance Distribution Function                         |
| Cal/Val    | Calibration and Validation                                              |
| CALIPSO    | Cloud-Aerosol Lidar and Infrared Pathfinder Satellite Observation       |
| CMEMS      | Copernicus Marine Environment Monitoring Service                        |
| CV         | Coefficient of Variation                                                |
| CWAC       | Clear Water Atmospheric Correction                                      |
| C2RCC      | Case-2 Regional CoastColour                                             |
| DPM        | Detail Processing Model                                                 |
| EPS-SG     | EUMETSAT Polar System Second Generation                                 |
| EUMETSAT   | European Organisation for the Exploitation of Meteorological Satellites |
| FCI        | Flexible Combined Imager                                                |
| FR         | Full Resolution (OLCI)                                                  |
| G-SOW      | Generic Statement of Work                                               |
| IOCCG      | International Ocean Color Coordinating Group                            |
| IODD       | Input Output Data Definition Document                                   |
| IP         | Implementation Plan                                                     |
| IPF        | Instrument Processing Facility                                          |
| L1B        | Level 1 B                                                               |
| L2         | Level 2                                                                 |
| l2gen      | L2 generation Ocean Colour processor                                    |

|         |                                                    |
|---------|----------------------------------------------------|
| LUT     | Look-up table                                      |
| MDB     | EUMETSAT Match-up DataBase                         |
| MERIS   | Medium Resolution Imaging Spectrometer             |
| MOBY    | Marine Optical Buoy                                |
| MODIS   | Moderate Resolution Imaging Spectroradiometer      |
| MSE     | Multiple Scattering Epsilon                        |
| MSG     | Meteosat Second Generation                         |
| MTG     | Meteosat Third Generation                          |
| NIR     | Near Infrared                                      |
| OC      | Ocean Colour                                       |
| OC-AAC  | Alternative (Deterministic) Atmospheric Correction |
| OC-BPC  | Ocean Colour Bright Pixel Correction               |
| OC-CCI  | Ocean Colour Climate Change Initiative (ESA)       |
| OC-DB   | Copernicus Ocean Colour In-situ Data Base          |
| OCR     | Ocean Colour Radiometry                            |
| OC-SAC  | Ocean Colour Standard Atmospheric Correction       |
| OC-SVC  | Ocean Colour System Vicarious Calibration          |
| OC-VCAL | Ocean Colour Vicarious Calibration                 |
| OLCI    | Ocean and Land Colour Instrument                   |
| OMAPS   | Multi-mission Ocean Colour Prototyping algorithm   |
| PACE    | Plankton, Aerosol, Cloud and ocean Ecosystem       |
| PM      | Progress meeting                                   |
| PMP     | Project Management Plan                            |
| POLYMER | Polynomial based algorithm applied to MERIS        |
| PVP     | Product Validation Plan                            |
| PVR     | Product Validation and evolution Report            |
| QA4EO   | Quality Assurance framework for Earth Observation  |
| RB      | Requirement Baseline Document                      |
| RD      | Reference Document                                 |
| RH      | Relative Humidity                                  |
| ROI     | Region Of Interest                                 |
| RR      | Reduced Resolution (OLCI)                          |
| RSP     | Remote Sensing and Products Division of EUMETSAT   |
| RTC     | Radiative Transfer Code                            |
| RTE     | Radiative Transfer Equation                        |

|          |                                                                    |
|----------|--------------------------------------------------------------------|
| RTM      | Radiative Transfer Model                                           |
| S3       | Sentinel-3                                                         |
| SACSO    | Spectral matching Atmospheric Correction for Sentinel Ocean colour |
| SeaWiFS  | Sea-viewing Wide Field-of-view Sensor                              |
| SNR      | Signal-to-Noise Ratio                                              |
| SoW      | Statement of Work                                                  |
| SPG      | South Pacific Gyre                                                 |
| SRF      | Spectral Response Function                                         |
| SSA      | Single Scattering Albedo                                           |
| SSE      | Single Scattering Epsilon                                          |
| SVC      | System Vicarious Calibration                                       |
| SVC-TOOL | OC-SVC software tool                                               |
| SWIR     | Short-wave Infrared                                                |
| S3VT     | Sentinel-3 Validation Team                                         |
| TBC      | To be confirmed                                                    |
| TOA      | Top of Atmosphere                                                  |
| VIIRS    | Visible Infrared Imaging Radiometer Suite                          |
| VIS      | VISible domain of the solar spectrum                               |
| WBS      | Work Breakdown Structure                                           |
| WM       | Working Meeting                                                    |
| WP       | Work Package                                                       |

## 1.6 NOTATIONS

The list of symbols is given below. Interpolation of a quantity  $y$  in a LUT  $y_{LUT}$  with respect to dimensions  $x_1 \dots x_n$  is simply noted:

$$y = y_{LUT}(x_1, \dots, x_n)$$

| Symbol    | Definition | Dimension/Unit                                          |
|-----------|------------|---------------------------------------------------------|
| $\lambda$ | Wavelength | nm (if not specified),<br>or $\mu\text{m}$ specifically |

| Symbol              | Definition                                                       | Dimension/Unit |
|---------------------|------------------------------------------------------------------|----------------|
| $\lambda_0$         | Reference wavelength in spectral models (865 nm for CWAC)        | nm             |
| $a_{cdm}(\lambda)$  | Dissolved and detrital materials absorption coefficient          | $m^{-1}$       |
| $a_p(\lambda)$      | Particulate absorption coefficient                               | $m^{-1}$       |
| $a_{ph}(\lambda)$   | Chlorophyll absorption coefficient                               | $m^{-1}$       |
| $a_p^*(\lambda)$    | Specific absorption coefficient                                  | $m^2/g$        |
| $a_{ph}^*(\lambda)$ | Specific chlorophyll absorption                                  | $m^2/mg$       |
| $b_{bp}(\lambda)$   | Particulate backscattering coefficient                           | $m^{-1}$       |
| $b_{bp}^*(\lambda)$ | Specific particulate backscattering                              | $m^2/g$        |
| $c_i, c_{i,j}$      | Coefficients for tabulating $\rho_a$ reflectance                 | dimensionless  |
| $\tilde{\beta}_p$   | Particulate phase function                                       | $sr^{-1}$      |
| $chl$               | Chlorophyll concentration                                        | $mg/m^3$       |
| $C_\rho$            | Variance-covariance matrix of any reflectance $\rho$             |                |
| $\varepsilon$       | Spectral variation of aerosol reflectance                        | dimensionless  |
| $F'$                | BRDF factor relating reflectance to single backscattering albedo | dimensionless  |
| $M$                 | Air mass fraction                                                | dimensionless  |
| $\eta_b$            | Ratio of pure water to total backscattering                      | dimensionless  |
| $\omega_b$          | Single backscattering albedo                                     | dimensionless  |
| $R_{rs}$            | Remote-sensing reflectance                                       | $sr^{-1}$      |

| Symbol                  | Definition                                                                                                           | Dimension/Unit              |
|-------------------------|----------------------------------------------------------------------------------------------------------------------|-----------------------------|
| $S_a$                   | Spectral slope of particulate absorption                                                                             | $\text{nm}^{-1}$            |
| $S_b$                   | Spectral slope of particulate backscattering                                                                         | dimensionless               |
| TSM                     | Total suspended matter                                                                                               | $\text{g/m}^3$              |
| $t_{atm}(\lambda)$      | Total transmittance (diffuse + direct) accounting for Rayleigh and aerosol, in downward + upward direction           | dimensionless               |
| $t_{down}(\lambda)$     | Total downward transmittance                                                                                         | dimensionless               |
| $t_{up}(\lambda)$       | Total upward transmittance                                                                                           | dimensionless               |
| $\mathbf{x}_a$          | Vector of atmospheric unknowns of the OC-BPC                                                                         | <i>cf.</i> explicit unknown |
| $\mathbf{x}_w$          | Vector of marine unknowns of the OC-BPC                                                                              | <i>cf.</i> explicit unknown |
| $\rho_a(\lambda)$       | Aerosol reflectance including multiple-scattering                                                                    | dimensionless               |
| $\rho_{gc}(\lambda)$    | TOA reflectance corrected for gaseous absorption, white-caps and sun glint                                           | dimensionless               |
| $\rho_{path}$           | Path reflectance (Rayleigh + aerosol)                                                                                | dimensionless               |
| $\rho_R(\lambda)$       | Rayleigh reflectance                                                                                                 | dimensionless               |
| $\rho_{Rc}(\lambda)$    | Rayleigh corrected reflectance, i.e. $\rho_{gc} - \rho_R$                                                            | dimensionless               |
| $\rho_w$                | Marine reflectance                                                                                                   | Dimensionless               |
| $\rho_{wN}$             | Fully-normalized marine reflectance                                                                                  | dimensionless               |
| $\rho_{wC2}$            | Marine reflectance in the NIR retrieved by BPC                                                                       | dimensionless               |
| $\rho_w^{mod}(\lambda)$ | Modelled marine reflectance                                                                                          | dimensionless               |
| $\boldsymbol{\rho}$     | Spectral vector of any reflectance $\rho$ e.g. $\boldsymbol{\rho}_R = (\rho_R(\lambda_1), \dots, \rho_R(\lambda_1))$ | dimensionless               |

| Symbol          | Definition                                                                             | Dimension/Unit |
|-----------------|----------------------------------------------------------------------------------------|----------------|
| $\alpha$        | Angstrom coefficient                                                                   | dimensionless  |
| $\tau_a$        | Aerosol optical thickness                                                              | dimensionless  |
| $\tau_R$        | Rayleigh optical thickness                                                             | dimensionless  |
| $m_r, m_i$      | Real and imaginary parts of the aerosol index of refraction                            | dimensionless  |
| $\nu$           | Junge aerosol size distribution parameter                                              | dimensionless  |
| $\theta_s$      | Sun zenith angle                                                                       | degree         |
| $\theta_v$      | View zenith angle                                                                      | degree         |
| $\Delta\varphi$ | Relative azimuth angle                                                                 | degree         |
| $\mu_s$         | Cosine of sun zenith angle                                                             | dimensionless  |
| $\mu_v$         | Cosine of view zenith angle                                                            | dimensionless  |
| $\Omega$        | Shorthand for $(\theta_s, \theta_v, \Delta\varphi)$ or $(\mu_s, \mu_v, \Delta\varphi)$ | As angles      |
| $\chi^2$        | Cost-function metrics in optimization problem                                          | dimensionless  |
| $z_a$           | Aerosol height                                                                         | km             |

## 2 PRODUCT OVERVIEW

### 2.1 PRODUCT DESCRIPTION

The main Level-2 product of the OC-SAC at pixel level is the directional marine reflectance (sometimes referred to as water-leaving reflectance, [AD-5]),  $\rho_w(\lambda)$ , provided at all spectral bands  $\lambda$  outside the strong gaseous absorption channels. This reflectance is not normalised for the bidirectional reflectance distribution function (BRDF), i.e. it is given in the viewing and illumination conditions of each pixel.

As detailed hereafter, marine reflectance comes from the correction of the satellite top-of-atmosphere (TOA) measurement for gaseous absorption, surface effects (white-caps, sun glint) and atmospheric path reflectance (Rayleigh and aerosols). This latter step combines the Bright Pixel Correction (BPC) to deal with sediment-loaded waters [AD-6] and the Clear Water Atmospheric Correction (CWAC) to detect the amount and type of aerosols in the Near-infrared (NIR). From this process, OC-SAC provides also two other Level-2 by-products related to the aerosol identification [AD-5]: aerosol optical thickness (AOT) at 865 nm,  $\tau_a(865)$ , and aerosol Ångström exponent,  $\alpha$ , computed between 779 and 865 nm.

Finally, OC-SAC produces Level-2 quality and science flags, MEGLINT, HIGHGLINT, WHITECAPS, ICE\_HIGHAERO, HIINLD, BPAC\_ON, CASE2\_S, WHITE\_SCATT, AC\_FAIL and annotations flags RWNEG\_O01 to RWNEG\_O21, ANNOT\_ABSOA, ANNOT\_TAU and ANNOT\_MIXR1, further described in section 4.3.2.16. Note that two other flags, LOWRW and HIGHRW, also depend on the output of the OC-SAC module but are not computed inside the module.

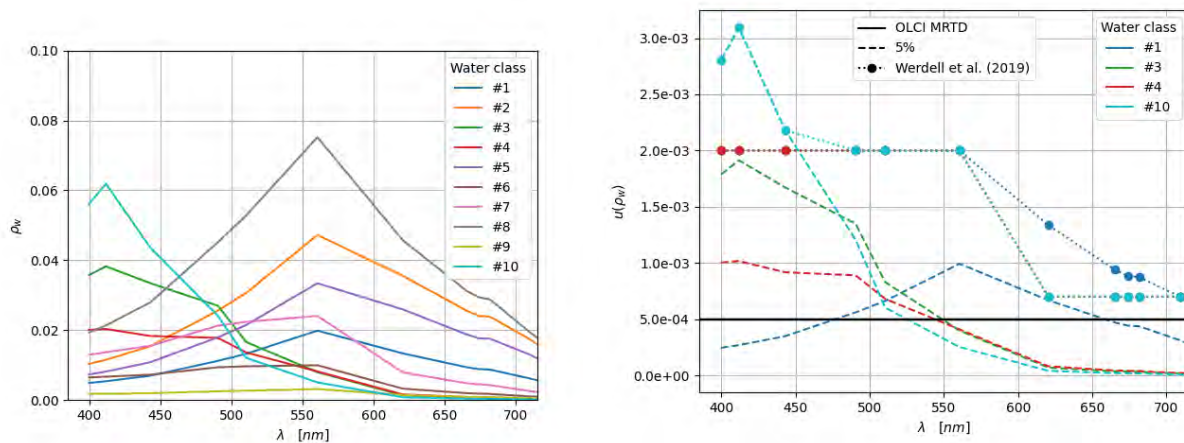
### 2.2 PRODUCT REQUIREMENTS

The historical requirement introduced in the 90's was to retrieve marine reflectance within 5% uncertainty in the blue-green bands, for clear waters (Hooker et al. 1992, Gordon 1997). This corresponds to an absolute uncertainty of  $1 \times 10^{-3}$  for a marine signal of amplitude 0.002, i.e. dominated by Chlorophyll absorption. This target of 5% has been widely used by the ocean colour community (IOCCG 2010, IOCCG 2012) and is a formal requirement of GCOS in the context of climate data records (GCOS, 2016). Antoine and Morel (1999) have rigorously justified absolute requirements to discriminate 30 classes of chlorophyll between 0.03 and 30 mg/m<sup>3</sup> in Case-1 waters with a band-ratio algorithm. They came to requirement of  $1 \times 10^{-3}$  at 443 nm and  $5 \times 10^{-4}$  at 490 nm, the more stringent value being due to small or high chlorophyll concentration (either below 0.3 mg/m<sup>3</sup> or above 3 mg/m<sup>3</sup>). It is important to highlight that these requirements were defined in very specific and ideal conditions, and thus shall be understood as target in similar conditions:

- i. Clear waters over the open ocean, whose optical characteristics can be parameterised by chlorophyll only (Case-1 water);
- ii. No contamination from the bottom, by clouds or surrounding coast (adjacency effects) or sun glint;
- iii. Atmosphere with only weakly absorbing aerosol (Gordon, 1997).

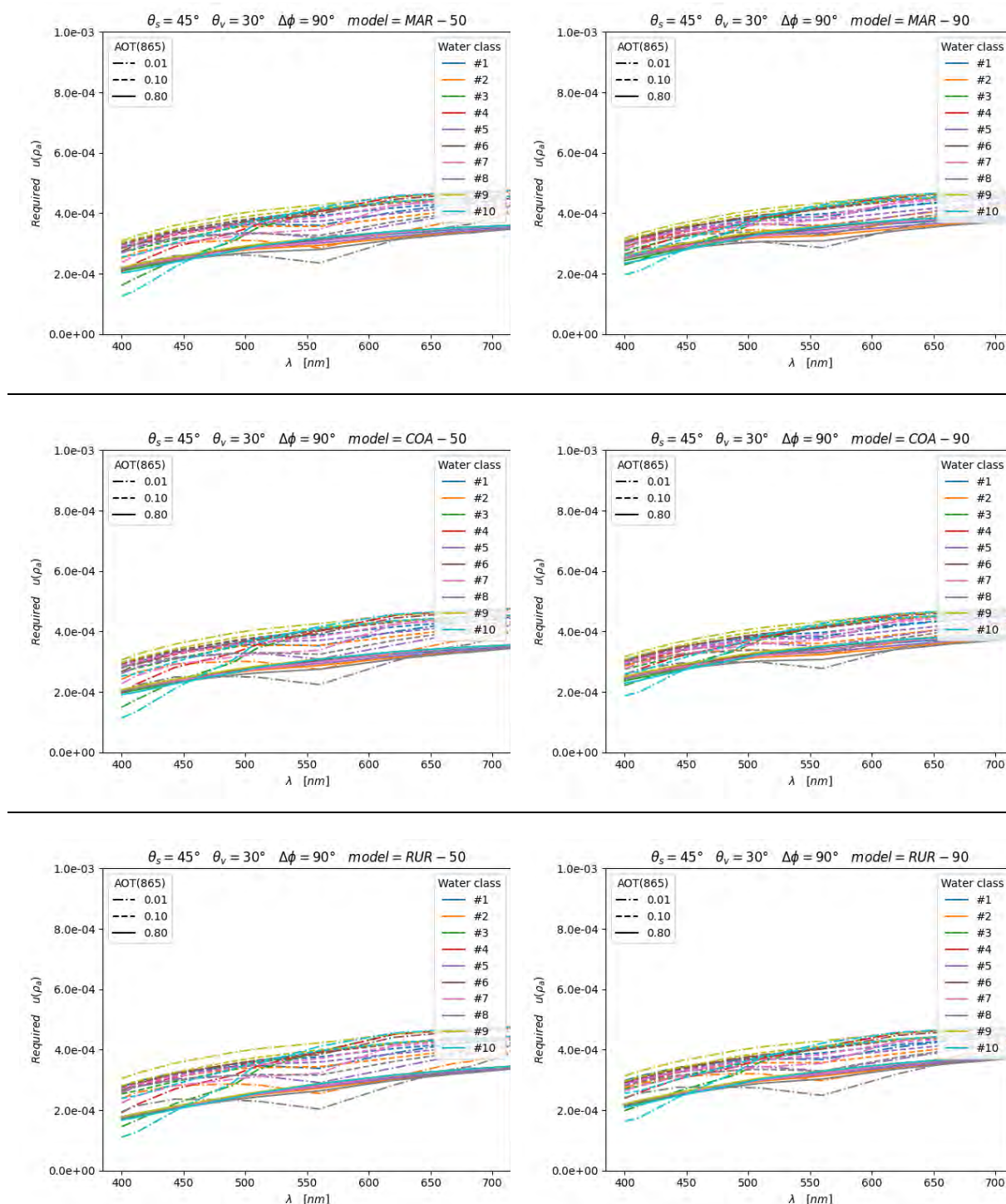
The absolute uncertainty of  $5 \times 10^{-4}$  introduced by Antoine and Morel (1999) in these very specific conditions and at 490 nm has become a global mission requirement for OLCI (Sentinel-3 Mission Requirements Traceability Document, MRTD, Donlon, 2011), without, however, any justification for other wavelengths or more complex waters. More recently, Werdell et al. (2019) have defined

requirements for PACE in a more subtle way, handling both absolute and relative uncertainties. The applicable uncertainties are defined as the maximum of  $2 \times 10^{-3}$  (absolute) and 5% (relative) between 400 and 600 nm, and the maximum of  $7 \times 10^{-4}$  (absolute) and 10% (relative) from 600 to 710 nm. Note that this is still limited to most of the deep ocean (depth  $\geq 1000$  m). This yields relaxed values compared to OLCI mission requirements, probably more achievable for non-oligotrophic waters. For instance, for a marine reflectance of about 0.02 in the blue, the 5% target would imply an absolute uncertainty of  $1 \times 10^{-3}$ , while Werdell et al. (2019) allow twice this value (i.e. 10% in relative unit). This is summarised in Figure 1, right.



**Figure 1 Left: Marine reflectance spectra,  $\rho_w$ , representative of 10 water classes (SACSO project). Right: required absolute uncertainty,  $u(\rho_w)$ , for 4 representative Case-1 spectra (#1, #3, #4 and #10) from different sources: as defined in OLCI MRTD (solid black line), from standard relative 5% (dashed lines) and following Werdell et al. (2019) (dotted lines).**

The uncertainty analysis conducted in [AD-1] has shown that the historical goal of 5% over very clear waters in the blue is achievable with an uncertainty on retrieved aerosol reflectance of about  $10^{-3}$  (and less in the green bands). However, it would need an uncertainty twice smaller for more mesotrophic waters (water classes #4) and seems unattainable for the most complex water (e.g. water classes #6, #9). This conclusion is problematic for OC-SAC because, by definition, the algorithm is not supposed to depend on any water modelling in the visible bands. In fact, the requirement of OCR expressed in relative uncertainty does not seem to be justified beyond the clear water case. It is thus advocated in this study to keep a target in absolute reflectance, and take here the very conservative value of  $5 \times 10^{-4}$  (Donlon, 2011). Considering the most stringent water and atmospheric cases, this objective requires an accuracy of aerosol reflectance,  $\rho_a$ , of  $2 \times 10^{-4}$  in the blue,  $3 \times 10^{-4}$  in the green and around  $3.5 \times 10^{-4}$  in the red bands (Figure 2). This constitutes the baseline requirement for OC-SAC aerosol retrieval, and has been used as an objective criterion in the optimisation of aerosol Look-up tables (see Appendix 1: LUT grid optimisation).



**Figure 2: Required absolute uncertainty on aerosol reflectance,  $u(\rho_a)$ , as a function of wavelength, to get a targeted absolute uncertainty of  $5 \cdot 10^{-4}$  on  $\rho_w$ . Colours refer to water classes (see Figure 1). Line types refer to three AOTs at 865 nm (0.01, 0.1 and 0.8, see top left legend). Aerosol models varies from top to bottom (maritime, coastal, rural) for two relative humidity values (left 50%, right 90%). From [AD-1].**

## 2.3 SCIENTIFIC STATE-OF-THE-ART

We refer to [AD-1] for an extended critical review of the various OC-SAC components and their modelling assumptions. Here we reproduce only material relevant to the CWAC algorithm (not its underlying physical models), which is the core of the new OC-SAC module.

### 2.3.1 STANDARD AEROSOL MODELS DETECTION

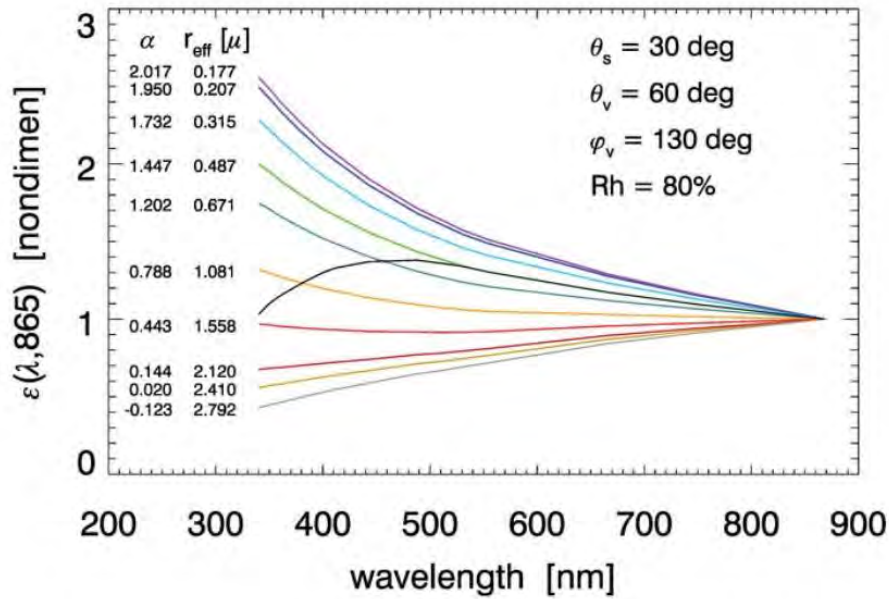
Given a set of candidate aerosol models (weakly absorbing) tabulated for a representative range of geometry and optical thickness, the purpose of CWAC is to select which model (or mixture of models) correspond to the actual acquisition, at pixel level. Various schemes have been proposed and three of them of major importance in the present development are summarised below (note that [AD-1] reviews seven published methods). The important characteristics of these various schemes are:

- i. The representation of the aerosol reflectance (including multiple scattering), generally given by a polynomial fit versus AOT or versus the reflectance at another band;
- ii. The continuity and non-ambiguity between models in a generally 2-dimensional domain (see Figure 3, Figure 4, Figure 5);
- iii. And the mixing between two models in this space, and its spectral dependence (generally neglected).

Gordon and Wang (1994) have proposed to detect the models through the so-called single scattering epsilon (SSE), defined between two bands by the ratio of single scattering aerosol reflectance,  $\rho_{as}$ :

$$\varepsilon(\lambda_1, \lambda_2) = \frac{\rho_{as}(\lambda_1)}{\rho_{as}(\lambda_2)} \quad (SSE) \quad (1)$$

The idea is that SSE characterises unambiguously the aerosol inherent properties, for standard (weakly absorbing) models (see Figure 3, coloured curves). Knowledge of the actual  $\varepsilon(\lambda_s, \lambda_l)$  given by two NIR bands  $\lambda_s < \lambda_l$  allows identification of two bracketing models in the SSE domain. This approach requires the link between the single scattering reflectance and the multiple scattering reflectance, this latter only referring to the real physics and observation; this link is tabulated through polynomial relationships, in both directions ( $MSE \leftrightarrow SSE$ ), for all aerosol models. It follows that the method cannot compute directly the  $\varepsilon(\lambda_s, \lambda_l)$  from the radiometry: the input  $\rho_a$  at  $\lambda_s$  and  $\lambda_l$  is first converted to  $\rho_{as}$  for each model, then SSE is computed also for each model, and finally the actual SSE is approximated by averaging SSEs of all existing models. Another major assumption, part of the aerosol correction, is that the interpolation coefficient (or mixing ratio) between the multiple scattering aerosol reflectance of the bracketing models can be computed directly on the SSE in the NIR, and kept fixed for all wavelengths in the VIS.

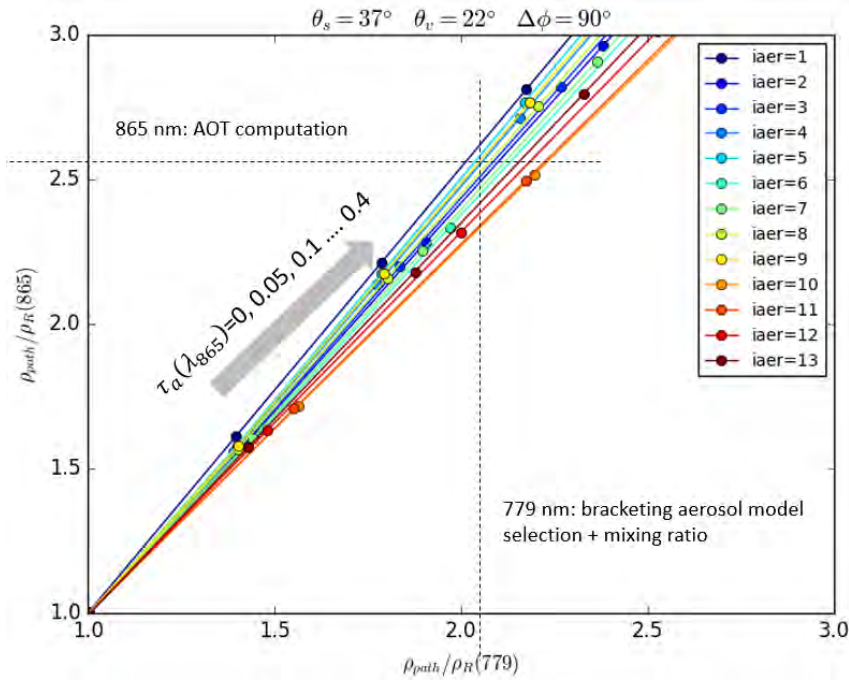


**Figure 3: Single-scattering epsilon (SSE) as a function of wavelength for various standard aerosol models (coloured curves, see legend for Angstrom and effective radius) and for a blue-absorbing aerosol (black curve). Reproduced from Mobley et al. (2016).**

Antoine and Morel (1999) have proposed an algorithm for MERIS which is still the baseline of current OLCI processing. Contrary to Gordon and Wang (1994), the aerosol detection is made directly in the multiple scattering domain, but through the total path reflectance scaled by Rayleigh,  $\xi$ :

$$\xi(\lambda) = \frac{\rho_{\text{path}}(\lambda)}{\rho_R(\lambda)} = \frac{\rho_R(\lambda) + \rho_a(\lambda)}{\rho_R(\lambda)} \quad (2)$$

This ratio, tabulated as a function of  $\tau_a$  for all aerosol models, expresses the relative change in the path reflectance brought by addition of aerosol within an atmosphere initially free from aerosols. The aerosol mixing is also computed in the NIR, on  $\xi(\lambda_s)$ , and is applied indifferently to  $\rho_a(\lambda)$  at all other wavelengths. Although supposed to be robust to pressure variation, this formalism may induce ambiguity between the models and be too sensitive to noise (Figure 4), hence may explain spatial discontinuity in the OLCI aerosol products and marine reflectance.



**Figure 4: Aerosol detection of current OLCI OC-SAC. Curves represent the  $\rho_{path}/\rho_R$  ratio for the 13 standard models (colours) parameterized as a function of growing optical thickness at 865 nm (y-axis, used for AOT computation) and 779 nm (x-axis, used for model and mixing identification).**

More recently, Ibrahim et al. (2019) have brought a significant extension to Gordon and Wang (1994) by using more bands in the NIR-SWIR (Multiband Atmospheric Correction, MBAC). The method starts from a first attempt of Ahmad and Franz (2018) to also identify aerosols directly in the multiple scattering domain (Figure 5). The multiple scattering epsilon (MSE) is simply defined by:

$$\varepsilon(\lambda_1, \lambda_2) = \frac{\rho_a(\lambda_1)}{\rho_a(\lambda_2)} (MSE) \quad (3)$$

Schematically, the MBAC minimizes a  $\chi^2$  metric defined as the weighted sum, over all available NIR-SWIR bands, of the difference between observed and modelled aerosol reflectance. The optical thickness is however directly retrieved at 869 nm, and not part of the inversion, what may not be optimal. The weights are defined in a very empirical way, according to the number of iterations of the Bailey et al. (2010) scheme: more iterations suggest more turbid waters and give higher weights to SWIR bands.

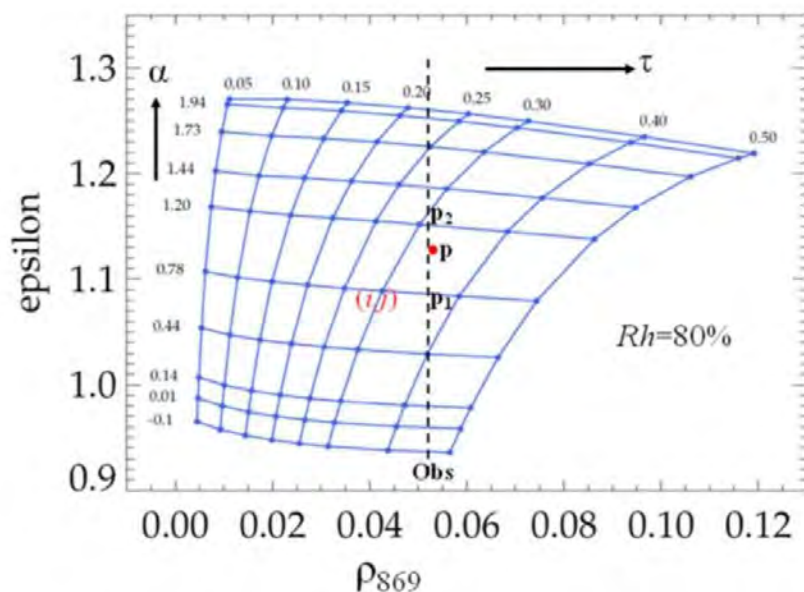


Figure 5: Aerosol detection based on multiple scattering epsilon (MSE), reproduced from Ahmad and Franz (2018). The blue grid shows variation of  $MSE = \rho_a(748)/\rho_a(869)$  as a function of  $\rho_a(869)$  for growing AOT (left to right) and growing Angstrom (bottom to top). Point p (red dot) represents the actual observation, falling between the bracketing models  $\alpha=0.78$  and  $\alpha=1.2$ .

### 2.3.2 STRONGLY ABSORBING AEROSOL MODELS DETECTION

Detection of strongly absorbing aerosols is a known issue of the CWAC, because they cannot be distinguished from other models in the NIR bands (see Figure 3, black curve). Various attempts, starting from Gordon et al. (1997), have consisted in using the full spectrum and a marine model, which is out of scope of the CWAC definition. One interesting trade-off was proposed in Antoine and Morel (1999) and further tested in Nobileau and Antoine (2005) through the use of only one band in the visible, 510 nm. For oceanic Case 1 waters, the marine reflectance is expected to be very stable at this band with respect to chlorophyll content (the hinge point, Clarke et al., 1970). When the reflectance at 510 nm retrieved from standard (weakly absorbing) aerosol diverges from a tabulated climatology, another pass is achieved with a new set of strongly absorbing models.

After spectral binning, OLCI provides radiometric measurement at 21 bands of mostly 10 nm width, whose nominal (theoretical) wavelengths are reported in Table 1. It is important to notice that these theoretical values do not correspond to the actual central wavelengths, which are detector dependent and require knowledge of the Spectral Response Function (SRF) of each detector at each channel; this is further discussed below. A single sensor SRF per band, averaged over all detectors after being shifted to the nominal centre, can be used to produce representative averaged central wavelengths, as given for OLCI-A in Table 3 of section 4.3.

**Table 1 OLCI nominal spectral bands and usage. From Donlon et al. (2012).**

| Band | Nominal wavelength [nm] | Width [nm] | Function                                                                                                   | Marine reflectance |
|------|-------------------------|------------|------------------------------------------------------------------------------------------------------------|--------------------|
| Oa01 | 400                     | 15         | Aerosol correction, improved water constituent retrieval                                                   | Yes                |
| Oa02 | 412.5                   | 10         | Yellow substance and detrital pigments (turbidity)                                                         | Yes                |
| Oa03 | 442.5                   | 10         | Chlorophyll absorption maximum, biogeochemistry, vegetation                                                | Yes                |
| Oa04 | 490                     | 10         | High Chlorophyll,                                                                                          | Yes                |
| Oa05 | 510                     | 10         | Chlorophyll, sediment, turbidity, red tide                                                                 | Yes                |
| Oa06 | 560                     | 10         | Chlorophyll reference (Chlorophyll minimum)                                                                | Yes                |
| Oa07 | 620                     | 10         | Sediment loading                                                                                           | Yes                |
| Oa08 | 665                     | 10         | Chlorophyll (2nd Chlorophyll absorption maximum), sediment, yellow substance/vegetation                    | Yes                |
| Oa09 | 673.75                  | 7.5        | For improved fluorescence retrieval and to better account for smile together with the bands 665 and 680 nm | Yes                |
| Oa10 | 681.25                  | 7.5        | Chlorophyll fluorescence peak, red edge                                                                    | Yes                |
| Oa11 | 708.75                  | 10         | Chlorophyll fluorescence baseline, red edge transition                                                     | Yes                |
| Oa12 | 753.75                  | 7.5        | O2 absorption/clouds, vegetation                                                                           | No                 |
| Oa13 | 761.25                  | 2.5        | O2 absorption band/aerosol correction.                                                                     | No                 |
| Oa14 | 764.375                 | 3.75       | Atmospheric correction                                                                                     | No                 |
| Oa15 | 767.5                   | 2.5        | O2A used for cloud top pressure, fluorescence over land                                                    | No                 |
| Oa16 | 778.75                  | 15         | Atmos. corr./aerosol corr.                                                                                 | Yes                |
| Oa17 | 865                     | 20         | Atmospheric correction/aerosol correction, clouds, pixel co-registration                                   | Yes                |
| Oa18 | 885                     | 10         | Water vapour absorption reference band. Common reference band with SLSTR instrument. Vegetation monitoring | Yes                |
| Oa19 | 900                     | 10         | Water vapour absorption/vegetation monitoring (maximum reflectance)                                        | No                 |
| Oa20 | 940                     | 20         | Water vapour absorption, Atmospheric correction/aerosol correction                                         | No                 |
| Oa21 | 1020                    | 40         | Atmospheric correction/aerosol correction                                                                  | Yes                |

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## 3.2 OLCI BENEFITS AND CAPABILITIES FOR OC-SAC

### 3.2.1 GEOMETRY FEATURES

OLCI cameras are tilted by about 12° westward from the nadir view in order to minimize the effect of Sun glint. However, OLCI images are still contaminated by glint, in camera 4 and 5 essentially. Hence, a glint correction is necessary, although it is not the focus of the present study.

A consequence of the tilt is that a significant part of OLCI swath is observed in backward mode (West side of the swath, backscattering angle approaching 180°), contrary for instance to what occurs for MERIS. The aerosol retrieval is then more sensitive to the size distributions of aerosol models tabulated in OC-SAC: large particles scatter less light in the backward direction and, if they are overrepresented in the algorithm, they tend to overestimate the aerosol optical thickness (vice-versa for small particles).

### 3.2.2 SPECTRAL CAPABILITIES

The purpose of OLCI measurements over water is to provide reflectance at the 16 bands outside the absorption channels between UV and SWIR, for various marine applications (Table 1). Hence atmosphere must be corrected at all these bands. However, the aerosol detection of OC-SAC is by definition limited to measurements in the NIR bands, to avoid perturbation from the water signal [AD-1]. OLCI has five bands in the NIR, outside absorption channels: 709, 754, 779, 865 and 885 nm. The current operational CWAC from Antoine and Morel (1999) uses only two bands (779 and 865 nm) and it is here advised to make the most from the five available NIR bands. Furthermore, OLCI benefits from the 1020 nm channel in the SWIR, which is already used by the OC-BPC to process very turbid waters [AD-6] and shall be used optionally in OC-SAC to extend the spectral range of aerosol detection.

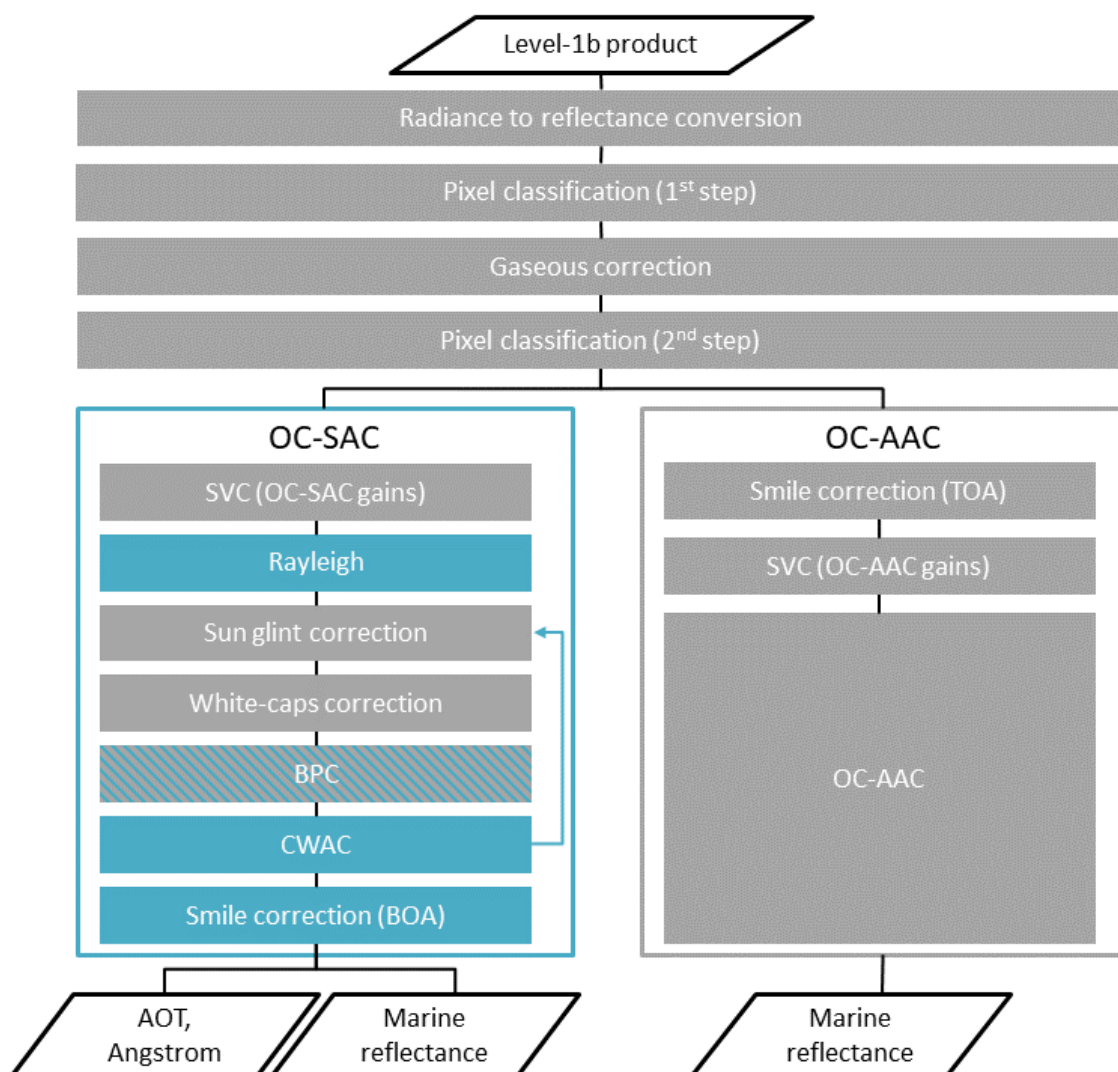
Last, three bands in the O<sub>2</sub>-A spectral region, 761, 764 and 767 nm, give further possibilities to detect the mean altitude of aerosols, especially in the case of strongly absorbing models (dust or biomass burning).

## 4 ALGORITHM DESCRIPTION

### 4.1 PROCESSING OUTLINE

#### 4.1.1 LEVEL-2 PROCESSOR OVERVIEW

An overview of the OLCI Level-2 processing chain is given in Figure 7. It corresponds essentially to the current operational processor (OLCI Collection 3), but with a clarified structure for the two aerosol corrections, OC-SAC and OC-AAC (neural network inversion), now totally parallel. As described hereafter, the new OC-SAC module uses the exact detector wavelengths, so that the TOA smile-correction becomes only relevant for the OC-AAC. The sole common precorrection between the two ACs is thus the gaseous correction.



**Figure 7. Overview of the OLCI Level-2 processing chain and OC-SAC components. In grey, processing steps without any change from Collection 3. In blue, new algorithms. In blue/grey, processing steps with small algorithmic updates.**

#### 4.1.2 OC-SAC OUTLINE

The OC-SAC components shown in Figure 7 are based on the definition introduced in the Requirement Baseline [AD-1]:

- The Clear Water Atmospheric Correction (CWAC) is defined as the method allowing detection and correction of aerosols, i.e.  $\rho_a(\lambda)$ , at pixel level, with minimum assumption on the water optical properties, i.e., essentially based in the NIR-SWIR spectral range under the black pixel assumption (clear waters). CWAC refers to the historical methods operationally used for decades by agencies, such as Gordon and Wang (1994) or Antoine and Morel (1999), and the present new algorithm.
- To be effective in all remote-sensing conditions, CWAC must be preceded by various corrections. The Bright Pixel Correction (BPC) removes the effect of residual marine signal in the NIR-SWIR, essentially due to sediment scattering. Sun glint and white-caps corrections, traditionally considered as independent pre-corrections of the AC, are more and more included in the AC process itself (e.g. Frouin et al., 2019); this is physically justified because the aerosol contribution in the direct and diffuse transmittance requires, strictly speaking, a coupling with the aerosol identification.
- OC-SAC is defined as the sequence of corrections comprising sun-glint correction, white-caps correction, BPC and CWAC. A possible coupling exists between these corrections because of aerosol transmittance (arrow in Figure 7 going back from CWAC to glint correction). Furthermore, System Vicarious Calibration (SVC) has to be applied with gains specific to this AC and is thus considered as part of OC-SAC too, with clear distinction with the other specific SVC gains for OC-AAC. Finally, a BOA smile correction has to be added at the end of the OC-SAC process, as discussed below.

The smile correction used up to Collection 3 was developed in the MERIS and OLCI processors to spectrally tune the TOA radiometry because the CWAC was only defined at instrument theoretical nominal bands. Smile correction is thus inherently linked to the inability of (current) CWAC to deal with the exact detector wavelengths. The correction uses a very simplistic linear interpolation of the Rayleigh corrected reflectance, without taking into account the real spectral variation of the target (e.g. water absorption) and, to our knowledge, has never been scientifically validated. As justified in [AD-1], it is more rigorous to conduct the processing as much as possible at the exact detector wavelengths, as proposed with the new CWAC. The impact on existing routines is minor:

- Sun glint and white-caps:
  - Need to compute at exact wavelength the transmittances (i.e. Rayleigh and aerosol optical thicknesses).
  - The Sun glint reflectance is supposed to be spectrally white (assumption of current operational processor), so no impact.
  - The white-caps reflectance at sea level has a spectral dependence (Frouin et al., 1996), however the variation with a few nm is neglected.
- BPC: in Collection 3, the BPC already starts from a non-smile corrected signal in the NIR bands and is supposed to handle the exact wavelength throughout the algorithm. This is in particular

achieved for the aerosol component, while the marine model is approximated at theoretical nominal bands, with the uncertainty expected to be lower than the uncertainty of the marine model itself.

Hence, the atmospheric correction inherently produces marine reflectance at the exact detector wavelengths. A spectral adjustment is required in order to provide users with data at nominal wavelengths. This is referred to as a new BOA smile correction.

The sun glint correction could be part of the CWAC, as the glint reflectance is additive with the path reflectance and its propagation to TOA depends on the amount of aerosol; however, for the sake of simplicity, it is kept in a usual separated step and the alternative options are discussed.

#### 4.1.3 CWAC OUTLINE

CWAC is the core component of the new OC-SAC module. It has been completely revised during the study, but it is still relying on tabulated radiative transfer simulations of a set of pre-determined aerosol models. Its main goal is to retrieve two bracketing aerosol models, their mixing ratio and the aerosol load (aerosol reflectance at 865 nm,  $\rho_{a0}$ ) from the observed radiometry in the NIR, and then propagate this information to the visible in order to correct the radiometry for the atmosphere and get the marine reflectance. It comprises schematically six main steps, starting from a family of standard aerosol models (Figure 8):

- Step 1: Computation of aerosol reflectance at 865 nm,  $\rho_{a0}$ , based on the observation at 865 nm or possibly more bands in the NIR, for all candidate models;
- Step 2: Aerosol identification, based on a spectral matching algorithm, to retrieve two aerosol models and their mixing that best match the observation;
- Step 3: Computation of AOT from  $\rho_{a0}$ , for the selected models;
- Step 4: Assessment of ALH thanks to OLCI O2-A bands, for the selected models;
- Step 5: Propagation of aerosol reflectance at all bands, computation of transmittance and atmospheric correction in the visible bands to get marine reflectance.
- Step 6: Detection of strongly absorbing aerosols in the visible band, based on climatological values of marine reflectance. If such situation occurs, then the five previous steps are run one more time in a 2<sup>nd</sup> pass, with a second family of predefined strongly absorbing models. The difference in the aerosol identification (step 2) is that bands in the VIS are used, with a weighing associated to the climatological uncertainty, so that AOT (step 3) and ALH (step 4) must be computed beforehand for all candidate models.

The algorithm stops either after the 1<sup>st</sup> pass with standard aerosols, or after the 2<sup>nd</sup> pass.

As described hereafter (section 4.3.1.11), the aerosol reflectance modelling relies strongly on tabulated polynomial coefficients, whose multilinear interpolation for a given pixel (geometry, ancillary data), given aerosol model, given ALH and given band is very costly. The implementation minimizes the number of these interpolations in the following way (Figure 8):

- In both the 1<sup>st</sup> and 2<sup>nd</sup> pass, considering that ALH does not impact the aerosol reflectance in the NIR bands (see section 4.3.2.9 hereafter), coefficients are computed in the NIR for a default ALH (0.2 km) and all candidate models;
- Then in the 1<sup>st</sup> pass, coefficients are recomputed at all bands with an updated ALH only for the two selected models.
- In the 2<sup>nd</sup> pass, which uses bands in the visible for aerosol identification, it is mandatory to first assess ALH. Hence coefficients are computed at all bands for all models, what is much costlier than for the 1<sup>st</sup> pass. However, coefficients of the two selected models are then ready for the atmospheric correction.

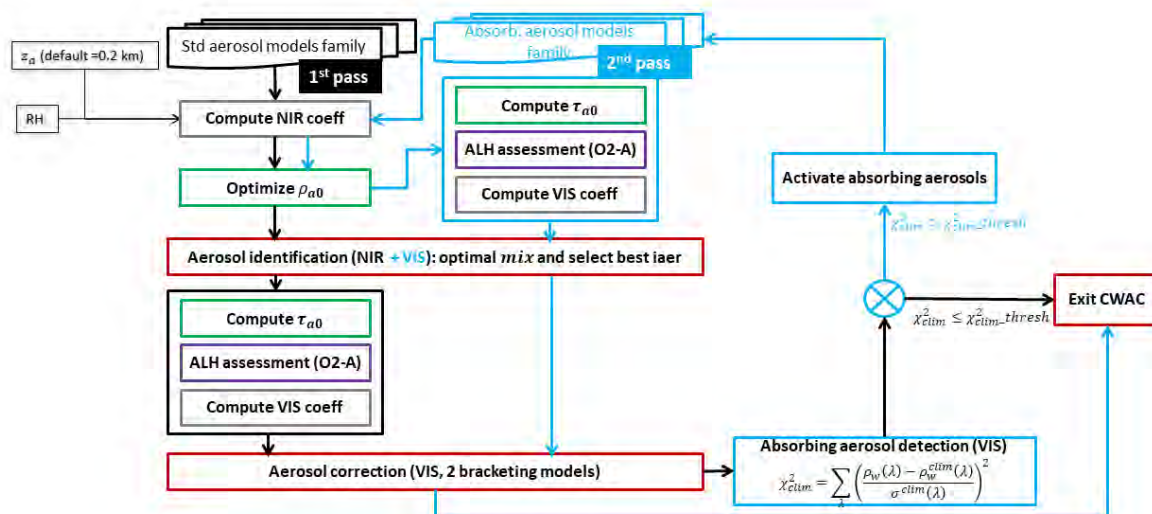


Figure 8. Detailed view of the CWAC module. Arrows in black refer to the 1<sup>st</sup> pass with standard aerosol models, and arrows in blue to the 2<sup>nd</sup> pass with strongly absorbing models.

## 4.2 ALGORITHM INPUT

Inputs of OC-SAC module are listed in Table 2.

**Table 2 OC-SAC algorithm inputs**

| Variable                                     | Description                                                                                  | Unit          | Range or reference   |
|----------------------------------------------|----------------------------------------------------------------------------------------------|---------------|----------------------|
| $\rho_{ng}(\lambda)$                         | TOA reflectance corrected for gaseous absorption                                             | <i>dl</i>     | All OLCI wavelengths |
| $C_{\rho_t}$                                 | Variance-covariance matrix of TOA radiometry $\rho_t$ (currently based on radiometric noise) | <i>dl</i>     | NIR bands            |
| $\lambda_1, \lambda_2, \dots, \lambda_{21},$ | Exact detector wavelengths (per pixel)                                                       | <i>nm</i>     | All OLCI wavelengths |
| $\theta_s$                                   | Sun zenith angle                                                                             | <i>degree</i> |                      |
| $\theta_v$                                   | View zenith angle                                                                            | <i>degree</i> |                      |
| $\mu_s$                                      | Cosine of Sun zenith angle                                                                   | <i>dl</i>     | [0, 1]               |
| $\mu_v$                                      | Cosine of view zenith angle                                                                  | <i>dl</i>     | [0, 1]               |
| $\Delta\varphi$                              | Relative azimuth angle                                                                       | <i>degree</i> | [0, 180°]            |
| $w_s$                                        | Wind speed modulus                                                                           | <i>m/s</i>    |                      |
| $p$                                          | Atmospheric pressure at sea level                                                            | <i>hPa</i>    |                      |
| RH                                           | Relative Humidity                                                                            | %             | [0, 100]             |
| <i>lat</i>                                   | latitude                                                                                     | <i>degree</i> | [-90°, 90°]          |
| <i>lon</i>                                   | longitude (towards East)                                                                     | <i>degree</i> | [-180°, 180°]        |
| <i>day</i>                                   | Day of acquisition in the year (from 0)                                                      | <i>int</i>    | [0, 365]             |

## 4.3 THEORETICAL DESCRIPTION

### 4.3.1 PHYSICAL DESCRIPTION

#### 4.3.1.1 SPECTRAL SAMPLING

Rayleigh wavelength dependency is accounted for implicitly through the optical depth, which is the input of the LUT (see sections 4.3.1.3 and 4.3.1.9).

For aerosols, the optical depth, the single scattering albedo and the phase function, used in the radiative transfer simulations to generate the LUT, are defined at each OLCI central bands (defined as the spectral integration over mean OLCI spectral response function), see Table 3. In the present version, only OLCI-A bands were considered for the simulations. As described in section 4.3.1.11, the final CWAC LUTs do not store directly the RT simulation at these specific band, but fitting coefficients with respect to wavelength, so that the aerosol formulation is a smooth function of wavelength and can account for both per-pixel spectral variation ( $\pm 1.5$  nm max) and differences between OLCI-A and OLCI-B.

**Table 3 Central wavelength of the inherent properties of aerosol used in the LUT generation.**

| Band              | Oa01      | Oa02      | Oa03      | Oa04      | Oa05      | Oa06      | Oa07      | Oa08       |
|-------------------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|------------|
| $\lambda$<br>[nm] | 400.30316 | 411.84534 | 442.96259 | 490.49301 | 510.46756 | 560.45026 | 620.40924 | 665.27441  |
| Band              | Oa09      | Oa10      | Oa11      | Oa12      | Oa16      | Oa17      | Oa18      | Oa21       |
| $\lambda$<br>[nm] | 674.02515 | 681.5705  | 709.11487 | 754.18134 | 779.25671 | 865.42969 | 884.30835 | 1015.79919 |

#### 4.3.1.2 GEOMETRICAL SAMPLING AND FUNCTIONAL RELATIONSHIPS

The variation of atmospheric scattering functions (reflectance, transmittance) with respect to geometry and possibly other dimensions (e.g. wind speed) and variables (e.g. optical thickness) has been investigated in details through an extended optimisation procedure. The goal is to identify the coarser grid that satisfies the radiometric requirements (section 2.2). The complexity resides in the multidimensional aspect of the physics (i.e. size of the LUTs storing the radiative transfer quantities), with constraints in terms of memory and CPU demand. For a given axis, a very high-resolution LUT is computed and serves as reference, while the other axes are restricted to only a few representative test values. An optimal tabulation is searchable on this axis. The process is then run successively on each axis. The tabulation can be of two types:

- Either a direct tabulation along the given axis, with an optimal grid;

- ii. Or a functional relationship with respect to the given variable, which means that the LUT stores only the fitting coefficients (typically polynomial coefficients); the fit can still be done on the high-resolution grid, not stored.

Angular and wind speed dimensions are stored in an optimal grid, while variation with respect to the aerosol load is stored through fitting coefficients (see section 4.3.1.11). More details about the optimization procedure are given in the Appendix 1: LUT grid optimisation. The grid actually selected is detailed in Table 4.

**Table 4 Grid of atmospheric LUTs ( $\rho_{a\_LUT}$ ,  $\rho_{R\_LUT}$ ,  $t_{down\_LUT}$ ,  $t_{up\_LUT}$ )**

| Axis            | Unit   | Size | Nodes                                                                                                                                                                                                                                                                |
|-----------------|--------|------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| $\mu_s$         | dl     | 24   | 0.07912548, 0.1175082, 0.1558909, 0.1942736, 0.2326563, 0.271039, 0.3094217, 0.3478044, 0.3861871, 0.4245698, 0.4629525, 0.5013351, 0.5397179, 0.5781006, 0.6164833, 0.654866, 0.6932487, 0.7316314, 0.770014, 0.8083968, 0.8467795, 0.8851622, 0.9235449, 0.9619276 |
| $\mu_v$         | dl     | 7    | 0.5264885, 0.5763318, 0.6510968, 0.8006267, 0.8753917, 0.9501567, 1                                                                                                                                                                                                  |
| $\Delta\varphi$ | degree | 16   | 0, 12, 24, 36, 48, 60, 72, 84, 96, 108, 120, 132, 144, 156, 168, 180                                                                                                                                                                                                 |
| $w_s$           | m/s    | 3    | 2, 7, 16                                                                                                                                                                                                                                                             |
| RH              | %      | 6    | 30, 50, 70, 75, 85, 95                                                                                                                                                                                                                                               |
| FMF             | dl     | 9    | 0, 0.04, 0.1, 0.2, 0.3, 0.4, 0.6, 0.8, 1                                                                                                                                                                                                                             |
| $z_a$           | km     | 3    | 0.2, 2, 5                                                                                                                                                                                                                                                            |
| $\tau_{a0}$     | dl     | 7    | 0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6                                                                                                                                                                                                                                      |

#### 4.3.1.3 RAYLEIGH OPTICAL THICKNESS AND PRESSURE

Rayleigh optical thickness (ROT) is computed at the wavelength, latitude and pressure of any pixel following Bodhaine et al. (1999). Hence, dependency on pressure is always handled through ROT, and there is no other dedicated pressure correction in the OC-SAC module.

As explained in section 4.3.1.9, the Rayleigh LUT comes from spherical shell radiative transfer simulations solved over a sampling of ROT, independently of the wavelength. The optical depth profile follows the US62 standard pressure profile.

#### 4.3.1.4 IOPS OF STANDARD AEROSOLS

Ahmad et al. (2010) have derived a set of aerosol models based on AERONET climatology, and these models are used in operation at NASA instead of the older modelling of Shettle and Fenn (1979). These aerosol models are simplified and consist of a mixture of a fine and a coarse mode, with a bi-modal log normal size distribution. The absorbing fine mode is composed of a mixture of soot, water soluble and dust aerosols while coarse size mode is optically spherical and minimally absorbing (consistent with sea salt). The size and real refractive index of both modes are defined by water uptake associated with eight relative humidity (RH) values between 30% and 95%. These eight fine mode aerosols are combined with the coarse mode at ten different fractions, for a total of eighty aerosol models. These fractions are expressed as the relative volume concentration of the fine mode to the total particle volume concentration, with values of 0%, 1%, 2%, 5%, 10%, 20%, 30%, 50%, 80% or 95%. Table 5 provides the size distribution as a function of RH.

The aerosol optical properties thus depend on the aerosol optical thickness  $\tau_a(\lambda_{\text{ref}})$  at one reference wavelength  $\lambda_{\text{ref}}$ , the fine-mode fraction in volume  $f_v$ , and RH. The Angström exponent and the Single Scattering Albedo  $\omega_o(\lambda)$  can be derived from the microphysics quantities.

Aerosol optical properties are integrated in OLCI spectral response functions. Due to its limit in spectral sampling, we do not use the refractive index as described in Ahmad et al. (2010). Instead, we use the refractive index from the Optical Properties of Aerosols and Clouds (OPAC) database (Hess et al., 1998) corresponding to the same material: water, soot, sea salt and mineral (called dust like in Ahmad et al., 2010). The OPAC refractive index extends over a larger spectral range covering the SRF of OLCI bands and it offers a better spectral resolution (Figure 9). Note however, that the spectral resolution is still limited and does not allow to capture the full variability at the scale of bands FWHM. The resulting extinction coefficients and single scattering albedo are shown in Figure 10 and Figure 11, for coarse and fine mode, respectively. The most significant difference in using the OPAC refractive index is for fine mode fraction = 1.0. The OPAC results in a more absorbing particle in the UV while being less absorbing after around 0.5 microns. All optical properties are computed using the MOPSMAP tool (Modeled optical properties of ensembles of aerosol particles, Gasteiger, 2018).

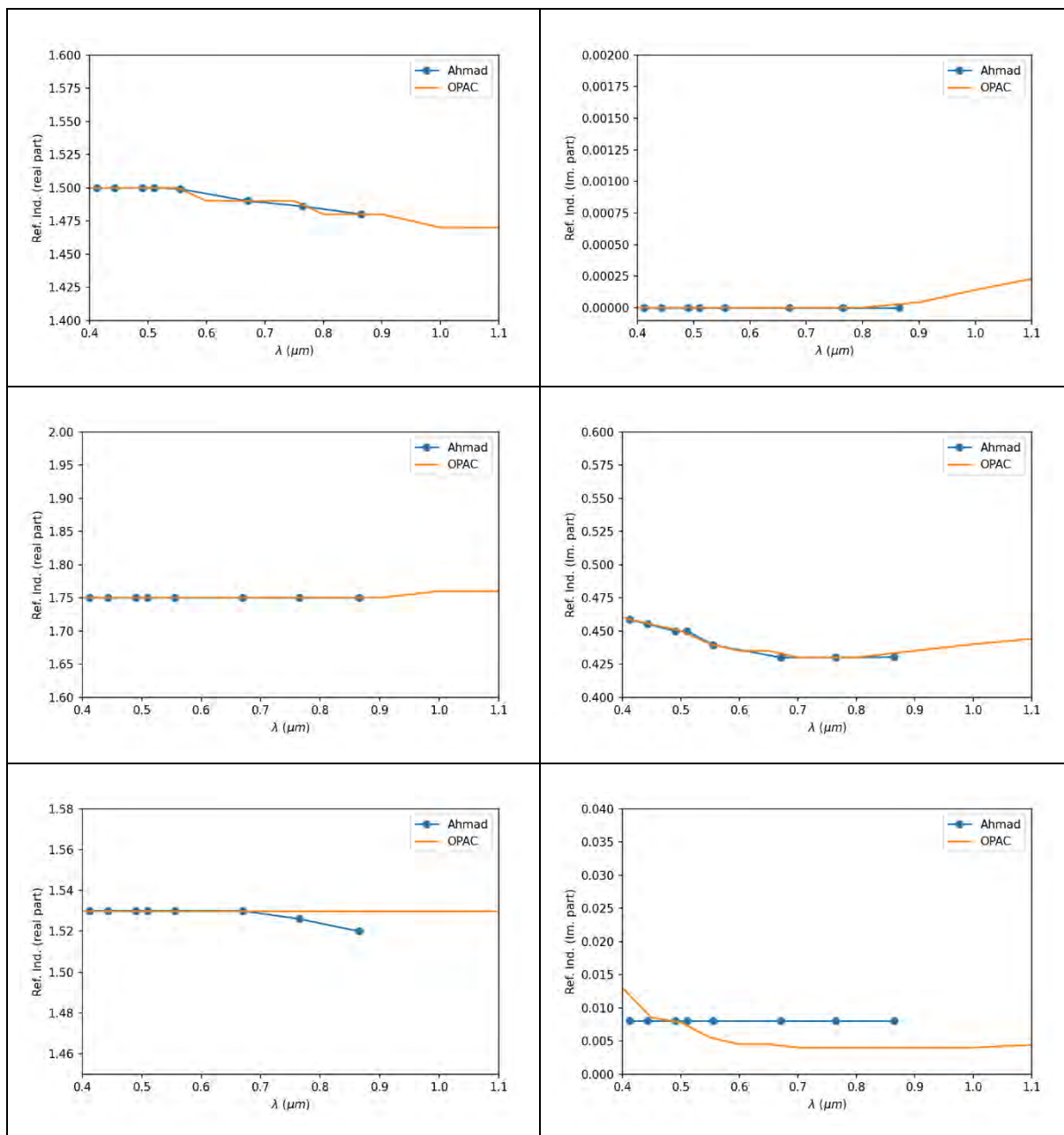
**Table 5. Size distribution of Ahmad et al. (2010) aerosol models with respect to RH.**

**Table 4. Modal Radii ( $r_{vf}, r_{vc}$ ), Standard Deviations ( $\sigma_f, \sigma_c$ ), and Ratios of Wet-to-Dry Aerosol Radius ( $r_{vf}/r_{ovf}, r_{vc}/r_{ovc}$ ) for Eight Values of Relative Humidity Used in This Study<sup>a</sup>**

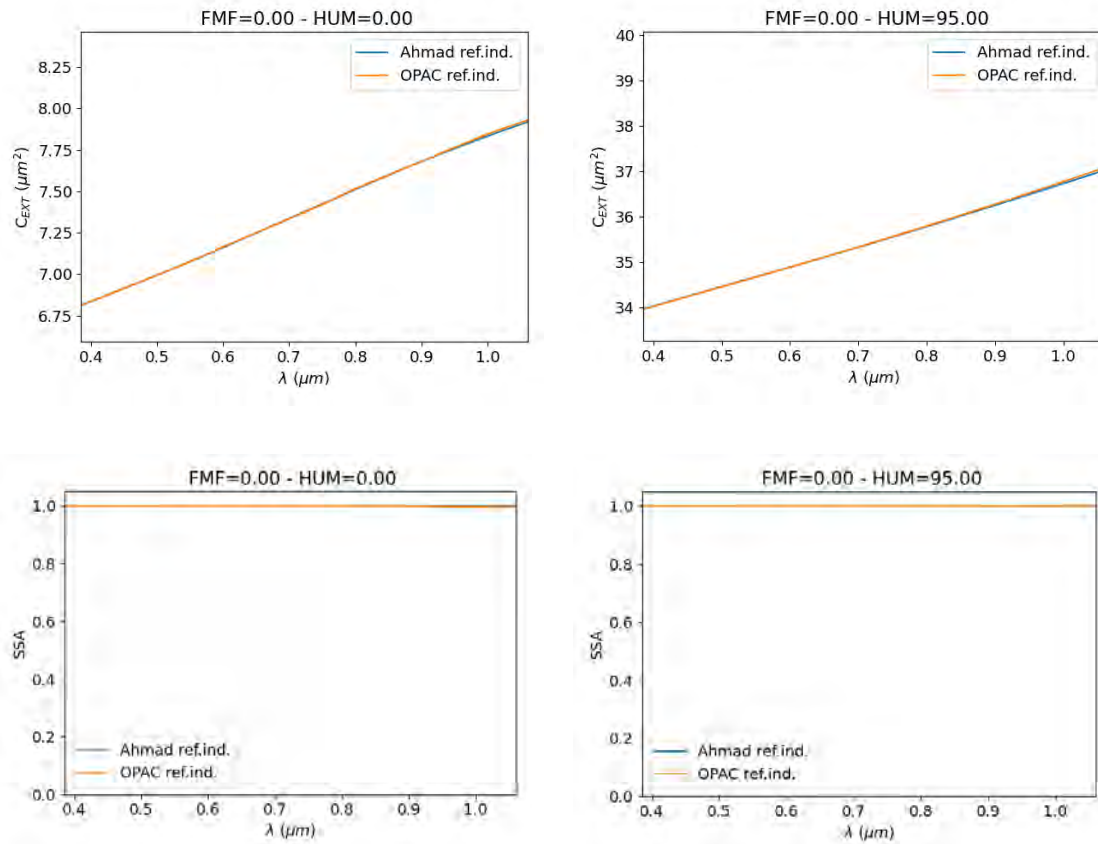
| $Rh$ | $r_{vf}$ | $\sigma_f$ | $r_{vc}$ | $\sigma_c$ | $r_{vf}/r_{ovf}$ | $r_{vc}/r_{ovc}$ |
|------|----------|------------|----------|------------|------------------|------------------|
| 0.30 | 0.150    | 0.437      | 2.441    | 0.672      | 1.006            | 1.009            |
| 0.50 | 0.152    | 0.437      | 2.477    | 0.672      | 1.019            | 1.024            |
| 0.70 | 0.158    | 0.437      | 2.927    | 0.672      | 1.063            | 1.210            |
| 0.75 | 0.167    | 0.437      | 3.481    | 0.672      | 1.118            | 1.439            |
| 0.80 | 0.187    | 0.437      | 3.966    | 0.672      | 1.255            | 1.639            |
| 0.85 | 0.204    | 0.437      | 4.243    | 0.672      | 1.371            | 1.753            |
| 0.90 | 0.221    | 0.437      | 4.638    | 0.672      | 1.486            | 1.917            |
| 0.95 | 0.246    | 0.437      | 5.549    | 0.672      | 1.648            | 2.293            |

<sup>a</sup>The subscripts  $v$ ,  $f$ , and  $c$ , respectively, refer to volume space, fine mode, and coarse mode of the aerosols

Contrary to OLCI aerosol models up to Collection 3, a key point of these new models is that they span continuously the multiple epsilon space, Eq (3), as shown on Figure 12. This justifies the core of the CWAC algorithm for aerosol detection and mixing, as detailed hereafter.



**Figure 9 Real (left) and imaginary (right) part of refractive indices of sea salt (top), soot (medium) and dust (bottom) from Ahmad et al. , 2010 (blue) and OPAC (orange).**



**Figure 10. Coarse mode optical properties (upper panel: extinction coefficient, lower panel: single scattering albedo) for two different relative humidity values (left panels humidity=0.0%, right panels humidity=95%). Results corresponding to two different refractive indices are shown: (i) the one of Ahmad et al., 2010 and (ii) the one of OPAC database (Hess et al., 1998)**

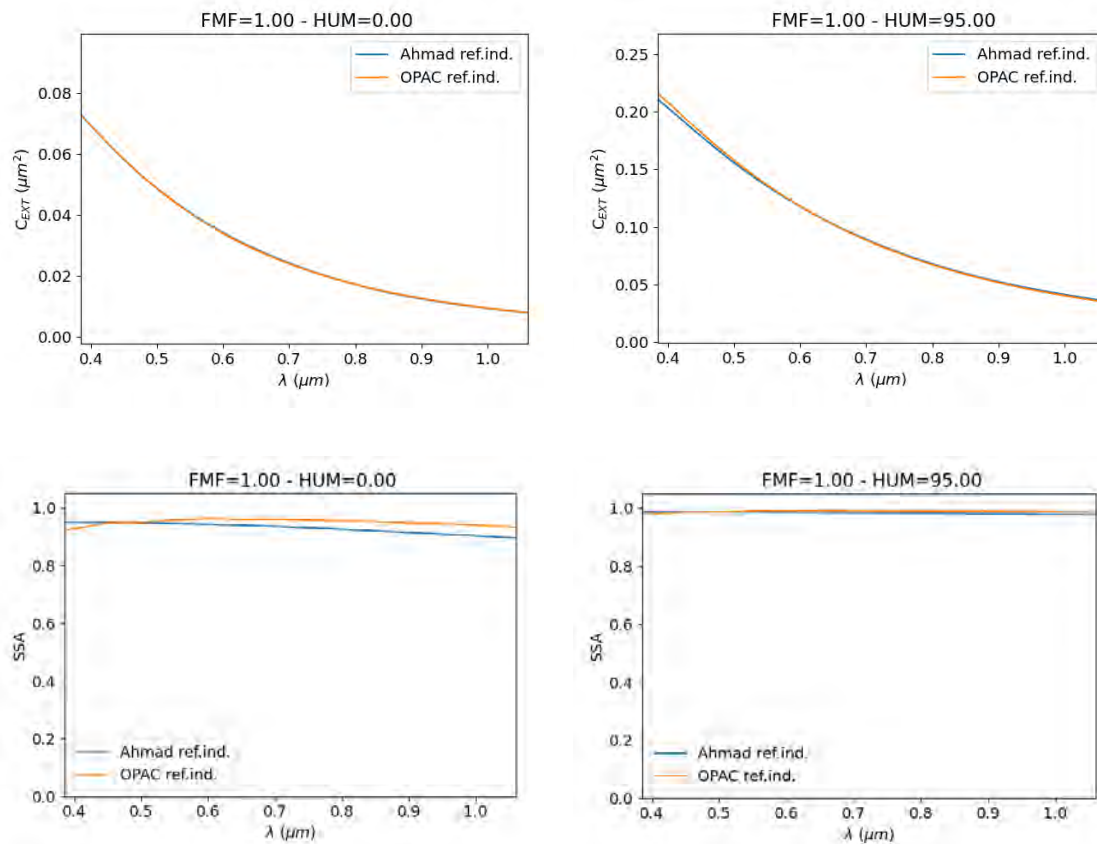


Figure 11. Same as Figure 10 but for Fine mode optical properties

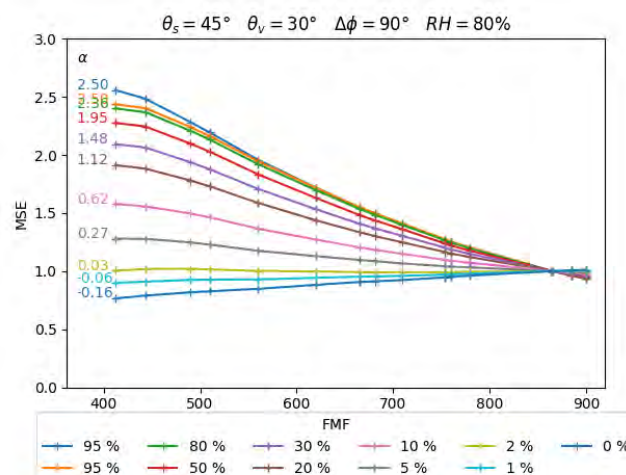


Figure 12. Multiple scattering epsilon (MSE) of the Ahmad et al. (2010) models defined for a relative humidity of 80%, for various FMF (colours).

#### 4.3.1.5 IOPS OF STRONGLY ABSORBING AEROSOLS

Additional aerosols models have to be introduced in order to account for strong absorption in the visible bands, like in dust episodes (Mobley et al., 2016; Moulin et al., 2001 for the OLCI dust models). An important constraint is to guarantee a smooth ordering of these new absorbing models (in the MSE space), as existing with the Ahmad et al. (2010) approach, in order to keep the core algorithm architecture of the aerosol retrieval. Therefore, we propose to introduce a new family as follows:

- We use the same Ahmad et al. (2010) approach, and create a second family by just modifying spectral refractive indices for fine and coarse mode, keeping the size distribution and its RH dependence.
- We adjust those new refractive indices to match the spectral Single Scattering Albedo published recently for biomass burning and dust transported zones (Di Biaggio et al., 2019, Pistone et al., 2019).

Different attempts to modify the spectral refractive indices are reported on Table 6. The philosophy is to keep the same refractive indices for the aerosol elementary components of Ahmad et al. (2010), i.e. sea salt, dust like, soot, but modify only the external mixing of these components in the composition of the fine and coarse modes (while keeping the same size distribution).

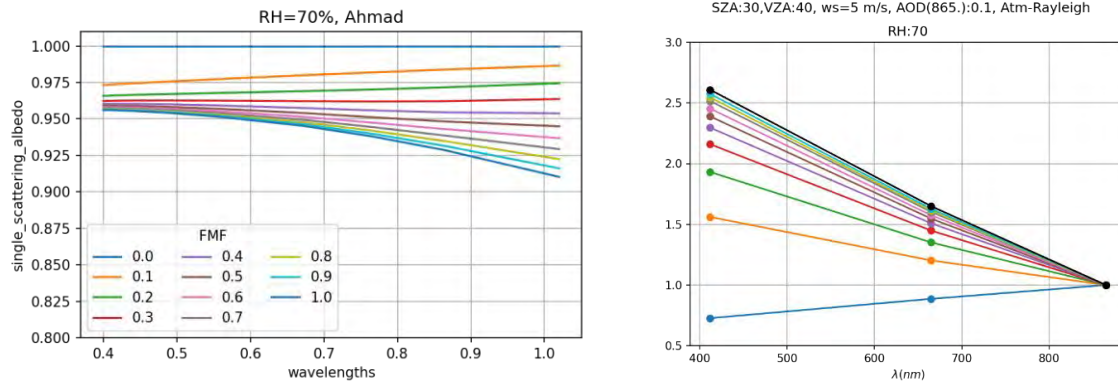
**Table 6 Tentative assemblages of the new strongly absorbing aerosol family (second and third main rows), starting from the standard model of Ahmad et al. (2010) (first row).**

| Family                                                        | Mode        | Component #1    | Component #2  |
|---------------------------------------------------------------|-------------|-----------------|---------------|
| <b>Standard Ahmad et al. (2010)</b>                           | Fine mode   | 99.5% dust like | 0.5% soot     |
|                                                               | Coarse mode | 100% sea salt   |               |
| <b>Fine mode extended</b>                                     | Fine mode   | 97.5% dust like | 2.5% soot     |
|                                                               | Coarse mode | 100% sea salt   |               |
| <b>Both modes extended (OC-SAC strongly absorbing models)</b> | Fine mode   | 95% dust like   | 5% soot       |
|                                                               | Coarse mode | 60% sea salt    | 40% dust like |

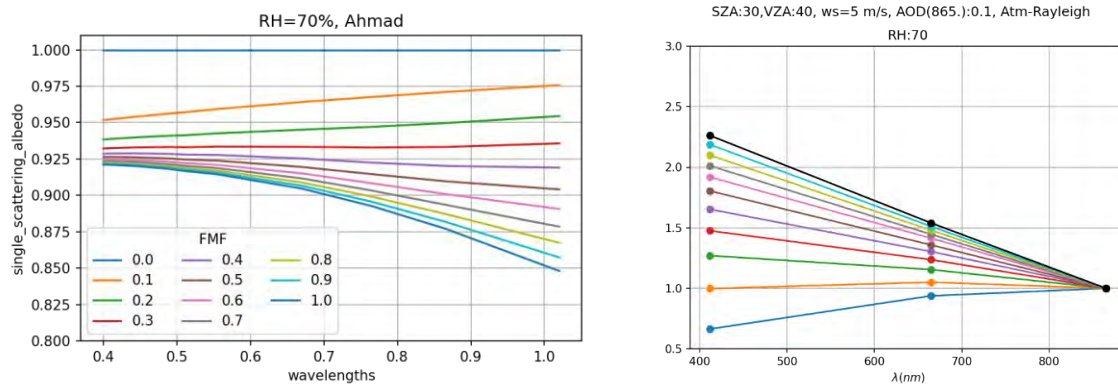
Figure 13, left, shows the corresponding single scattering albedo for RH=70%. The enhancement of the absorption of the fine mode is visible in the red and the NIR (consistent with a 'biomass burning type' aerosol) and the enhancement of the absorption of the coarse mode is visible in the blue (consistent with a 'dust type' aerosol). The spectral shape of the SSA is in relative agreement with the publication (see Figure 14).

Figure 13, right, reports the spectral dependence of the atmospheric reflectance corrected for Rayleigh. We see that the aerosol model ordering is unchanged, only the amplitude is varying as we expect. This confirms the validity of the proposed approach. The third row of Table 6 corresponds to the OC-SAC strongly absorbing models currently implemented. It would be required to fine tune the refractive index modifications to achieve a better agreement with the published properties of the strongly absorbing models, and compare notably to the current OLCI dust models.

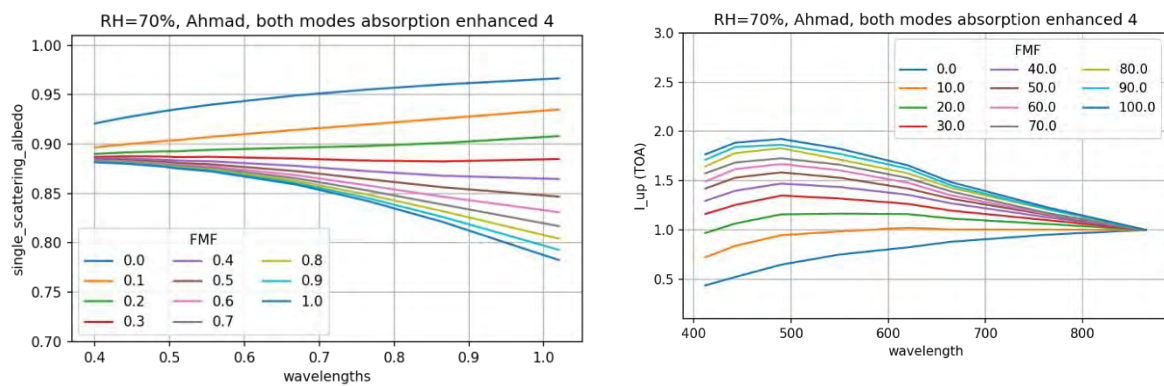
Original Ahmad et al. (2010)



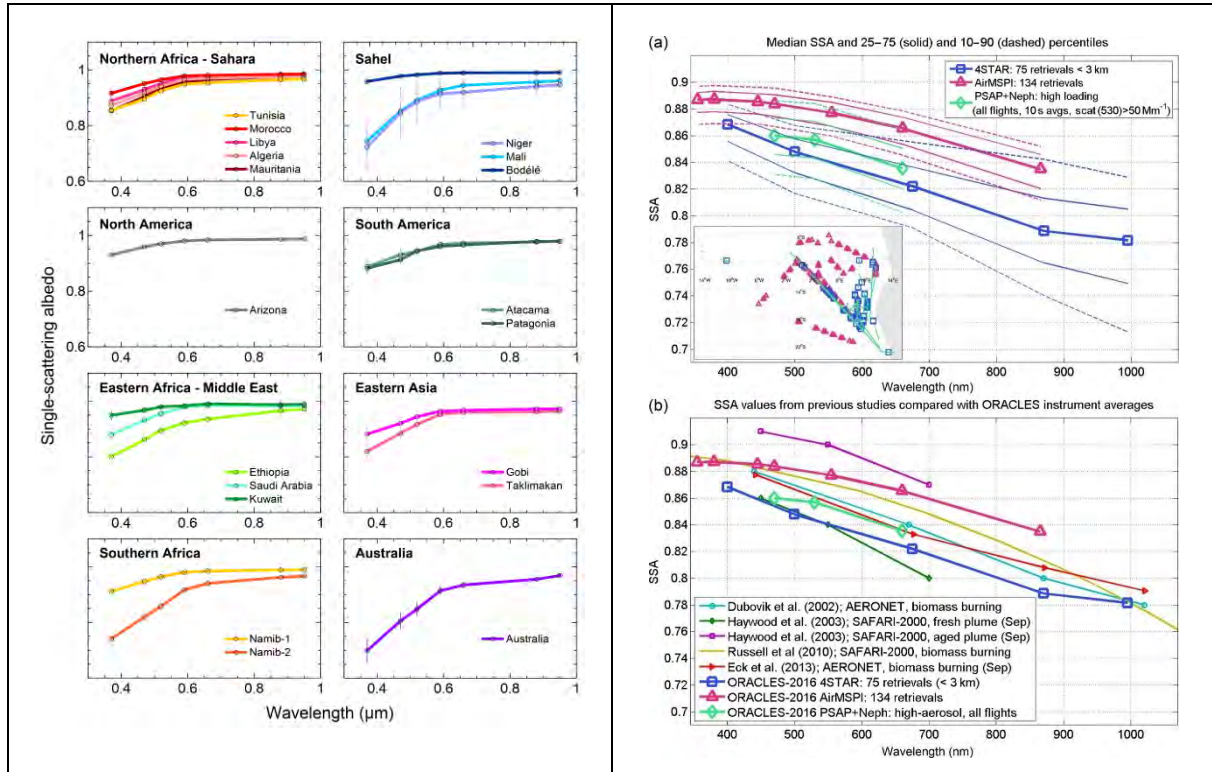
Ahmad et al. (2010) with fine mode enhanced absorption



Ahmad et al. (2010) with fine and coarse modes enhanced



**Figure 13 Spectral single scattering albedo (left) and spectral dependence (right) of the aerosol models for RH=70% as a function of the fine mode fraction for 3 assemblages (see Table 6).**



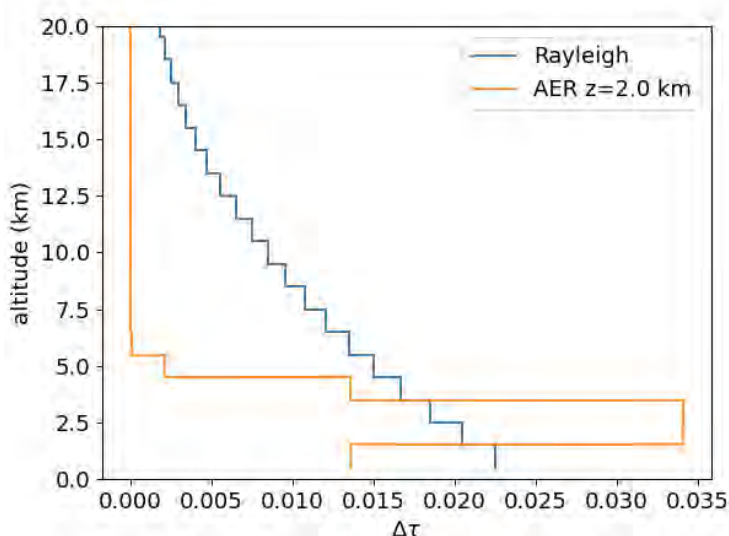
**Figure 14 Published spectral single scattering albedo for dust episodes (left, courtesy di Biaggio et al., 2019) or biomass burning (right, courtesy Pistone et al., 2019)**

#### 4.3.1.6 AEROSOL VERTICAL PROFILES

We intend to model the vertical profile of the aerosol extinction coefficient as a Gaussian centered on the altitude  $z_a$  with a width  $\sigma_a$ :

$$k_{ext}(z) = k_{ext}(0) + (k_{ext}(0) - k_{ext}(z_a)) * e^{-\frac{(z-z_a)^2}{\sigma_a^2}} \quad (4)$$

The standard deviation of the Gaussian is set to 1 km and  $z_a$  is sampled following the optimization procedure (see Appendix). Current tabulation contains three altitudes: 0.5, 2 and 5 km. Figure 15 shows an example of profile for  $z_a = 2$ km.



**Figure 15. Example of atmospheric profiles. Total Rayleigh optical depth is 0.2 and total aerosol optical depth is 0.1. The layering is the same as the one used for the radiative transfer solving.**

#### 4.3.1.7 RADIATIVE TRANSFER CODES

Two different codes are used to solve the radiative transfer for Rayleigh and aerosol. Except for the special case of O<sub>2</sub> bands, no gas absorption is accounted for, as it is supposed to be corrected for before the OC-SAC module.

**Plane parallel assumption (PPA)** – For the computation of the aerosol reflectance (including coupling with the Rayleigh), ARTDECO is used, and the radiative transfer is solved in plane parallel. ARTDECO (Atmospheric Radiative Transfer Database for Earth Climate Observation) is a numerical tool that gathers models and data for the 1D simulation of Earth atmosphere radiance and radiative fluxes as observed with passive sensors in the UV to thermal IR range. It is developed and maintained by LOA/HYGEOS and was initially developed at LOA and funded by the TOSCA program of the French space agency (CNES). It properly accounts for the absorption / scattering coupling in the atmosphere as well as for the surface / atmosphere coupling. It is available at <https://www.icare.univ-lille.fr/artdeco/>. The vertical distribution of aerosols and clouds can be arbitrarily defined as an input. The user can choose among available models, giving several methods for the truncation of the phase matrix and several RTE solvers, to compute radiative quantities corresponding to the scene. Technical parameters (e.g. number of computational angle) for these models are also accessible through input files. The accuracy / computing time ratio can then be easily adjusted. For the present project, an adding and doubling code (de Haan et al., 1987) is used. It properly accounts for the polarization and surface atmosphere coupling. For radiance computation, the first order of scattering correction (Nakajima and Tanaka, 1988) is applied for both the surface and atmosphere contribution.

**Spherical Shell Assumption (SSA)** – For the computation of pure Rayleigh reflectance, SMART-G is used, and the radiative transfer is solved using the spherical shell assumption. SMART-G is a Monte-Carlo code, developed by HYGEOS (Ramon et al., 2019), validated and used in several studies involving the coupled ocean-atmosphere system (Chowdhary et al., 2020), a spherical shell atmosphere and adjacency effects (Chowdhary et al., 2019).

**PPA/SSA hybrid method** – The spherical effect is mostly due to high altitude Rayleigh scattering and is partly due to i) the change of air masses between SSA and PPA for Rayleigh single scattering and ii) the increase of the escape probability for Rayleigh multiple scattering. The multiple scattering between aerosols and molecules occurs at the bottom of the atmosphere and is less influenced by the curvature of the atmosphere.

It is thus proposed to approximate the total path reflectance (aerosols + Rayleigh) in SSA geometry by:

$$\rho_{path}^{SSA} \approx \rho_r^{SSA} - \rho_r^{PPA} + \rho_{path}^{PPA} \quad (5)$$

We consider in that modelling that the spherical effect is completely due to the Rayleigh scattering. It is very practical as it implies only to perform calculations in SSA for the Rayleigh scattering. It reduces dramatically the dimensionality of the atmospheric path radiances computations in SSA.

An example of the accuracy of such modelling is given in Figure 16 and Figure 17. The accuracy of Eq. (5) seems to be very good and stable for a broad range of OZA, SZA outside the principal plane, and also aerosol model and AOD.

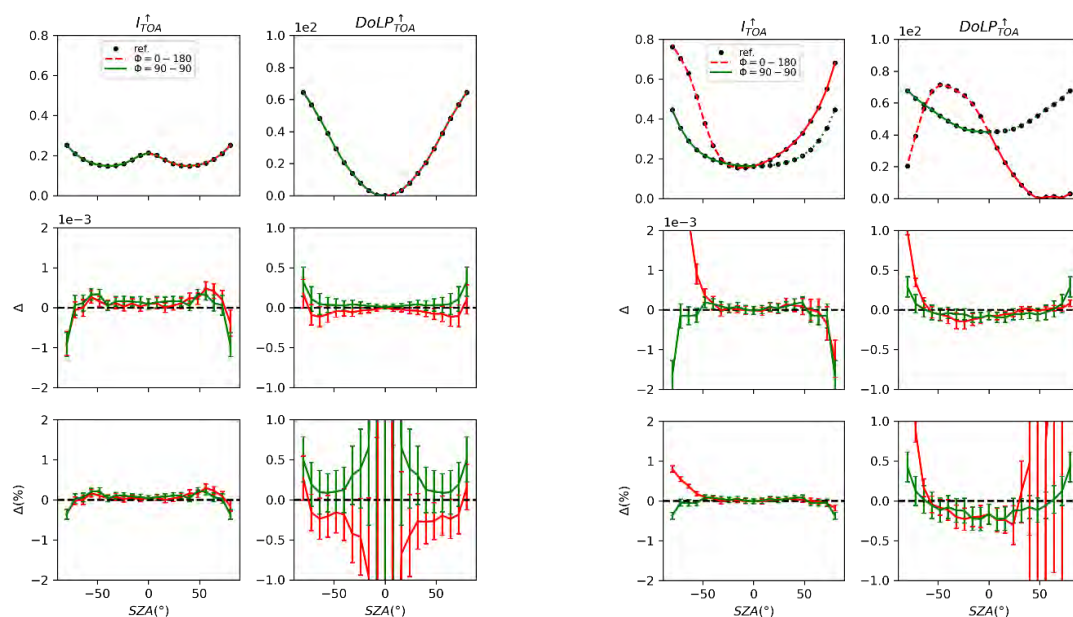
An equivalent formulation of Eq. (5), used in the OC-SAC module, is:

$$\rho_{path}^{SSA} \approx \rho_r^{SSA} + \rho_a^{PPA} \quad (6)$$

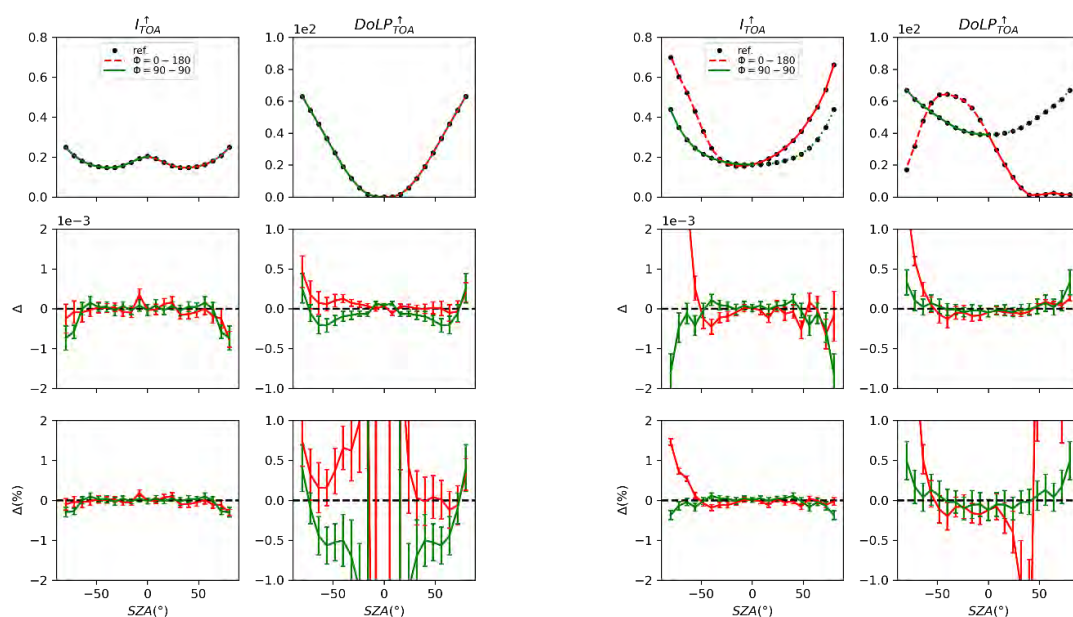
Where  $\rho_a^{PPA}$  is simply given by  $\rho_{path}^{PPA} - \rho_r^{PPA}$ . The quantity  $\rho_r^{PPA}$  is actually a special case of  $\rho_{path}^{PPA}$  simulations when AOT is zero. To summarise, the Rayleigh correction is done in SSA while the aerosol LUT (including coupling with Rayleigh) used in the CWAC is generated in PPA.

**Code for O2 band.** – Specific LUTs are computed for aerosol altitude retrieval that accounts for the O<sub>2</sub> absorption (see algorithm described in section 4.3.2.9: ALH assessment). The correlated k-distribution parametrisation is used in ARTDECO. We computed a set of coefficients using our tool PyKdis that was developed by HYGEOS and the Laboratoire d'Optique Atmosphérique. The coefficients of the parametrisation are computed using the instrument SRF and solar spectral flux to weight the gas absorption (see Edwards and Francis, 2000). We use the “idealized atmosphere” line-by-line coefficients described in Hogan and Matricardi (2020) as an input of PyKdis. It was computed using version 12.8 of LBLRTM (Line-By-Line Radiative Transfer Model, Clough et al., 2005) developed at Atmospheric & Environmental Research (AER). Continuum for the collision-induced bands of O<sub>2</sub> and N<sub>2</sub> is included in the computations. The spectroscopic input parameters have been taken from the Atmospheric and Environmental Research (AER) line parameter database, version 3.6 (<http://rtweb.aer.com>), which is largely drawn from HITRAN 2012 (Rothman et al., 2013) but with AER customized modifications, most notably for H<sub>2</sub>O, CO<sub>2</sub>, and O<sub>2</sub>.

**Relative azimuth convention** – ARTDECO and SMART-G use a different convention for relative azimuth angle than OLCI. As a reminder, OLCI defines forward scattering geometry with  $\Delta\varphi = 180^\circ$  (Sun in front of the sensor) and backward scattering geometry with  $\Delta\varphi = 0^\circ$  (Sun behind the sensor). Hence, all RTM simulations are reversed with respect to  $\Delta\varphi$  when tabulated in the OLCI ADF.



**Figure 16: Accuracy of Eq. (5) at 412 nm for an AOD of 0.2 at 550 nm,  $w_s = 5$  m/s, two azimuth angles (colours) and two OZA (nadir view, left plots and OZA=56°, right plots). Top: values of radiance  $I_{TOA}$  (left) and degree of linear polarization  $DoLP_{TOA}$  (right). Middle: absolute error. Bottom: relative error.**



**Figure 17: Same as Figure 16 but for an atmosphere with desert dust with AOD at 550 nm of 0.4.**

#### 4.3.1.8 SEA SURFACE

In ARTDECO, the surface reflectance is defined as in Mishchenko and Travis 1997, considering an isotropic surface with a mean square surface slope of  $\sigma^2 = 0.003 + 5.12 \times 10^{-3} w_s$  where wind-speed ( $w_s$ ) is in m/s. To account for shadowing effect by the surface waves, a bidirectional shadowing function as described Tsang et al., 1985 is used. The refractive index of pure water (Hale and Query, 1973) is used with a correction of the real part depending on the salinity  $nr = nr_{\text{purewater}} + 0.006 x_{\text{sal}}/34.3$ , with  $x_{\text{sal}}$  being the salinity in ppt. The used salinity for computation is 34.3 ppt.

No white caps are accounted for, as they are pre-corrected before the CWAC module. For the computation of aerosol and Rayleigh reflectance, the water is assumed black. For the computation of reflectance in bands affected by the O<sub>2</sub> absorption (aerosol altitude retrieval), the water reflectance is a dimension of the LUT.

#### 4.3.1.9 RAYLEIGH LUT

Rayleigh is computed with SMART-G, in SSA, for a range of optical thicknesses covering a realistic spectrum (400 nm to 1020 nm) and change in pressure. For all geometries and wind speeds, the LUT contains the coefficients of a 4<sup>th</sup> order polynomial fitting versus  $\tau_R$ :

$$\rho_R = a * \tau_R^3 + b * \tau_R^2 + c * \tau_R + d \quad (7)$$

This generic LUT shall be read with the Rayleigh optical thickness at a given band and a given pressure, following Bodhaine et al. (1999). Examples of the polynomial fit are shown in Appendix 1: LUT grid optimisation.

#### 4.3.1.10 AEROSOL SPECTRAL DEPENDENCE LUT

Linear dependency with extinction coefficients is assumed:

$$\tau_a^{iaer}(\lambda, \tau_{a0}) = c^{iaer}(\lambda, \lambda_0) * \tau_{a0} \quad (8)$$

The coefficient is computed for all OLCI central wavelengths  $\lambda_i$  (Table 3) and models. To account for the spectral variation between pixel, the extinction coefficients is converted and tabulated into an Angstrom exponent  $\alpha(\lambda_i, iaer)$ , so that  $\tau_a$  can be computed at any (non-nominal) wavelength  $\lambda_{pix}$  corresponding to channel  $\lambda_i$  with a power law:

$$\tau_a(\lambda_{pix}) = \tau_a(865) \left( \frac{\lambda_{pix}}{865} \right)^{-\alpha(\lambda_i, iaer)} \quad (9)$$

#### 4.3.1.11 ATMOSPHERIC REFLECTANCE LUT

For a given model and geometry, aerosol reflectance at any wavelength shall be computed through functional relationships with respect to the aerosol load at a reference band in the NIR ( $\lambda_0 = 865 \text{ nm}$ ). In [AD-1], a review of published relationships was conducted. The most common option, used in current OLCI algorithm (Antoine and Morel, 1999) and in Ibrahim et al. (2019), consists in expressing  $\rho_a(\lambda)$  as a polynomial of  $\tau_{a0}$ :

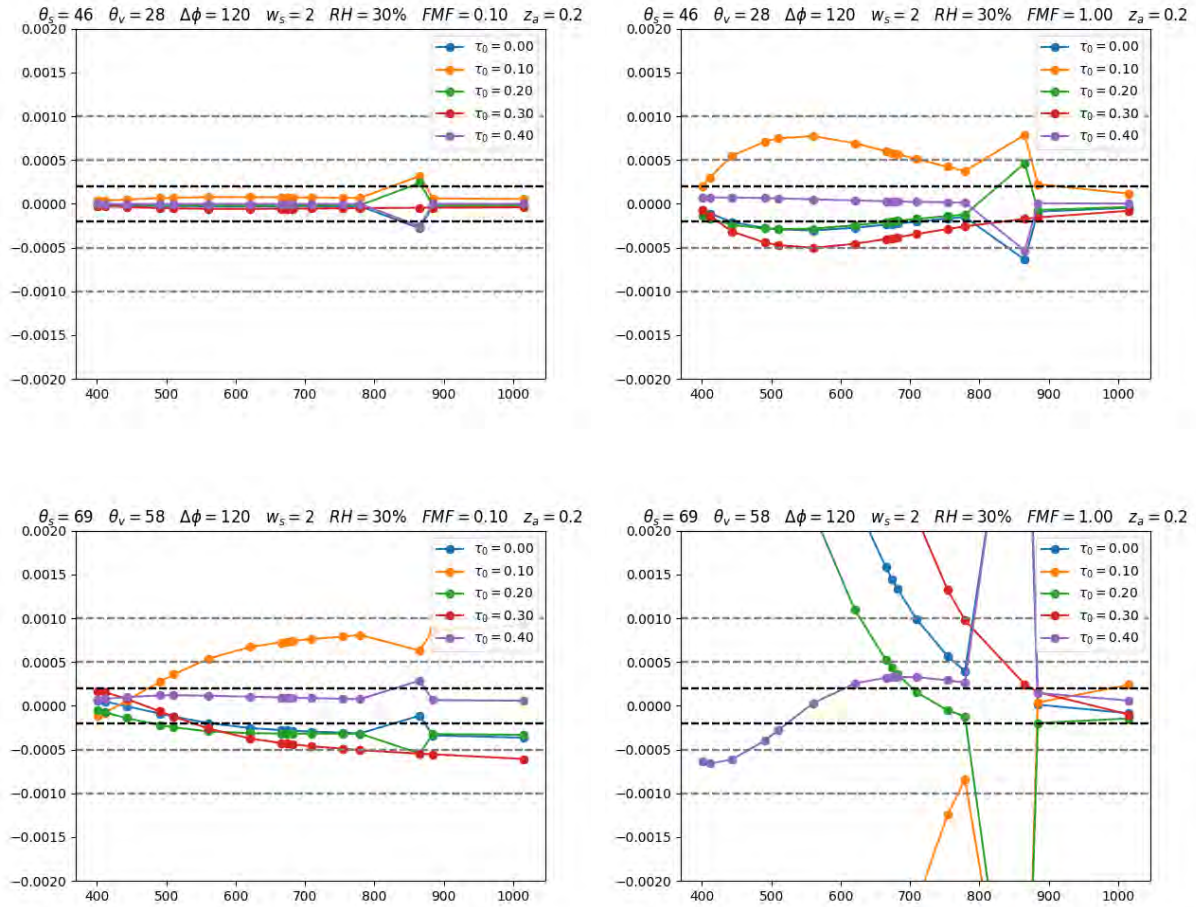
$$\rho_a^{iaer}(\lambda, z_a, \tau_R, \mathbf{\Omega}, w_s, \tau_{a0}) = \begin{cases} \sum_{i=0}^3 c_i(\lambda, iaer, z_a, \tau_R, \mathbf{\Omega}, w_s) * \tau_{a0}^i & \lambda \neq 865 \text{ nm} \\ \sum_{i=0}^2 c_i(\lambda, iaer, z_a, \tau_R, \mathbf{\Omega}, w_s) * \tau_{a0}^i & \lambda = 865 \text{ nm} \end{cases} \quad (10)$$

A detail in Eq. (10) is that the fit at any wavelength is made against  $\tau_{a0}$ , and not  $\tau_a^{iaer}(\lambda, \tau_{a0})$  as usually done (Antoine and Morel, Ibrahim et al. 2019), so that extinction coefficients are implicitly handled in the polynomial coefficients and there is no need to compute them at this stage. The polynomials are classically of 2<sup>nd</sup> order at 865 nm for easy inversion of  $\tau_{a0}$ . Contrary to Antoine and Morel (1999), they are here extended to 3<sup>rd</sup> order at all other bands for a more accurate fitting (see Appendix 1: LUT grid optimisation). In fact, fitting with respect to AOT would need even higher order, e.g. 4<sup>th</sup> order as in Ibrahim et al. (2019), but this becomes more critical in terms of storage and LUT interpolations. Indeed, the LUT contains coefficients  $c_i$  for all combination of  $(\lambda, iaer, z_a, \tau_R, \mathbf{\Omega}, w_s)$  and a multilinear interpolation is done along all these axes. In the multiband approach considered for the new CWAC, computing aerosol reflectance at 5 NIR bands for 9 candidate models requires  $5*9*4=180$  interpolations with 3<sup>rd</sup> order polynomials, what is three times more costly than the current 2-band OLCI algorithm based on 2<sup>nd</sup> order polynomials ( $2*9*3=54$ , for a same number of aerosol models). Further considerations on CPU and RAM performance will be given in section 4.5.2: Numerical computation considerations. Reducing the order of the polynomials while keeping strong accuracy is achieved by another formulation, expressed in term of  $\rho_{a0}$  instead of  $\tau_{a0}$ , as proposed by Ahn et al. (2016):

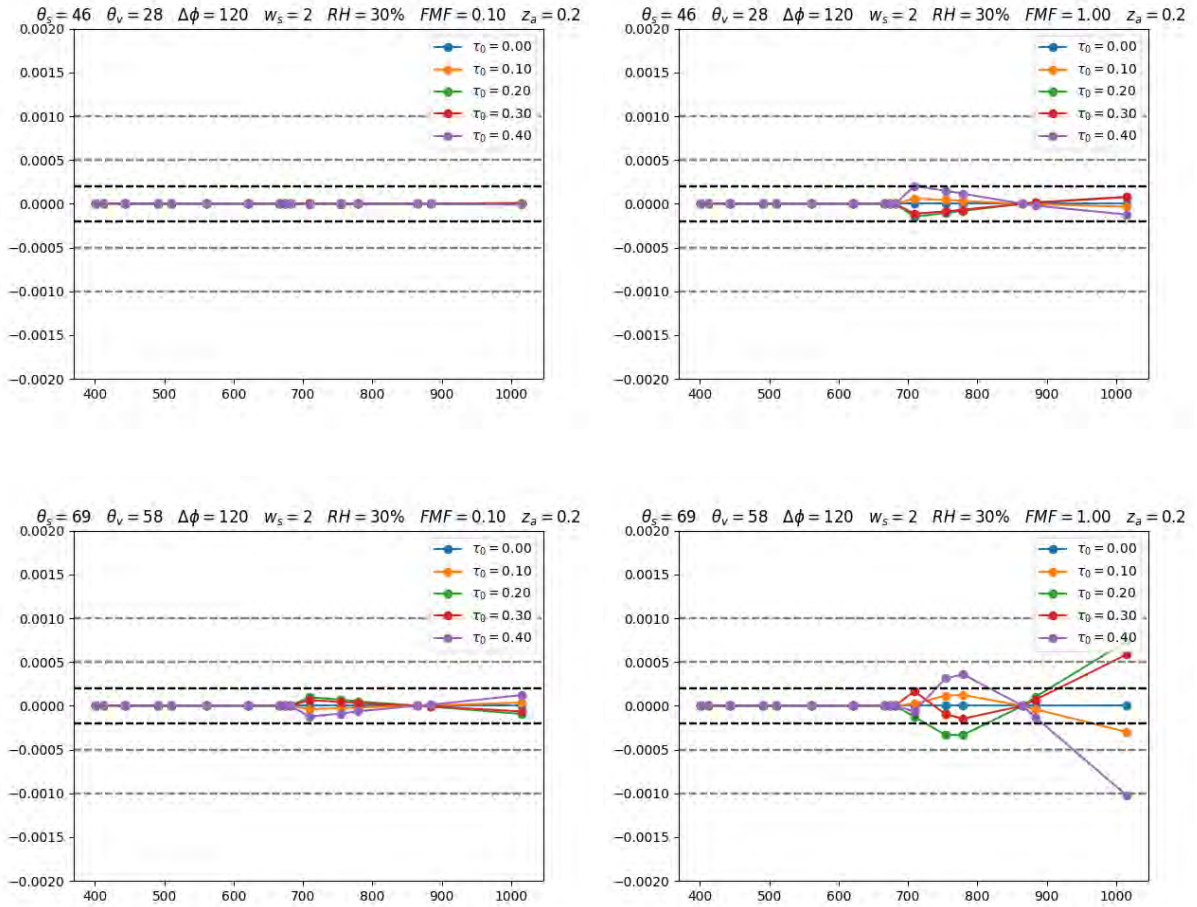
$$\rho_a^{iaer}(\lambda, z_a, \tau_R, \mathbf{\Omega}, w_s, \rho_{a0}) = \begin{cases} \sum_{i=1}^4 c_i(\lambda, iaer, z_a, \tau_R, \mathbf{\Omega}, w_s) * \rho_{a0}^i & \lambda \leq 681 \text{ nm} \\ \sum_{i=1}^2 c_i(\lambda, iaer, z_a, \tau_R, \mathbf{\Omega}, w_s) * \rho_{a0}^i & \lambda \geq 709 \text{ nm} \end{cases} \quad \begin{matrix} \text{(OP-SAC-} \\ \text{CWAC-} \\ \text{RHOA-1)} \end{matrix}$$

Another difference with Eq. (10) is that the 0<sup>th</sup> order coefficients are assumed to be strictly zero (no signal without any aerosol content), what saves storage and interpolations. Coefficients  $c_i$  are computed by fitting RT simulations up to an AOT of 0.4 at 865 nm.

Figure 18 shows that the formulation with respect to  $\tau_{a0}$ , given by Eq. (10), does not meet the required accuracy of  $2 \times 10^{-4}$  in the visible bands for large FMF, even for standard OLCI observation conditions and an AOT of 0.1 (top right images). Interestingly, the error increases with the air mass (bottom images) and can be largely above  $10^{-3}$  at various bands for the extreme OLCI condition reached at the edge of the swath and with Sun zenith angle of 70°. The error at 865 nm is also clearly higher than at any other band, for all situations, because of the 2<sup>nd</sup> order polynomial. On the contrary, a fit with respect to  $\rho_{a0}$  is much more accurate and robust to air mass (Figure 19), for an equivalent number of coefficients. The error remains below of  $2 \times 10^{-4}$  for all bands in the visible and all conditions, and even in the NIR for most cases. Clearly, the non-linearity of the reflectance due to increased aerosol load is weaker as a function of  $\rho_{a0}$  (which is already an apparent optical property) than as a function of AOT (which is an IOP). This principle is somehow used in the original Gordon and Wang (1994) algorithm, where the aerosol reflectance including multiple scattering was expressed as a polynomial with respect to single scattering reflectance.



**Figure 18. Absolute error of  $\rho_a(\lambda)$  versus  $\lambda$  when fitting radiative transfer simulations with respect to  $\tau_{a0}$  with Eq. (10). Left FMF=0.1, right FMF=1. Top: classical OLCI viewing condition (air mass=2.57); bottom: extreme viewing condition (air mass=4.68). Dashed horizontal lines represents errors of  $\pm 2 \times 10^{-4}$ ,  $\pm 5 \times 10^{-4}$  and  $\pm 10^{-3}$ .**



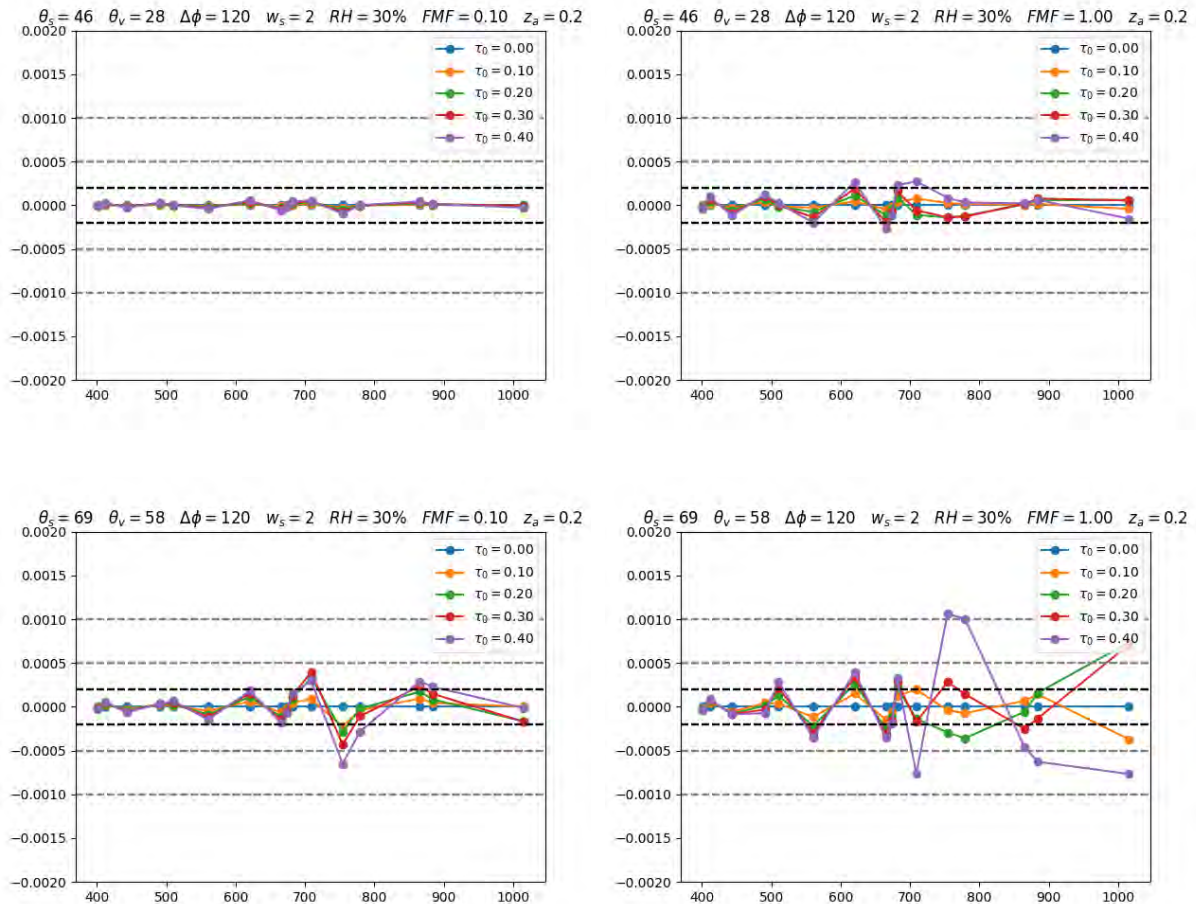
**Figure 19. Same as Figure 18 but when fitting radiative transfer simulations with respect to  $\rho_{a0}$  with Eq. (OP-SAC-CWAC-RHOA-1).**

A second step in the dimensionality reduction consists in fitting each coefficient  $c_i$  of Eq. (OP-SAC-CWAC-RHOA-1) as a function of wavelength. The best relationships identified so far distinguish again between the visible and NIR:

$$c_i(\lambda, iaer, z_a, \tau_R, \mathbf{\Omega}, w_s) = \begin{cases} \sum_{j=1}^7 c_{i,j}(iaer, z_a, \tau_R, \mathbf{\Omega}, w_s) * \lambda^{-j} & \lambda < 0.7 \mu m, 1 \leq i \leq 4 \\ \sum_{j=1}^3 c_{i,j}(iaer, z_a, \tau_R, \mathbf{\Omega}, w_s) * \lambda^{-j} & \lambda \geq 0.7 \mu m, 1 \leq i \leq 2 \end{cases} \quad \begin{matrix} \text{(OP-SAC-} \\ \text{CWAC-} \\ \text{RHOA-2)} \end{matrix}$$

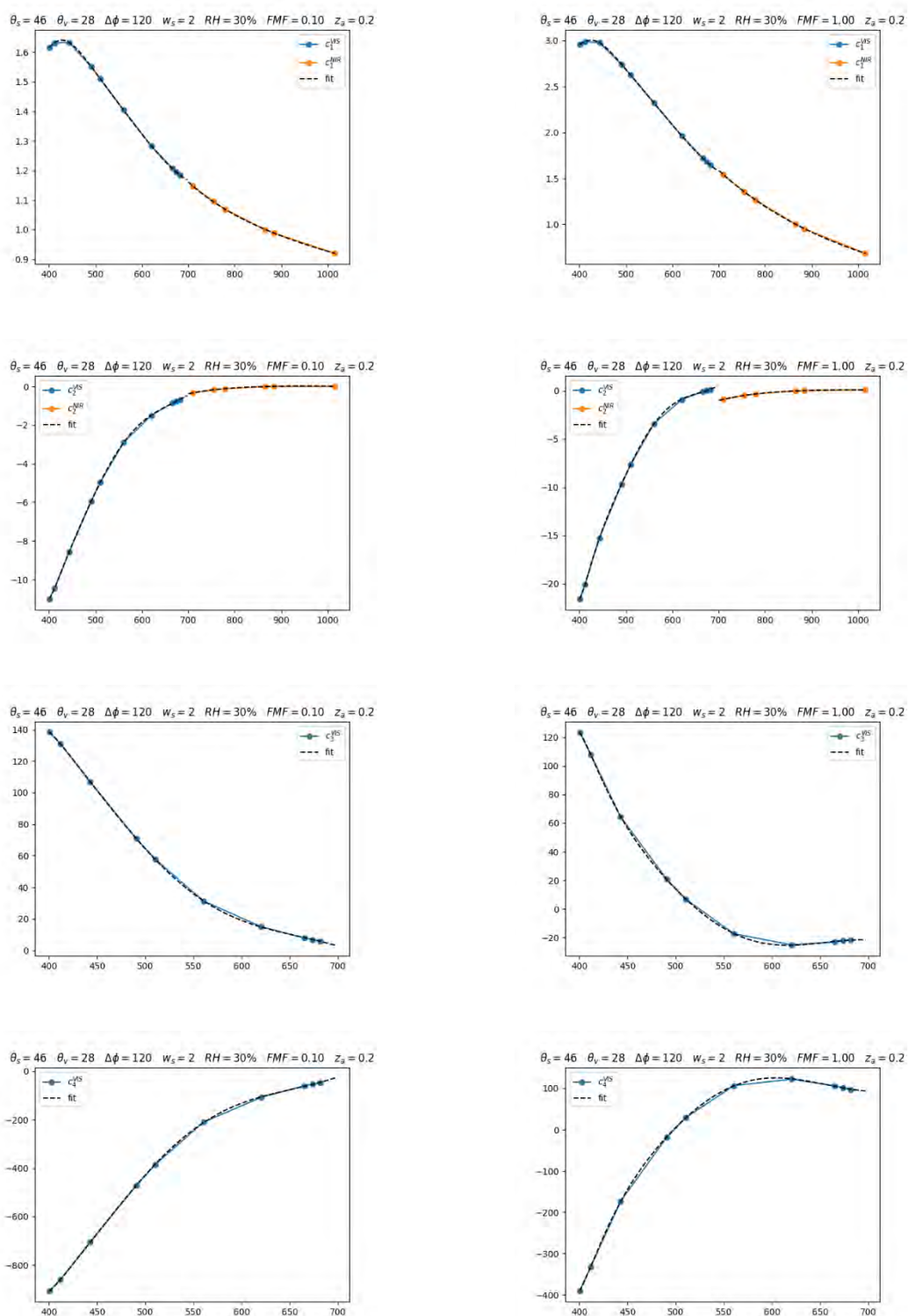
Importantly,  $\lambda$  is here expressed in  $\mu m$  for better numerical fitting. It is worth noting that the complete formulation Eqs. (OP-SAC-CWAC-RHOA-1)-(OP-SAC-CWAC-RHOA-2) is still linear with respect to the coefficients, hence multilinear interpolations still apply (care, however, for the interpolation with respect to  $\tau_R$ , which depends on wavelength). Now coefficients  $c_{i,j}$  do not depend any more on

wavelength, what saves many interpolations: computing aerosol reflectance at 5 NIR bands for 9 candidate models with this formulation requires  $9 \times 2 \times 3 = 54$  interpolations, like the current OLCI 2-band algorithm. The performance of the fit remains excellent (Figure 20 to be compared to Figure 18).



**Figure 20. Same as Figure 18 but with the complete fit with respect to  $\rho_{a0}$  given by Eqs. (OP-SAC-CWAC-RHOA-1)-(OP-SAC-CWAC-RHOA-2).**

A further interest of this formulation is that it can be applied to the exact detector wavelength. Figure 21 and Figure 22 show the smooth variation of the fitted coefficients  $c_i(\lambda)$ , over each spectral range (visible and NIR); note that the discontinuity between the two spectral domains is only due to the two different polynomials, Eq. (OP-SAC-CWAC-RHOA-1), what does not impact the reflectance itself, as shown by previous error plots.



**Figure 21. Coefficients  $c_i(\lambda)$  of Eq. (OP-SAC-CWAC-RHOA-1) versus  $\lambda$  (blue dots in the visible, orange dots in the NIR) and their spectral fitting through Eq. (OP-SAC-CWAC-RHOA-2) (dashed line), for a classical OLCI viewing conditions (air mass=2.57). Left FMF=0.1, right FMF=1.**

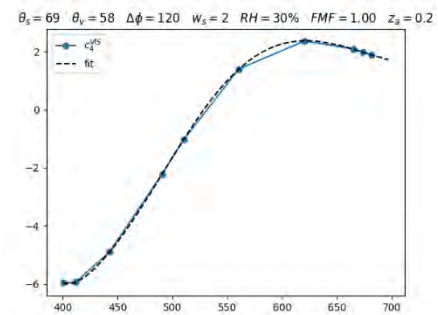
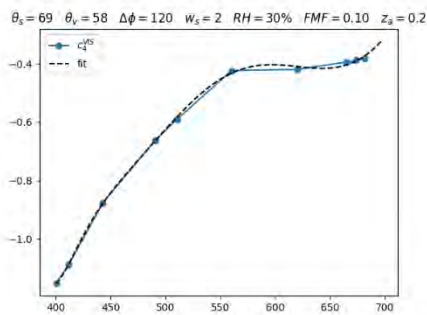
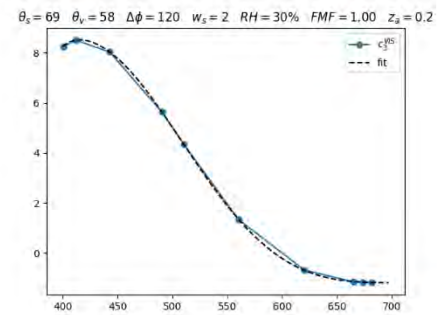
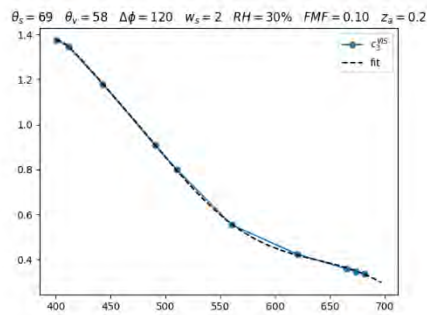
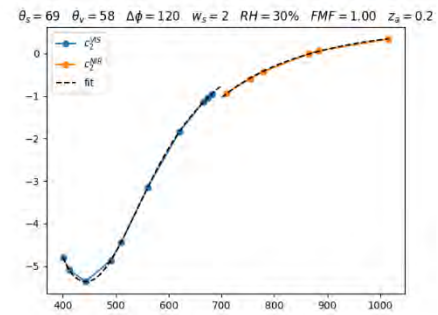
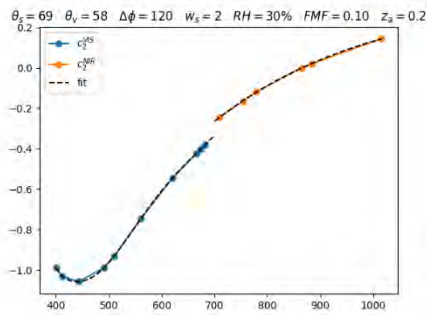
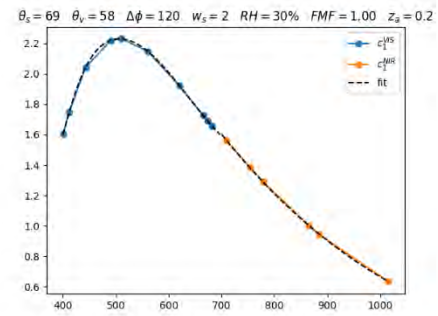
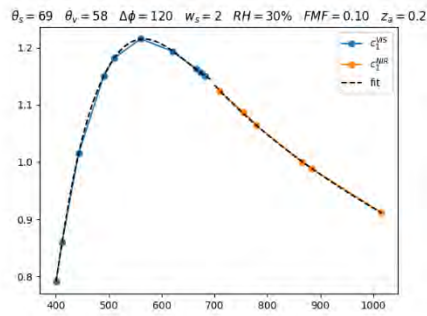


Figure 22. Same as Figure 21 but for an extreme viewing condition (air mass=4.68).

#### 4.3.1.12 ATMOSPHERIC TRANSMITTANCE LUT

Downward and upward transmittance LUTs are built on a similar grid as  $\rho_a$ , except that  $\tau_{a0}$  is also a dimension of the table (i.e. there are no functional relationships). The LUT is stored in logscale, what theoretically improves the linear interpolation with respect to Rayleigh optical thickness, aerosol optical thickness and air mass.

#### 4.3.1.13 AEROSOL MIXING

The mixing between two consecutive models (i.e. FMFs) is supposed to be linear, through a spectrally white mixing ratio:

$$\rho_a^{mod}(\lambda, iaer, \tau_{a0}, mix) = (1 - mix)\rho_a^{iaer}(\lambda, \tau_{a0}) + mix * \rho_a^{iaer+1}(\lambda, \tau_{a0}) \quad (11)$$

The justification is a smooth ordering of the aerosol model in the epsilon plane (Figure 3).

### 4.3.2 MATHEMATICAL DESCRIPTION

#### 4.3.2.1 SYSTEM VICARIOUS CALIBRATION (SVC)

In the Level-2 processor, SVC consists in applying multiplicative gains, fixed for a given spectral band:

$$\rho_{ng}^*(\lambda) = g(\lambda) * \rho_{ng}(\lambda) \quad (\text{OP-SAC-WPP-SVC-1})$$

The computation of the SVC gains is done offline, outside the processor, as described in Appendix 2: OC-SAC SVC gains computation.

#### 4.3.2.2 RAYLEIGH COMPUTATION

Rayleigh optical thickness is computed from Bodhaine et al. (1999), as a function of wavelength, CO<sub>2</sub> content, latitude, altitude and pressure:

$$\tau_R(\lambda) = \tau_{R\_bodhaine}(\lambda, CO_2, lat, z, p) \quad (\text{OP-SAC-WPP-RAY-1})$$

By default, the CO<sub>2</sub> content is taken as 400 ppm.

Rayleigh reflectance is computed as a 3<sup>rd</sup> order polynomial of  $\tau_R$ , where polynomial coefficients are interpolated at actual pixel geometry and wind speed:

$$c_R(i) = \rho_{R\_LUT}(i, \mu_s, \mu_v, \Delta\phi, w_s), \quad i = 0 \dots 3 \quad (\text{OP-SAC-WPP-RAY-2})$$

$$\rho_R(\lambda) = \sum_{i=0}^3 c_R(i) * \tau_R(\lambda)^i \quad (\text{OP-SAC-WPP-RAY-3})$$

#### 4.3.2.3 ITERATIVE TRANSMITTANCE

As shown on the OC-SAC workflow (Figure 7), an optional iterative process allows to take the best knowledge of aerosol from CWAC in order to compute the atmospheric transmittance in glint correction, white-caps correction and BPC. Setting variable `oc_sac_niter` to 1 simply discards the iterations (default option). At start, the first guess on AOT is given by an auxiliary data:  $\tau_a(865)_{init} = 0.1$  and Angstrom of  $\alpha_{init} = 1$ , to compute  $\tau_a(\lambda)$  at all bands, taking into account the exact detector wavelength:

$$\tau_a(\lambda) = \tau_a(865)_{init} * \left(\frac{\lambda}{865}\right)^{-\alpha_{init}} \quad (\text{OP-SAC-WPP-ITER-1})$$

The first computation of downward and upward diffuse transmittance follows the approximate formulation used so far in the OLCI processor ([AD-6]):

$$\begin{cases} t_{down}(\lambda) &= e^{-0.5 * (\tau_R(\lambda) + (1 - f_0(\lambda) \omega_0(\lambda)) \tau_a(\lambda)) / \mu_s} \\ t_{up}(\lambda) &= e^{-0.5 * (\tau_R(\lambda) + (1 - f_0(\lambda) \omega_0(\lambda)) \tau_a(\lambda)) / \mu_v} \end{cases} \quad (\text{OP-SAC-WPP-ITER-2})$$

where  $f_0(\lambda) \omega_0(\lambda)$  is fixed to 0.8. This expression is only applied to the NIR bands for BPC, and to all bands for white-caps, see Eq. (OP-SAC-WPP-WCP-2).

During the iteration,  $t_{down}(\lambda)$  and  $t_{up}(\lambda)$  are then computed with atmospheric LUTs as in the CWAC, see Eq. (OP-SAC-CWAC-COR-2).

The direct transmittance relevant for Sun glint correction is explicitly computed with the actual value of  $\tau_R(\lambda)$  and  $\tau_a(\lambda)$  at the given iteration, following Eq. (OP-SAC-WPP-GLT-5) below.

#### 4.3.2.4 SUN GLINT CORRECTION

Sun glint reflectance at sea level is interpolated from a LUT (only once, outside the iterative loop):

$$\rho_g = \rho_{R\_LUT}(\mu_s, \mu_v, \Delta\varphi, w_s) \quad (\text{OP-SAC-WPP-GLT-1})$$

Sun glint flags are raised according to thresholds:

If  $\rho_g < low_{glint\_threshold}$ :

$$\text{MEGLINT} = \text{False} \quad (\text{OP-SAC-WPP-GLT-2})$$

$$\text{HIGHLINT} = \text{False} \quad (\text{OP-SAC-WPP-GLT-3})$$

$$\text{ICE\_HIGHAERO} = \text{BRIGHT} \quad (\text{OP-SAC-WPP-GLT-4})$$

Direct transmittance is computed as a function of Rayleigh and aerosol optical thickness:

$$T(\lambda) = e^{-(\tau_R(\lambda) + \tau_a(\lambda)) * M} \quad (\text{OP-SAC-WPP-GLT-5})$$

Sun glint correction writes:

$$\rho_{gc}(\lambda) = \rho'_{ng}(\lambda) - T(\lambda)\rho_g \quad (\text{OP-SAC-WPP-GLT-6})$$

#### 4.3.2.5 WHITE-CAPS CORRECTION

White-caps computation is from Frouin et al.:

$$\rho_{wc}(\lambda) = \alpha_{wc}(\lambda) * (\min(w, w_{max}) - w_{min})^{Y_{wc}} \quad (\text{OP-SAC-WPP-WCP-1})$$

White-caps correction is then done by:

$$\rho_{gc}(\lambda) = \rho_{gc}(\lambda) - t_{down}(\lambda)t_{up}(\lambda)\rho_{wc}(\lambda) \quad (\text{OP-SAC-WPP-WCP-2})$$

#### 4.3.2.6 BRIGHT PIXEL CORRECTION

The BPC is fully detailed in [AD-6]. Only the inputs and outputs of the BPC module are described here. The Rayleigh correction writes:

$$\rho_{Rc}(\lambda) = \rho_{gc}(\lambda) - \rho_R(\lambda) \quad (\text{OP-SAC-BPC-1})$$

The input variance-covariance matrix  $\mathbf{C}_{\rho_{gc}}$  is computed as in [AD-6], i.e. is equal to the TOA radiometric uncertainty  $\mathbf{C}_{\rho_t}$  computed upstream OC-SAC (essentially radiometric noise, scaled at actual pixel radiance):

$$\mathbf{C}_{\rho_{gc}} = \mathbf{C}_{\rho_t} = \begin{pmatrix} \left(\frac{\pi}{\mu_s F_0(\lambda_1)}\right)^2 \sigma_{typ}^2(\lambda_1) \frac{L_t(\lambda_1)}{L_{typ}(\lambda_1)} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \left(\frac{\pi}{\mu_s F_0(\lambda_n)}\right)^2 \sigma_{typ}^2(\lambda_n) \frac{L_t(\lambda_n)}{L_{typ}(\lambda_n)} \end{pmatrix} \quad (\text{OP-SAC-BPC-2})$$

where  $\sigma_{typ}(\lambda_i)$  is the uncertainty of TOA signal at a typical radiance  $L_{typ}(\lambda_i)$ ,  $F_0(\lambda_i)$  the extra-terrestrial irradiance and  $L_t(\lambda_1)$  the actual per-pixel radiance. Using  $\mathbf{C}_{\rho_t}$  instead of  $\mathbf{C}_{\rho_{gc}}$  avoids propagating artifacts of the Level-2 precorrections in the BPC band weighting.

The main output of BPC, in the OC-SAC context, is the TOA marine signal in the NIR, computed by

$$t\rho_{wc2}(\lambda) = \rho_{Rc}(\lambda) - \rho_a(\lambda) \quad (\text{OP-SAC-BPC-3})$$

where importantly  $\rho_a(\lambda)$  is the one computed within BPC. As explained in [AD-6], this definition removes the residual water signal retrieved by the BPC optimisation scheme, and it provides to the CWAC a purely atmospheric and spectrally smooth reflectance, see Eq. (OP-SAC-CWAC-ID-1) below. A

small update is that the output marine reflectance is now directly at detector wavelength, not at theoretical bands.

Some outputs of BPC are further used by two new elements in OC-SAC:

1.  $t\rho_{WC2}$  is used as a boundary condition in the ALH assessment in the NIR.
2. The output uncertainties of  $t\rho_{WC2}$ , which form the variance-covariance matrix  $\mathbf{C}_{t\rho_{WC2}}$ , were not defined in previous BPC code; the matrix is now used to defined uncertainties of the observed signal in the NIR, for weighted chi-square minimization in case of strongly absorbing models (see section 4.3.2.12). In the present version, it is simply defined as the input uncertainty computed in the BPC, accounting for TOA and marine model uncertainty.

#### 4.3.2.7 AEROSOL LOAD COMPUTATION

The computation of  $\rho_{a0}$  presently follows the idea of Ibrahim et al. (2019), in the sense that it relies only on the 865 nm band, with the difference that our formulation is already in reflectance instead of AOT. Hence, the retrieval is simply achieved for all candidate aerosol models by:

$$\rho_{a0} = \rho_a^{obs}(865) \quad (\text{OP-SAC-CWAC-RHOA0-1})$$

Note that  $\rho_{a0}$  is set to zero in case of negative  $\rho_a^{obs}(865)$ . An advantage of this retrieval is its compatibility with SVC gain computation in the NIR, where 865 nm is assumed to be a reference band.

Using more bands, however, may improve the robustness of the AC. This alternative computation is achieved by minimizing the following weighted chi-square (we refer to section 4.3.2.10, *Standard aerosol identification*, for more context about the multi-band minimization):

$$\chi^2(\rho_{a0}) = \sum_{\lambda_{NIR}} w(\lambda) \left( \rho_a^{iaer}(\lambda, \rho_{a0}) - \rho_a^{obs}(\lambda) \right)^2$$

Thanks to the 2<sup>nd</sup> order polynomial dependence of  $\rho_a^{iaer}(\lambda)$  with respect to  $\rho_{a0}$  in the NIR, Eq. (OP-SAC-CWAC-RHOA-1), it can be shown that the minimum is the solution of a cubic equation:

$$\begin{aligned} & \left( 2 \sum_{\lambda_{NIR}} w(\lambda) c_2^2(\lambda) \right) \rho_{a0}^3 + \left( 3 \sum_{\lambda_{NIR}} w(\lambda) c_1(\lambda) c_2(\lambda) \right) \rho_{a0}^2 \\ & + \left( \sum_{\lambda_{NIR}} w(\lambda) \left( c_1^2(\lambda) - 2c_2(\lambda) \rho_a^{obs}(\lambda) \right) \right) \rho_{a0} \\ & - \left( \sum_{\lambda_{NIR}} w(\lambda) c_1(\lambda) \rho_a^{obs}(\lambda) \right) \end{aligned} \quad (\text{OP-SAC-CWAC-RHOA0-2})$$

In this equation, the dependence of  $c_i$  with respect to  $iaer$  has been omitted for brevity, but importantly  $\rho_{a0}$  is now different for each aerosol model. The cubic equation is solved numerically with the function `gsl_poly_solve_cubic` of the GSL library. It has either one real solution, or three; in the latter case, to avoid unrealistic value, the closest solution to  $\rho_a^{obs}(865)$  is selected. In practice, we have not observed significant differences between both formulations, either in terms of marine

reflectance or AOT. Equation (OP-SAC-CWAC-RHOA0-2) is thus currently by-passed in the code, and could be investigated in more details in future developments.

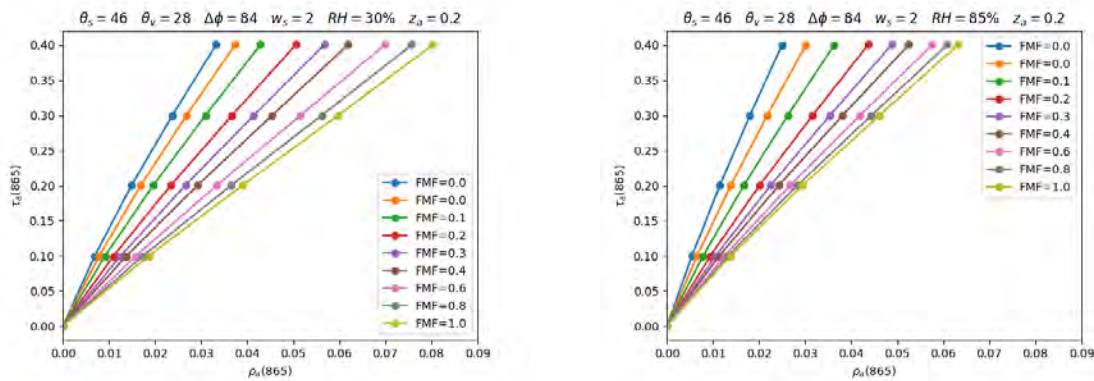
#### 4.3.2.8 AOT COMPUTATION

AOT at 865 nm (i.e.  $\tau_{a0}$ ) is required for the ALH assessment, the computation of atmospheric transmittance, and is also a Level-2 product. Since aerosol in the OC-SAC retrieval is formulated in terms of  $\rho_{a0}$ , a convenient way is to tabulate the relationship  $\tau_{a0} = P(\rho_{a0})$  for all grid. This is achieved by 3<sup>rd</sup> order polynomial, without a zero order term:

$$\tau_{a0} = \sum_{i=1}^3 d_i(iaer, z_a, \tau_R, \Omega, w_s) * (\rho_{a0})^i \quad (\text{OP-SAC-CWAC-AOT-1})$$

The polynomial fit was achieved up to an AOT of 0.4, similarly to the aerosol reflectance LUT nodes (see examples on Figure 23). In order to not apply the polynomial on its decreasing part, in case of too high reflectance, it is checked that its derivative is positive at given  $\rho_{a0}$ . If not, the maximum allowed AOT is given:

$$\tau_{a0} = \tau_{a0\_max} \text{ if } \sum_{i=1}^3 i * d_i(iaer, z_a, \tau_R, \Omega, w_s) * (\rho_{a0})^{i-1} < 0 \quad (\text{OP-SAC-CWAC-AOT-2})$$



**Figure 23. Aerosol optical thickness versus aerosol reflectance, both at 865, for various FMFs (see colours) and two values of relative humidity: left 30%, right 85%.**

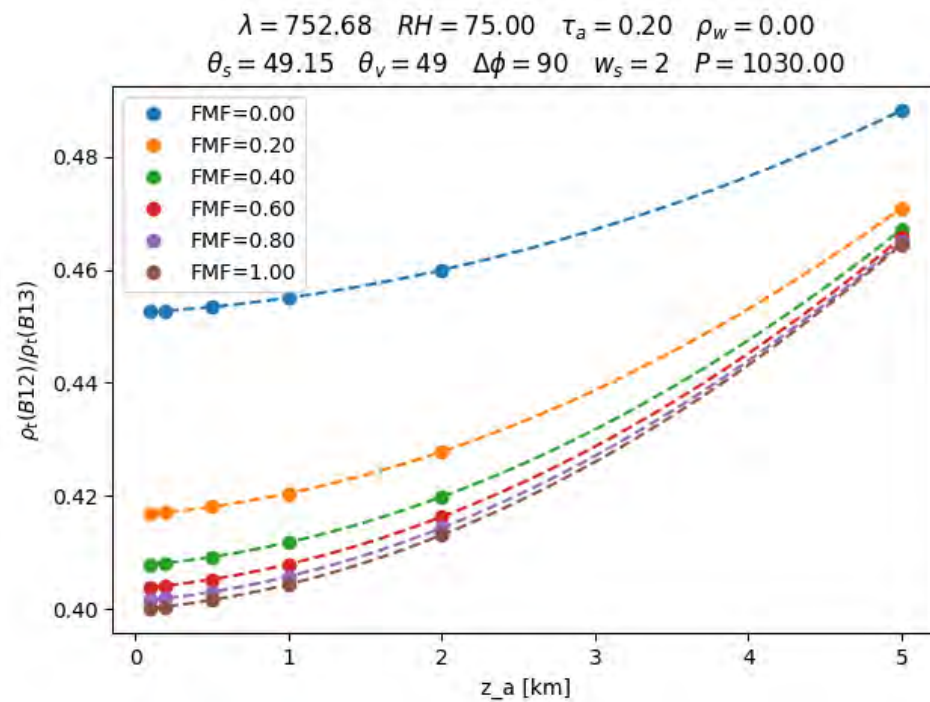
#### 4.3.2.9 ALH ASSESSMENT

The ALH algorithm follows the principle of Dubuisson et al. (2009), that relies on the tabulated relationship between ALH and the reflectance ratio of an absorbing channel and the non-absorbing channel Oa12. This approach usually needs an estimate of the aerosol amount ( $\tau_{a0}$ ) and type (SSA). Here the idea is to loop over the aerosol models (*iaer*), what gives the SSA, and take for each of them the first guess estimate  $\tau_{a0\_init}(iaer)$ . This gives a set of  $z_a(iaer)$ , to be used in the CWAC detection. The surface reflectance, which is also an input of the O<sub>2</sub> ratio LUT, is given by  $t\rho_{wC2}(754)$  from BPC, divided by the actual diffuse transmittance (i.e. first guess transmittance in the initial OC-SAC loop and for first standard aerosol pass, or from CWAC transmittance in all other cases).

The first version of the algorithm uses only one absorbing channel (Oa13) and a direct inversion of the Oa12/Oa13 ratio versus  $z_a$ :

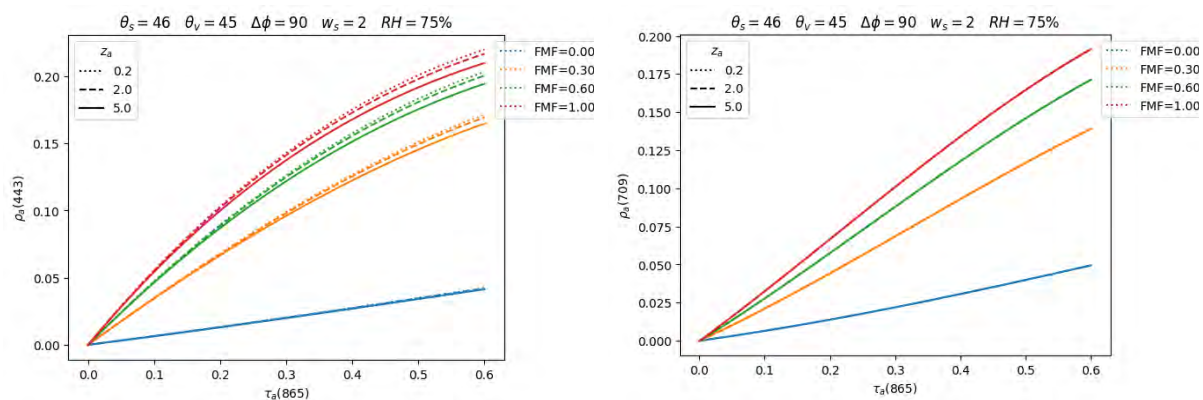
$$ratio = \frac{\rho_{ng}(760)}{\rho_{ng}(753)} \quad (OP-SAC-CWAC-ALH-1)$$

The inversion is achieved thanks to a 2<sup>nd</sup> order polynomial fitting (Figure 24). The input radiometry is only corrected for gaseous absorption but not for O<sub>2</sub> ( $\rho_{ng}$ , not corrected for O<sub>2</sub> at 754 and 761 nm). Improving the robustness to the surface contamination could be attempted with a more evolved inversion, like spectral fitting using the three OLCI available ratios.



**Figure 24. Relationship between O<sub>2</sub> ratio and  $z_a$ , for a specific parametrization (see title) and for various FMF (see colours).**

In practice, ALH only impacts the aerosol signal in the visible bands (see Figure 25). This is why a default ALH of 0.2 km can be considered for the aerosol retrieval in the NIR, and the ALH module is launched only for the relevant aerosol models used for atmospheric correction in the visible.



**Figure 25. Aerosol reflectance versus AOT, for various FMF (colour) and ALH (dotted, dashed, and solid lines). Left at 443 nm and right at 709 nm (no impact of ALH).**

#### 4.3.2.10 STANDARD AEROSOL IDENTIFICATION

The goal of the proposed method is to detect unambiguously the aerosol models, in the NIR-SWIR only for weakly absorbing models. The standard aerosol retrieval that we propose is inspired by the work of Ibrahim et al. (2019). The detection seeks to minimize the discrepancy between the observed radiometry and the modelled radiometry by radiative transfer. Because the Rayleigh correction is purely subtractive, this discrepancy can be defined equivalently either in terms of  $\rho_{path}$  or  $\rho_a$  (strict equivalence has been checked numerically in the inversion). Considering the fact that the aerosol signal is tabulated without Rayleigh (but still with Rayleigh coupling), it is more convenient to choose the formulation with respect to  $\rho_a$ . Definition of observation is thus defined by:

$$\rho_a^{obs}(\lambda) = \rho_{gc}(\lambda) - \rho_R(\lambda) - t\rho_{wc2}(\lambda) \quad (\text{OP-SAC-CWAC-ID-1})$$

The modelled aerosol signal,  $\rho_a^{mod}$ , depends on many variables, as reflected in the LUT (see section 4.3.1.11). Wavelength, ROT, geometry, wind speed and RH are known. With  $\rho_{a0}$  being already quantified (section 4.3.2.7), the remaining unknown is the fine mode fraction ( $f_v$ ). The method relies on the fact that the spectral behavior of the aerosol reflectance varies smoothly and monotonously with respect to the discrete fine mode fraction,  $f_v$ . In this sense, the combination of  $RH$  (known for a given observation) and  $f_v$  (unknown) defines a list of candidate models,  $iaer = \{RH, f_v\}$ , which are ordered under a physical relationship (basically in the MSE plane). Under this ordering, the candidate models inevitably result in a limited number of bracketing possibilities, noted schematically by two successive indices:  $(iaer; iaer + 1)$ . The aerosol reflectance model is a linear mixing between both, with interpolation coefficient noted  $mix$ . It follows that the two degrees of freedom are thus  $(iaer, mix)$ , for given  $\rho_{a0}$ :

$$\begin{aligned} \rho_a^{mod}(\lambda, \rho_{a0}, iaer, mix) \\ = (1 - mix)\rho_a^{iaer}(\lambda, \rho_{a0}) + mix * \rho_a^{iaer+1}(\lambda, \rho_{a0}) \end{aligned} \quad (\text{OP-SAC-CWAC-ID-2})$$

Where here only the dependency on wavelength is kept and  $\rho_a^{iaer}$  is computed for a given model  $iaer$  from the LUT and polynomial relationship with respect to  $\rho_{a0}$ .

The optimization problem is solved in two steps:

1. For each model  $iaer$  (and implicitly its successor  $iaer + 1$ ), minimize the cost function  $\chi_{iaer}^2$ , defined by a weighted average of the differences between observation and simulations at  $N_{NIR}$  bands in the NIR-SWIR:

$$\chi_{iaer}^2(mix) = \sum_{\lambda_{NIR}} w(\lambda) \left( \rho_a^{mod}(\lambda, \rho_{a0}, iaer, mix) - \rho_a^{obs}(\lambda) \right)^2 \quad (\text{OP-SAC-CWAC-ID-3})$$

2. Then select the two best bracketing models with lowest  $\chi_{iaer}^2$ .

The weights  $w(\lambda)$  are set to unity by default, but ideally come from a per-pixel uncertainty analysis (see section 4.3.2.15).

Due to linearity of the forward model on the mixing ratio, it is possible to compute the analytic solution of  $mix$  (which implicitly depends on  $\rho_{a0}$ ):

$$\begin{aligned}
& \text{mix} \\
& = \frac{\sum_{\lambda_{NIR}} w(\lambda) \left( \rho_a^{obs}(\lambda) - \rho_a^{iaer}(\lambda, \rho_{a0}) \right) \left( \rho_a^{iaer+1}(\lambda, \rho_{a0}) - \rho_a^{iaer}(\lambda, \rho_{a0}) \right)}{\sum_{\lambda_{NIR}} w(\lambda) \left( \rho_a^{iaer+1}(\lambda, \rho_{a0}) - \rho_a^{iaer}(\lambda, \rho_{a0}) \right)^2} \quad (\text{OP-SAC-CWAC-ID-4})
\end{aligned}$$

#### 4.3.2.11 STRONGLY ABSORBING AEROSOL DETECTION

The proposed detection of absorbing models is an extension of the initial approach of Nobileau and Antoine (2005) based on the “hinge point” at 510 nm, with a consolidated climatology of marine reflectance,  $\rho_w^{clim}$ , and a metric using more spectral bands.

We use the climatology from ESA OC-CCI (Sathyendranath et al., 2021; courtesy of PML), computed over 25 years of ocean colour data (see Figure 27). This climatology is constructed from monthly Level-3 products on a bin grid of 4km. The standard-deviation,  $\sigma^{clim}$ , hence only comprises the inter-annual variability (not intra-monthly).

The metric,  $\chi_{clim}^2$ , is defined by:

$$\chi_{clim}^2 = \frac{1}{N_{clim}} \sum_{\lambda} \left( \frac{\rho_w(\lambda) - \rho_w^{clim}(\lambda)}{3 * \sigma^{clim}} \right)^2 \quad (\text{OP-SAC-CWAC-ABS-1})$$

Examples for two cases are shown in Figure 26, when using 3 bands: 510, 560 and 665 nm. The dust event is well captured for large  $\chi_{clim}^2$ , typically higher than unity, while the scene with supposedly standard aerosol show value below unity. The detection is thus based on a threshold,  $\chi_{clim}^2_{thresh}$ , whose definitive value has to be tuned and check for marine and atmospheric conditions:

$$\chi_{clim}^2 > \chi_{clim}^2_{thresh} \quad (\text{OP-SAC-CWAC-ABS-2})$$

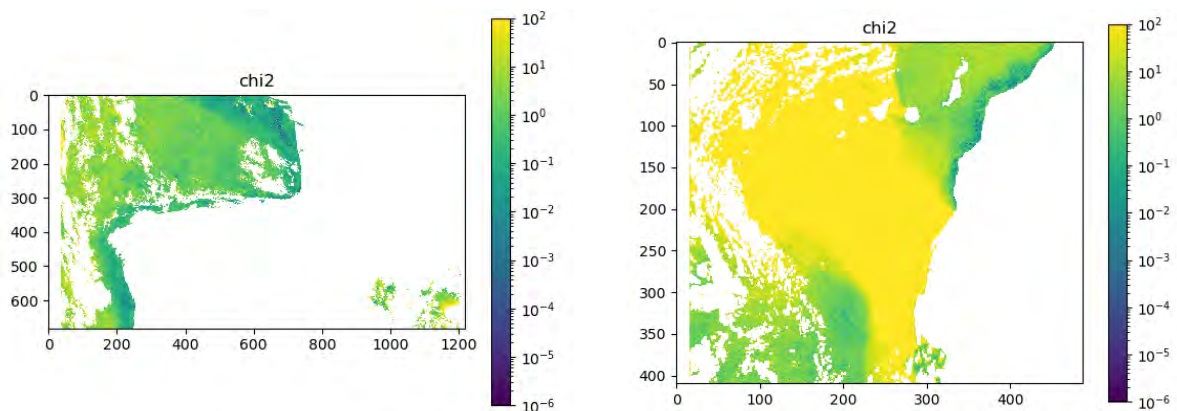


Figure 26. Maps of  $\chi_{clim}^2$  over two regions: Bay of Biscay (left, OLCI-A 23.01.2017) and a Saharan dust event (right, OLCI-A 05.02.2019)

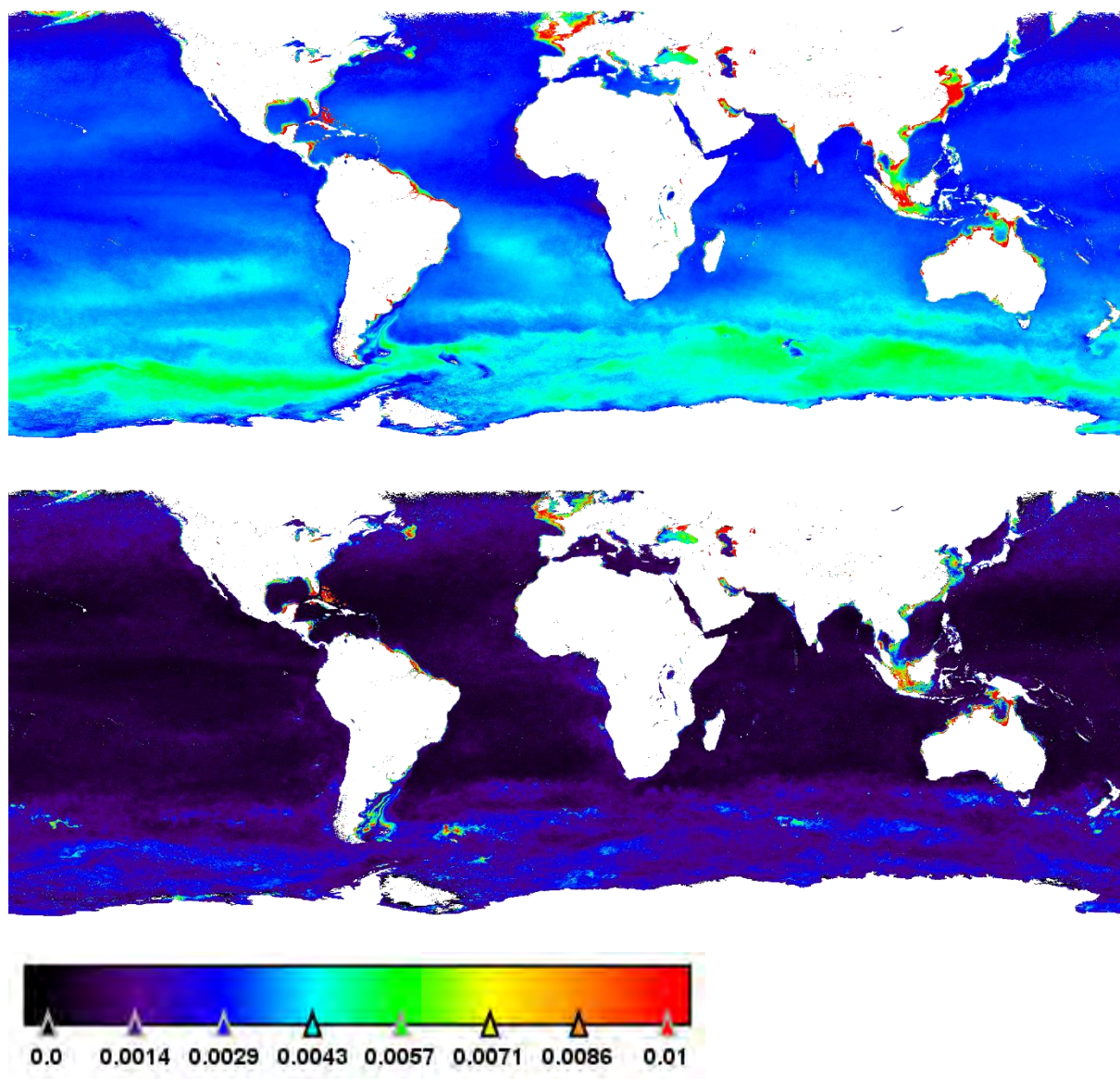


Figure 27. ESA OC-CCI climatology at 510 nm for January, top  $\rho_w^{clim}$ , bottom  $3 * \sigma^{clim}$  (same colour scale). Note that these maps are in unit of Rrs (sr-1).

#### 4.3.2.12 STRONGLY ABSORBING AEROSOL IDENTIFICATION

The core idea of the CWAC module is to use as much as possible the same methodology for standard and strongly absorbing models identification, i.e. a chi-square minimization, but use new bands in the visible in the second case:

$$\chi_{iaer}^2(mix) = \sum_{\lambda_{NIR} + \lambda_{VIS}} w(\lambda) \left( \rho_a^{mod}(\lambda, \rho_{a0}, iaer, mix) - \rho_a^{obs}(\lambda) \right)^2 \quad (OP-SAC-CWAC-ID-5)$$

The observation in the VIS comes now precisely from the climatology:

$$\rho_a^{obs}(\lambda_{VIS}) = \rho_{Rc}(\lambda_{VIS}) - t_{atm}(\lambda_{VIS}) \rho_w^{clim}(\lambda_{VIS}) \quad (OP-SAC-CWAC-ID-6)$$

While  $\rho_w^{clim}$  is known and fixed for a given pixel, there are two differences with the standard model identification:

- i. The total atmospheric transmittance,  $t_{atm}(\lambda)$ , now also depends on the unknown  $\tau_{a0, mix}$ . Hence, contrary to Eq. (OP-SAC-CWAC-ID-1), Eq. (OP-SAC-CWAC-ID-6) cannot be pre-computed for the current pixel outside the aerosol identification.
- ii.  $\rho_w^{clim}$  cannot be considered as an exact per-pixel value; its uncertainty is likely higher than  $t_{\rho_{WC2}}$  and must be included in the VIS-NIR band weighting.

The weighting uses the BPC and climatology uncertainties:

$$w(\lambda_{NIR}) = 1 / (\sigma_{t_{\rho_{WC2}}})^2 \quad (OP-SAC-CWAC-ID-7)$$

And

$$w(\lambda_{VIS}) = 1 / (3 * \sigma^{clim})^2 \quad (OP-SAC-CWAC-ID-8)$$

The mixing of atmospheric transmittance for two aerosols is done in log scale, as explained hereafter, and provided by Eq. (OP-SAC-CWAC-COR-5). This makes the chi-square minimization a non-linear problem. However, we have checked that a very good linear approximation is given by:

$$t_{atm}(\lambda) \approx t_{atm}^{ia1}(\lambda) * \left( 1 + mix * \ln \frac{t_{atm}^{ia2}(\lambda)}{t_{atm}^{ia1}(\lambda)} \right)$$

The partial derivative with respect to  $mix$  is given exactly by  $\frac{\partial t_{atm}}{\partial mix} = t_{atm} * \ln \frac{t_{atm}^{ia2}}{t_{atm}^{ia1}}$ . Then, it can be shown that minimizing  $\chi_{iaer}^2$  is equivalent to solving a quadratic equation with respect to  $mix$ :

$$\sum_{\lambda_{NIR} + \lambda_{VIS}} w(\lambda) (k_1(\lambda) + k_2(\lambda) * mix) (k_2(\lambda) + k_3(\lambda) * mix) \quad (OP-SAC-CWAC-ID-9)$$

$$\text{with } \begin{cases} k_1(\lambda) = \rho_a^{iaer}(\lambda, \rho_{a0}) - \rho_{Rc}(\lambda) + t_{atm}^{ia1}(\lambda) \rho_w^{clim}(\lambda) \\ k_2(\lambda) = \rho_a^{iaer+1}(\lambda, \rho_{a0}) - \rho_a^{iaer}(\lambda, \rho_{a0}) + \ln \frac{t_{atm}^{ia2}(\lambda)}{t_{atm}^{ia1}(\lambda)} t_{atm}^{ia1}(\lambda) \rho_w^{clim}(\lambda) \\ k_3(\lambda) = \left( \ln \frac{t_{atm}^{ia2}(\lambda)}{t_{atm}^{ia1}(\lambda)} \right)^2 t_{atm}^{ia1}(\lambda) \rho_w^{clim}(\lambda) \end{cases}$$

We recall the fact that, if the summation is limited to NIR bands with  $t_{atm}(\lambda) \rho_w^{clim}(\lambda) = t \rho_{wc2}(\lambda)$  (i.e. not depending on *mix* such that formally  $\ln \frac{t_{atm}^{ia2}(\lambda)}{t_{atm}^{ia1}(\lambda)} = 0$ ), then Eq. (OP-SAC-CWAC-ID-9) becomes a linear equation whose solution was given previously in the case of standard aerosol identification by Eq. (OP-SAC-CWAC-ID-4). This solution is actually selected when the quadratic equation has no solution, i.e., when:

$$\begin{aligned} & \left( \sum_{\lambda_{NIR} + \lambda_{VIS}} w(\lambda) (k_1(\lambda) k_3(\lambda) + k_2^2(\lambda)) \right)^2 \\ & - 4 \left( \sum_{\lambda_{NIR} + \lambda_{VIS}} w(\lambda) k_2(\lambda) k_3(\lambda) \right) \left( \sum_{\lambda_{NIR} + \lambda_{VIS}} w(\lambda) k_1(\lambda) k_2(\lambda) \right) < 0 \end{aligned} \quad (\text{OP-SAC-CWAC-ID-10})$$

#### 4.3.2.13 AEROSOL CORRECTION

The correction consists in first computing aerosol reflectance and atmospheric transmittance for both bracketing models *iaer* = ia1, ia2:

$$\rho_a^{iaer}(\lambda) = \sum_{i=1}^{2 \text{ or } 4} c_i(\lambda, iaer) * (\rho_{a0})^i \quad (\text{OP-SAC-CWAC-COR-1})$$

Atmospheric transmittance is computed by interpolation of the LUT stored in log scale:

$$\begin{cases} \ln t_{down}^{iaer}(\lambda) = \log t_{down\_LUT}(\lambda, iaer, z_a(iaer), RH, \tau_R(\lambda), \tau_{a0}, \mu_s, w_s) \\ \ln t_{up}^{iaer}(\lambda) = \log t_{up\_LUT}(\lambda, iaer, z_a(iaer), RH, \tau_R(\lambda), \tau_{a0}, \mu_v) \end{cases} \quad (\text{OP-SAC-CWAC-COR-2})$$

In practice, only the total atmospheric transmittance,  $t_{atm}$ , is useful:

$$\ln t_{atm}^{iaer}(\lambda) = \ln t_{down}^{iaer}(\lambda) + \ln t_{up}^{iaer}(\lambda) \quad (\text{OP-SAC-CWAC-COR-3})$$

Then these quantities are weighted with respect to the mixing ratio:

$$\rho_a(\lambda) = (1 - mix) * \rho_a^{ia1}(\lambda) + mix * \rho_a^{ia2}(\lambda) \quad (\text{OP-SAC-CWAC-COR-4})$$

$$t_{atm}(\lambda) = e^{(1-mix) * \ln t_{atm}^{ia1}(\lambda) + mix * \ln t_{atm}^{ia2}(\lambda)} \quad (\text{OP-SAC-CWAC-COR-5})$$

Finally, the marine reflectance can be computed:

$$\rho_w(\lambda) = \left( \rho_{gc}(\lambda) - \rho_R(\lambda) - \rho_a(\lambda) \right) / t_{atm}(\lambda) \quad (\text{OP-SAC-CWAC-COR-6})$$

#### 4.3.2.14 SPECTRAL CORRECTION (“BOA SMILE CORRECTION”)

It is required to implement a band-shift of marine reflectance at nominal bands in the IPF (RB section 3.2.4) because it can be too complicated for users to handle it per detector. Band-shift ideally requires a full marine spectral model (Mélin and Sclep, 2015; Steinmetz 2020 for SACSO). This is however out of scope of the OC-SAC module per se.

A cubic spline interpolation is here implemented for the OC-SAC validation, as it is shown to already produce better results than the nominal TOA smile correction. This first needs to define the interpolation grid  $\lambda^{ex}$  and interpolated vector  $\rho_w^{ex}$ :

$$\begin{cases} \lambda^{ex} &= (\lambda_1, \dots, \lambda_{NBANDS\_OC}) \\ \rho_w^{ex} &= (\rho_w(\lambda_1), \dots, \rho_w(\lambda_{NBANDS\_OC})) \end{cases} \quad (\text{OP-SAC-SC-1})$$

where for OLCI  $NBANDS\_OC=16$  and refers to all bands outside absorption channels. To ease the implementation, the spline computation relies on the GLS library:

$$gsl\_spline\_init(spline, \lambda^{ex}, \rho_w^{ex}, NBANDS\_OC) \quad (\text{OP-SAC-SC-2})$$

where *spline* is the GSL object containing the spline interpolator. Then, marine reflectance at any theoretical band  $\lambda^{theo}$  is simply evaluated by:

$$\rho_w(\lambda^{theo}) = gsl\_spline\_eval(spline, \lambda^{theo}) \quad (\text{OP-SAC-SC-3})$$

Note that currently bands 400 and 1020 nm cannot be corrected with this GSL implementation because they are on the edge of the interpolation grid; this shall be handled in a next version of the algorithm.

#### 4.3.2.15 PER-PIXEL UNCERTAINTIES

The uncertainty of marine reflectance in the visible is estimated following the law of uncertainty propagation given by the GUM (BIPM, 2018). The interest of such formalism is to provide an analytical expression of the uncertainty per pixel, fast in term of CPU. Here we assume that uncertainties propagate only in the aerosol terms, and not in the Rayleigh component, but this latter contribution could be added to the present budget if known. Starting from the fundamental equation (OP-SAC-CWAC-COR-6), the generic term of the variance-covariance matrix  $C_{\rho_w}$  is given by:

$$u(\rho_w(\lambda_i), \rho_w(\lambda_j)) = \mathbf{v}(\lambda_i) \begin{pmatrix} u(\rho_{gc}(\lambda_i), \rho_{gc}(\lambda_j)) & u(\rho_{gc}(\lambda_i), \rho_a(\lambda_j)) & u(\rho_{gc}(\lambda_i), t_{atm}(\lambda_j)) \\ u(\rho_a(\lambda_i), \rho_{gc}(\lambda_j)) & u(\rho_a(\lambda_i), \rho_a(\lambda_j)) & u(\rho_a(\lambda_i), t_{atm}(\lambda_j)) \\ u(t(\lambda_i), \rho_{gc}(\lambda_j)) & u(t(\lambda_i), \rho_a(\lambda_j)) & u(t_{atm}(\lambda_i), t_{atm}(\lambda_j)) \end{pmatrix} \mathbf{v}(\lambda_j)^T \quad (12)$$

With  $\mathbf{v}(\lambda_i) = 1/t_{atm}(\lambda_i)(1, -1, -\rho_w(\lambda_i))$ . This general formulation simplifies because there is no error correlation between  $\rho_{gc}$  in the visible and the output of the atmospheric correction ( $\rho_{path}$  and  $t_{atm}$ , computed in the NIR), i.e.  $u(\rho_{gc}, \rho_a) = u(\rho_{gc}, t_{atm}) = 0$ . On the contrary, we expect a full anti-correlation between errors of path reflectance and transmittance, since both come from the same amount and type of aerosols, i.e.  $u(\rho_a, t_{atm}) = -u(\rho_a) * u(t_{atm})$ , as shown for instance in Liberti et al. (2020). The diagonal terms can be more explicitly written as:

$$u^2(\rho_w(\lambda_i)) = \frac{1}{t_{atm}} \left( u^2(\rho_{gc}(\lambda_i)) + \left( u(\rho_a(\lambda_i)) - \rho_w * u(t_{atm}(\lambda_i)) \right)^2 \right) \quad (13)$$

This expression shows that the correlation of errors between  $\rho_a$  and  $t_{atm}$  tends to decrease uncertainty on  $\rho_w$ , as one would expect: if for instance the aerosol load is erroneously too high, the error on  $\rho_w$  increases (negatively) due to that on  $\rho_a$ , but this growth is partially compensated by the division with a higher transmittance (closer to unity).

The uncertainty of  $\rho_a$  can also be computed from the law of propagation of uncertainties applied to Eq. (OP-SAC-CWAC-COR-4). This equation shows that aerosol reflectance depends solely on  $\rho_a^{obs}$  in the NIR, on the one hand through the mixing ratio  $mix$  (Eq. OP-SAC-CWAC-ID-4) and on the other hand through  $\rho_{a0}$ , which, in the present version, is exactly equal to  $\rho_a^{obs}(\lambda_0)$ . The input uncertainty required in this computation is thus the variance-covariance matrix  $\mathbf{C}_{\rho_a^{obs}}$  defined in the NIR, and is given by the upstream BPC with  $\mathbf{C}_{\rho_a^{obs}} = \mathbf{C}_{t\rho_{wc2}}$ . Considering the spectral dimension of the problem, with  $\boldsymbol{\rho}_a = (\rho_a(\lambda_{VIS,1}), \dots, \rho_a(\lambda_{VIS,M}))$  and  $\boldsymbol{\rho}_a^{obs} = (\rho_a(\lambda_{NIR,1}), \dots, \rho_a(\lambda_{NIR,N}))$ , the variance-covariance matrix  $\mathbf{C}_{\rho_a}$  is given by the matrix product:

$$\mathbf{C}_{\rho_a} = \left( \frac{\partial \boldsymbol{\rho}_a}{\partial \boldsymbol{\rho}_a^{obs}} \right) \mathbf{C}_{\rho_a^{obs}} \left( \frac{\partial \boldsymbol{\rho}_a}{\partial \boldsymbol{\rho}_a^{obs}} \right)^T \quad (14)$$

Where  $\left( \frac{\partial \boldsymbol{\rho}_a}{\partial \boldsymbol{\rho}_a^{obs}} \right)$  is the Jacobian matrix of size  $M \times N$  defined by:

$$\left( \frac{\partial \boldsymbol{\rho}_a}{\partial \boldsymbol{\rho}_a^{obs}} \right) = \begin{pmatrix} \frac{\partial \rho_a(\lambda_{VIS,1})}{\partial \rho_a^{obs}(\lambda_{NIR,1})} & \dots & \frac{\partial \rho_a(\lambda_{VIS,1})}{\partial \rho_a^{obs}(\lambda_{NIR,N})} \\ \vdots & \ddots & \vdots \\ \frac{\partial \rho_a(\lambda_{VIS,M})}{\partial \rho_a^{obs}(\lambda_{NIR,1})} & \dots & \frac{\partial \rho_a(\lambda_{VIS,M})}{\partial \rho_a^{obs}(\lambda_{NIR,N})} \end{pmatrix} \quad (15)$$

To ease the notations, we will use  $\rho_{a0}$  instead of  $\rho_a^{obs}(\lambda_0)$  in the following. From Eq. (OP-SAC-CWAC-COR-4), these partial derivatives are computed as follows:

$$\frac{\partial \rho_a(\lambda_i)}{\partial \rho_a^{obs}(\lambda_j)} = \begin{cases} \frac{\partial mix}{\partial \rho_a^{obs}(\lambda_j)} * (\rho_a^{ia2}(\lambda_i) - \rho_a^{ia1}(\lambda_i)) & \text{if } \lambda_j \neq \lambda_0 \\ \frac{\partial mix}{\partial \rho_{a0}} * (\rho_a^{ia2}(\lambda_i) - \rho_a^{ia1}(\lambda_i)) + (1 - mix) \frac{\partial \rho_a^{ia1}(\lambda_i)}{\partial \rho_{a0}} + mix \frac{\partial \rho_a^{ia2}(\lambda_i)}{\partial \rho_{a0}} & \text{if } \lambda_j = \lambda_0 \end{cases} \quad (16)$$

Computation of  $\frac{\partial mix}{\partial \rho_a^{obs}}$  is the most cumbersome but can still be achieved analytically:

$$\frac{\partial mix}{\partial \rho_a^{obs}(\lambda_j)} = \frac{w(\lambda_j)(\rho_a^{ia2}(\lambda_j) - \rho_a^{ia1}(\lambda_j))}{\sum_{\lambda_{NIR}} w(\lambda)(\rho_a^{ia2}(\lambda) - \rho_a^{ia1}(\lambda))^2} \text{ if } \lambda_j \neq \lambda_0 \quad (17)$$

And

$$\frac{\partial mix}{\partial \rho_{a0}} = \frac{\frac{\partial U}{\partial \rho_{a0}} * V - U * \frac{\partial V}{\partial \rho_{a0}}}{V^2} \quad (18)$$

With

$$\begin{cases} U(\rho_{a0}) &= \sum_{\lambda_{NIR}} w(\lambda) (\rho_a^{obs}(\lambda) - \rho_a^{ia1}(\lambda, \rho_{a0})) (\rho_a^{ia2}(\lambda, \rho_{a0}) - \rho_a^{ia1}(\lambda, \rho_{a0})) \\ V(\rho_{a0}) &= \sum_{\lambda_{NIR}} w(\lambda) (\rho_a^{ia2}(\lambda, \rho_{a0}) - \rho_a^{ia1}(\lambda, \rho_{a0}))^2 \\ \frac{\partial U}{\partial \rho_{a0}} &= \sum_{\lambda_{NIR}} w(\lambda) (\rho_a^{obs}(\lambda) - \rho_a^{ia1}(\lambda, \rho_{a0})) \left( \frac{\partial \rho_a^{ia2}}{\partial \rho_{a0}}(\lambda, \rho_{a0}) - \frac{\partial \rho_a^{ia1}}{\partial \rho_{a0}}(\lambda, \rho_{a0}) \right) \\ &\quad - w(\lambda) \frac{\partial \rho_a^{ia1}}{\partial \rho_{a0}}(\lambda, \rho_{a0}) (\rho_a^{ia2}(\lambda, \rho_{a0}) - \rho_a^{ia1}(\lambda, \rho_{a0})) \\ \frac{\partial V}{\partial \rho_{a0}} &= 2 \sum_{\lambda_{NIR}} w(\lambda) (\rho_a^{ia2}(\lambda, \rho_{a0}) - \rho_a^{ia1}(\lambda, \rho_{a0})) \left( \frac{\partial \rho_a^{ia2}}{\partial \rho_{a0}}(\lambda, \rho_{a0}) - \frac{\partial \rho_a^{ia1}}{\partial \rho_{a0}}(\lambda, \rho_{a0}) \right) \end{cases} \quad (19)$$

Finally, the derivatives  $\frac{\partial \rho_a^{ia}(\lambda_i)}{\partial \rho_{a0}}$  with  $\lambda_i$  in the visible can be explicitly computed thanks to the polynomial formulation, Eq. (OP-SAC-CWAC-COR-1):

$$\frac{\partial \rho_a^{ia}(\lambda_i)}{\partial \rho_{a0}} = \sum_{i=1}^4 c_i(\lambda, iaer) * i * (\rho_{a0})^{i-1} \quad (20)$$

Computing uncertainties of the total transmittance  $t_{atm}$  follows the same principles. The variance-covariance matrix  $C_t$  is given by the matrix product:

$$C_t = \left( \frac{\partial t_{atm}}{\partial \rho_a^{obs}} \right) C_{\rho_a^{obs}} \left( \frac{\partial t_{atm}}{\partial \rho_a^{obs}} \right)^T \quad (21)$$

Where  $\left( \frac{\partial t_{atm}}{\partial \rho_a^{obs}} \right)$  is the Jacobian matrix of size MxN defined by:

$$\left( \frac{\partial t_{atm}}{\partial \rho_a^{obs}} \right) = \begin{pmatrix} \frac{\partial t_{atm}(\lambda_{VIS,1})}{\partial \rho_a^{obs}(\lambda_{NIR,1})} & \dots & \frac{\partial t_{atm}(\lambda_{VIS,1})}{\partial \rho_a^{obs}(\lambda_{NIR,N})} \\ \vdots & \ddots & \vdots \\ \frac{\partial t_{atm}(\lambda_{VIS,M})}{\partial \rho_a^{obs}(\lambda_{NIR,1})} & \dots & \frac{\partial t_{atm}(\lambda_{VIS,M})}{\partial \rho_a^{obs}(\lambda_{NIR,N})} \end{pmatrix} \quad (22)$$

Each partial derivative is computed by:

$$\frac{\partial t_{atm}(\lambda_i)}{\partial \rho_a^{obs}(\lambda_j)} = \begin{cases} \frac{\partial mix}{\partial \rho_a^{obs}(\lambda_j)} * \ln \frac{t_{atm}^{ia2}(\lambda_i)}{t_{atm}^{ia1}(\lambda_i)} & \text{if } \lambda_j \neq \lambda_0 \\ \frac{\partial mix}{\partial \rho_{a0}} * \ln \frac{t_{atm}^{ia2}(\lambda_i)}{t_{atm}^{ia1}(\lambda_i)} + (1 - mix) \frac{1}{t_{atm}^{ia1}(\lambda_i)} \frac{\partial t_{atm}^{ia1}(\lambda_i)}{\partial \rho_{a0}} & \\ + mix \frac{1}{t_{atm}^{ia2}(\lambda_i)} \frac{\partial t_{atm}^{ia2}(\lambda_i)}{\partial \rho_{a0}} & \text{if } \lambda_j = \lambda_0 \end{cases} \quad (23)$$

The partial derivatives of  $mix$  with respect to  $\rho_a^{obs}$  have already been provided above. The only difference with the analytical computation of  $\partial \rho_a^{ia}(\lambda_i) / \partial \rho_{a0}$  given by Eq. (20) is that  $t_{atm}^{ia}$  is interpolated in a LUT with respect to  $\tau_{a0}$ . To avoid numerical differentiation in the LUT, we can assume that transmittance varies exponentially with  $\tau_{a0}$ , so that we have:

$$\begin{aligned} \frac{1}{t_{atm}^{ia}(\lambda_i)} \frac{\partial t_{atm}^{ia}(\lambda_i)}{\partial \rho_{a0}} &= \frac{1}{t_{atm}^{ia}(\lambda_i)} \frac{\partial t_{atm}^{ia}(\lambda_i)}{\partial \tau_{a0}} \frac{\partial \tau_{a0}}{\partial \rho_{a0}} \\ &= \frac{\ln t_{atm}^{ia}(\lambda_i)}{t_{atm}^{ia}(\lambda_i)} \frac{\partial \tau_{a0}}{\partial \rho_{a0}} \end{aligned} \quad (24)$$

The derivative  $\frac{\partial \tau_{a0}}{\partial \rho_{a0}}$  has already been expressed in Eq. (OP-SAC-CWAC-AOT-2), what completes the uncertainty propagation.

#### 4.3.2.16 FLAGGING

The following flags are handled in OC-SAC:

MEGLINT (medium glint): raised if the Sun glint reflectance (at sea level) is higher than a threshold.

HIGHGLINT: raised if Sun glint reflectance is higher than a threshold (relative to the gaseous corrected TOA reflectance at 865 nm) or if the glint correction yields any negative reflectance from 400 to 1020 nm.

WHITECAPS: raised if wind speed is higher than a threshold.

HIINLD: raised if pressure is below a threshold. Note that the name could be changed because it is not self-explanatory.

BPAC\_ON: raised when BPC is applied and successful. Note that it could be changed to BPC\_ON for consistency with the name of the processing step.

CASE2\_S: raised when TSM computed by BPC is higher than a threshold.

WHITE\_SCATT (white scatterers, e.g. coccoliths): raised when the slope of Rayleigh corrected radiometry between 620 and 709 nm is below a threshold.

ICE\_HIGHAERO: raised outside glint if Level-1 BRIGHT flag is raised, or if the glint corrected reflectance at 412 nm is higher than a threshold (geometry dependent); deactivated if WHITE\_SCATT is raised.

AC\_FAIL: raised when BPC failed (i.e. not BPAC\_ON). Note that the CWAC is launched even if AC\_FAIL is raised. In IPF of Collection 3, AC\_FAIL was raised for the following reasons, which do not longer apply:

- i.  $\rho_{gc}(\lambda) - t\rho_{wc2}(\lambda) < \rho_R(\lambda)$  at  $\lambda = 779$  or  $865$  nm, which is equivalent to  $\rho_a^{obs}(\lambda) < 0$ ; now the spectral matching algorithm can deal with negative observation.
- ii. No candidate model; now there is always a couple of best bracketing models identified.
- iii. Negative optical thickness: this is impossible as  $\tau_{a0}$  is bounded in a positive domain and the spectral dependence cannot produce negative values.
- iv. Negative  $\rho_a^{mod}(\lambda)$  at any band in the visible, or  $\tau_a(\lambda)$  higher than the value where 2<sup>nd</sup> order polynomial is maximum; now  $\rho_a^{mod}$  cannot be negative and the polynomial relationship is given at all bands with respect to  $\tau_{a0}$ .

*Update of ACFAIL with respect to chi2 to be considered in future version.*

F\_ORINP0: for consistency with current operational CWAC, this internal flag is raised when a LUT interpolation returns a no-zero status (e.g. when the point to interpolate is outside the range of the tabulated grid); note however that this internal flag is never used in the IPF.

Annotation flags as existing in OLCI products of Collection 3 are implemented as follows:

RWNEG\_O01 to RWNEG\_O21: raised when marine reflectance is below a threshold (allows slightly negative value).

ANNOT\_ABSOA: raised when strongly absorbing aerosol is detected.

ANNOT\_ALPHA: raised If Angstrom cannot be computed because of negative AOT at 779 and 865 nm; note that this is now impossible (see above). Hence this flag could be removed.

ANNOT\_MIXR1: raised if mixing ratio is 0 or 1.

ANNOT\_TAU: raised if AOT at 865 nm is greater than a threshold (currently 0.4, stored in ADF).

ANNOT\_AERO\_B and ANNOT\_AERO\_D: not implemented since OC-SAC does not distinguish blue and dust models. Hence this flag could be removed.

ANNOT\_ACLIM: not implemented as consistency between the existing climatology and new Ahmad et al. (2010) models was not checked. Hence this flag could be removed.

ANNOT\_DROUT: not implemented as the test at 510 nm is now replaced by a more complex chi-square test on various bands. Hence this flag could be removed.

#### 4.4 ALGORITHM OUTPUT

The outputs of the OC-SAC algorithm are listed in Table 7. These fields are part of the IPF pix\_t structure.

**Table 7 OC-SAC algorithm outputs. In column Type, *o* and *b* refers to *output* variables (included directly or indirectly in Level-2 product) and *breakpoints* (intermediate data), respectively, as handled in the OLCI Level-2 processor.**

| Processing step | Variable               | Description                                                                          | Type     | Unit             |
|-----------------|------------------------|--------------------------------------------------------------------------------------|----------|------------------|
| OP-SAC-WPP-SVC  | $\rho_{ng}^*(\lambda)$ | TOA reflectance corrected for gaseous absorption and SVC gains, at pixel wavelengths | <i>b</i> | dl               |
| OP-SAC-WPP-RAY  | $\tau_R(\lambda)$      | Rayleigh optical thickness corrected for pressure, at pixel wavelengths              | <i>b</i> | dl               |
|                 | $\rho_R(\lambda)$      | Rayleigh reflectance at pixel wavelengths                                            | <i>b</i> | dl               |
| OP-SAC-WPP-GLT  | $\rho_G$               | Sun glint reflectance (at sea level)                                                 | <i>b</i> | dl               |
|                 | $T\rho_G(\lambda)$     | TOA glint reflectance at pixel wavelengths                                           | <i>b</i> | dl               |
|                 | $\rho_{gc}(\lambda)$   | Glint corrected reflectance at pixel wavelengths (first step)                        | <i>b</i> | dl               |
| OP-SAC-WPP-WCP  | $\rho_{wc}(\lambda)$   | White-caps reflectance at pixel wavelengths                                          | <i>b</i> | dl               |
|                 | $t\rho_{wc}(\lambda)$  | TOA white-caps reflectance at pixel wavelengths                                      | <i>b</i> | dl               |
|                 | $\rho_{gc}(\lambda)$   | Glint corrected reflectance at pixel wavelengths (second step)                       | <i>b</i> | dl               |
| OP-SAC-BPC      | $b_{bp0}$              | Particulate backscattering at 779 nm                                                 | <i>b</i> | m <sup>-1</sup>  |
|                 | <i>TSM</i>             | Total suspended matter, used for CASE2_S flag                                        | <i>b</i> | g/m <sup>3</sup> |
|                 | $\rho_w(\lambda)$      | Marine reflectance at pixel wavelengths in the NIR                                   | <i>b</i> | dl               |
|                 | $t\rho_{wc2}(\lambda)$ | TOA marine reflectance at pixel wavelengths in the NIR                               | <i>b</i> | dl               |
|                 | chisq                  | BPC cost function at convergence                                                     | <i>b</i> | dl               |
|                 | bpc_niter              | Number of BPC iterations                                                             | <i>b</i> | dl               |

| Processing step | Variable          | Description                                                         | Type     | Unit |
|-----------------|-------------------|---------------------------------------------------------------------|----------|------|
| OP-SAC-CWAC-ALH | $z_a$             | ALH                                                                 | <i>b</i> | km   |
| OP-SAC-CWAC-ID  | cwac_niter        | Number of iterations for the retrieved bracketing models            | <i>b</i> | dl   |
|                 | ia1               | FMF index of lower bracketing model                                 | <i>b</i> | dl   |
|                 | ia2               | FMF index of upper bracketing model                                 | <i>b</i> | dl   |
|                 | aer_mix           | Mixing ratio between bracketing models                              | <i>b</i> | dl   |
| OP-SAC-CWAC-COR | $\rho_a(\lambda)$ | Aerosol reflectance at pixel wavelengths                            | <i>b</i> | dl   |
|                 | $\tau_a(\lambda)$ | Aerosol optical thickness at nominal wavelengths                    | <i>b</i> | dl   |
|                 | $\tau_a(865)$     | Aerosol optical thickness at nominal 865 nm band                    | <i>o</i> | dl   |
|                 | $\alpha$          | Angstrom exponent between 779 and 865 nm                            | <i>o</i> | dl   |
|                 | $t_d(\lambda)$    | Downward transmittance at pixel wavelengths                         | <i>b</i> | dl   |
|                 | $t_u(\lambda)$    | Upward transmittance at pixel wavelengths                           | <i>b</i> | dl   |
|                 | $\rho_w(\lambda)$ | Directional marine reflectance at pixel wavelengths (first step)    | <i>b</i> | dl   |
|                 | chi2              | CWAC cost function at convergence                                   | <i>b</i> | dl   |
| OP-SAC-CWAC-SML | $\rho_w(\lambda)$ | Directional marine reflectance at nominal wavelengths (second step) | <i>o</i> | dl   |

## 4.5 PRACTICAL CONSIDERATIONS

### 4.5.1 HIGH-LEVEL DESCRIPTION OF THE PROTOTYPED SOFTWARE

The detailed description of the OC-SAC and CWAC modules is given in [AD-3]. Briefly, the software architecture (Figure 28) follows exactly the algorithm design already presented in section 4.1. The module has been integrated into both the OLCI operational processor at EUMETSAT (IPF) and the SACSO prototype processor [AD-4], adapted and renamed as OC-SAC-SACSO prototype. The module is simply plugged-in the IPF code thanks to the use of following variables:

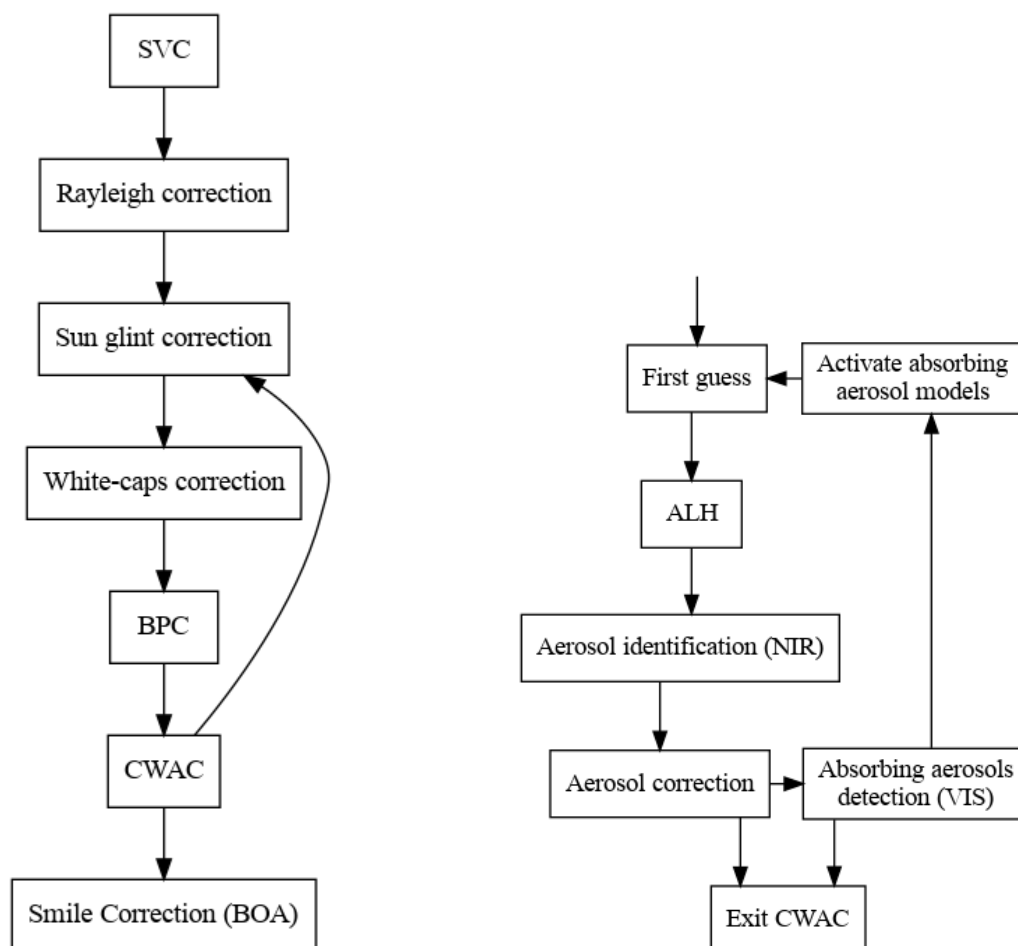
1. *pixel* structure (*pix\_t* pointer defined in *pixel.h*): main object containing inputs at pixel level for all OC-SAC modules and functions. This structure keeps all fields required by the processor beyond OC-SAC (TOA radiometry, geometry, etc.) and is cleaned/updated for the specific OC-SAC fields. The SACSO processor deals with the same structure but use only the relevant fields.
2. *adf* structure (defined in *olci\_adh.h*): global variable containing the required auxiliary data.

LUTs interpolation routines are those already existing in the IPF. Hence, the data formats of the multidimensional auxiliary variables also follow those of the IPF (either *S\_LUT* structure or one-dimensional array). The SACSO prototype uses its own routines, with same signatures, for perfect compatibility of the OC-SAC routines shared in both processors.

Data storage of new LUTs follows the existing S3 specifications: netCDF file with XML manifest. The list of updated ADFs is given in Table 8. Note that new SVC gains were not included in this version of ADF while they were used in the OC-SAC-SACSO prototype to generate all results.

**Table 8 ADFs required in OC-SAC module**

| ADF ID | Filenames (OLCI-A, OLCI-B)                                                                                                                                                     | Update from Collection 3                                                                      |
|--------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------|
| ACP    | S3A_OL_2_CLP_AX_20160216T000000_20991231T235959_20220726T100000_____MPC_D_AL_003.SEN3<br>S3B_OL_2_ACP_AX_20180425T000000_20991231T235959_20220920T100000_____EUM_D_AL_004.SEN3 | Aerosol LUTs, CWAC parameters (number of iterations, etc.), ALH LUT                           |
| CLP    | S3A_OL_2_CLP_AX_20160216T000000_20991231T235959_20220726T100000_____MPC_D_AL_003.SEN3<br>S3B_OL_2_CLP_AX_20180425T000000_20991231T235959_20220726T100000_____MPC_D_AL_001.SEN3 | Marine reflectance climatology (mean and std-dev)                                             |
| PPP    | S3A_OL_2_PPP_AX_20160216T000000_20991231T235959_20220413T100000_____MPC_O_AL_006.SEN3<br>S3B_OL_2_PPP_AX_20180425T000000_20991231T235959_20220413T100000_____MPC_D_AL_002.SEN3 | Transfer of Rayleigh LUTs existing in previous ACP ADF of Collection 3 to a new "smile" group |



**Figure 28 Outline of the OC-SAC (left) and CWAC (right) modules.**

#### 4.5.2 NUMERICAL COMPUTATION CONSIDERATIONS

Aside from BPC, whose numerical details are fully described in [AD-6], the core algorithm of OC-SAC is the aerosol identification inside the CWAC module. The algorithm is numerically very simple, since the optimization of the mixing ratio is done analytically, without any iterative algorithm. A profiling tool (callgrind) has shown that the costliest component in term of CPU was the interpolation of polynomial coefficients used to model the aerosol reflectance. The main concern of the new CWAC is thus the way the physics is stored, to minimize the number of interpolations as well as the RAM, directly related to the size of the LUTs. After various attempts, the formulation proposed in section 4.3.1.11 has proven to be successful. The performance measured at EUMETSAT for the processing of a global full day OLCI-A acquisition (Full Resolution) is comparable to that of current operational processor (Table 9): about +17% in CPU and -20% in RAM.

**Table 9 IPF performance in RAM & CPU assessed on an OLCI-A benchmark (see text)**

| Processor                      | RAM: Maximum resident set size | CPU: User time (mean per PDU) |
|--------------------------------|--------------------------------|-------------------------------|
| Operational IPF (Collection 3) | 8.02 GB $\pm$ 0.28             | 44.5 min $\pm$ 29.9           |
| IPF with present OC-SAC        | 6.39 GB $\pm$ 0.70             | 52.0 min $\pm$ 38.9           |

#### 4.5.3 PROGRAMMING AND PROCEDURAL CONSIDERATIONS

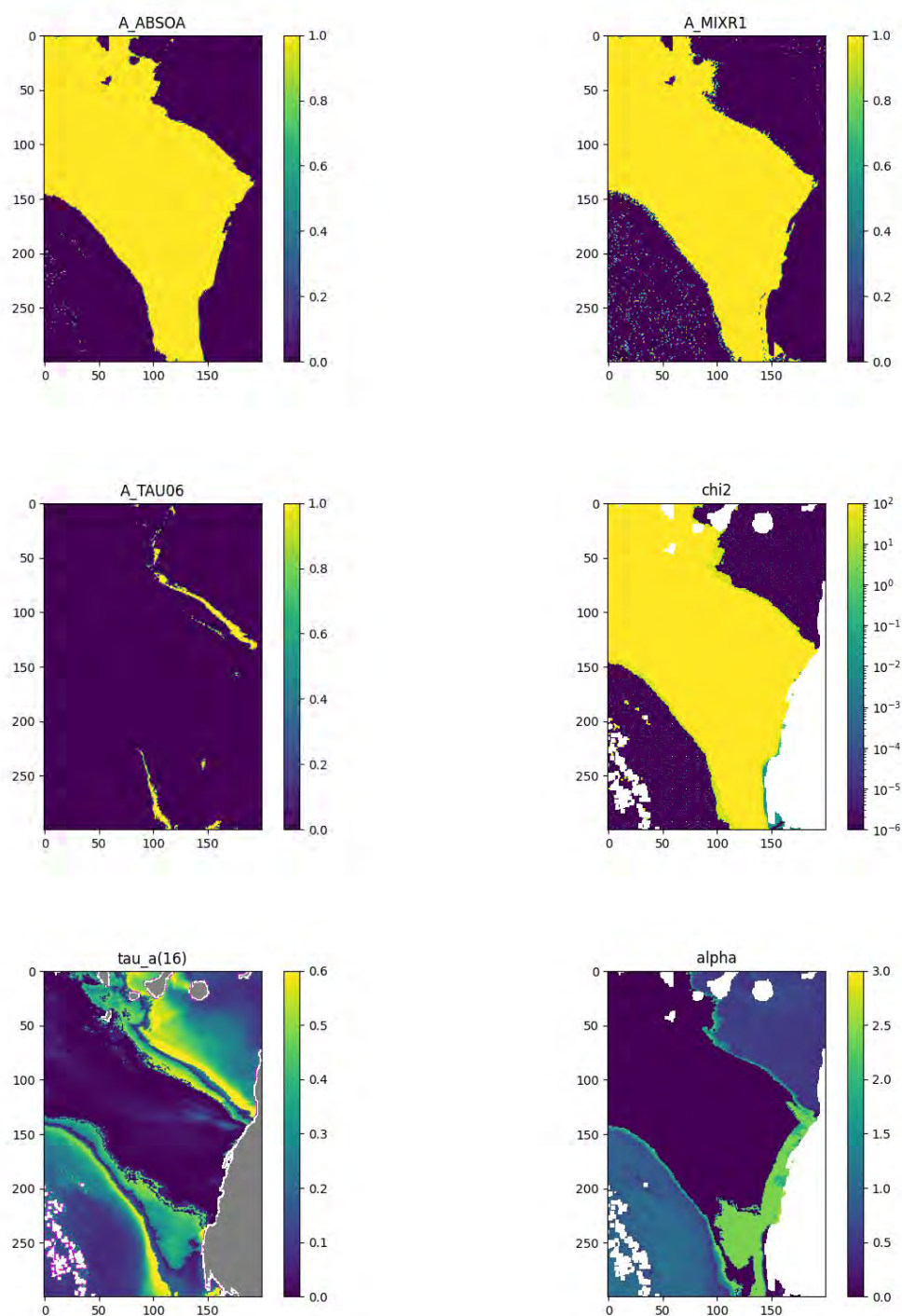
The OC-SAC module is written in C language (C++ for the BPC component) and interfaces with the operational OLCI Level-2 processor in C language. It calls the GNU Scientific Library (GSL, version  $\geq 2.5$ , <https://www.gnu.org/software/gsl/doc/html/index.html>) to use vectors, matrixes and linear algebra routines (in particular for the uncertainty computation in BPC) and core minimization method in CWAC (Brent minimization algorithm).

#### 4.5.4 QUALITY ASSESSMENT AND DIAGNOSTIC

Quality of OC-SAC can be assessed through annotation flags and the normalized  $\chi^2$  at convergence, Eq. OP-SAC-CWAC-ID-3. A subtlety in the current code is that the  $\chi^2$  is not normalised for standard aerosol detection while it is for strongly absorbing models. Hence, its interpretation on a scene mixing both types of models should be cautious. An example of failure is shown on Figure 29 for the complex case of Saharan dust. The ANNOT\_ABSOA flag is raised over the plume as expected. ANNOT\_MIXR1 is also raised, what shows problematic aerosol identification (here strongly absorbing models). ANNOT\_TAU is marginally raised on the edge of the plume, actually where standard aerosol models are identified. The unnormalized  $\chi^2$  over the standard aerosol region remains very low (below  $10^{-5}$ ), proving likely good inversion, as shown on the map of AOT (high values) and Angstrom. On the contrary, the normalised  $\chi^2$  over the strongly absorbing models is very large (higher than 100) and values of AOT and Angstrom are unrealistic. Hence the analysis of annotation flags can be used as reliable diagnostic in Level-2 products. Note that the  $\chi^2$  is currently only an internal variable and does not impact the Level-2 flags or downstream processing.

#### 4.5.5 EXCEPTION HANDLING

*To be completed in a future version of the document*



**Figure 29. CWAC diagnostic over Saharan dust (OLCI-A, 2019-02-05). From top to bottom, left to right: ANNOT\_ABSOA, ANNOT\_MIXR1, ANNOT\_TAU, chi2, aerosol optical thickness at 865 nm and Angstrom.**

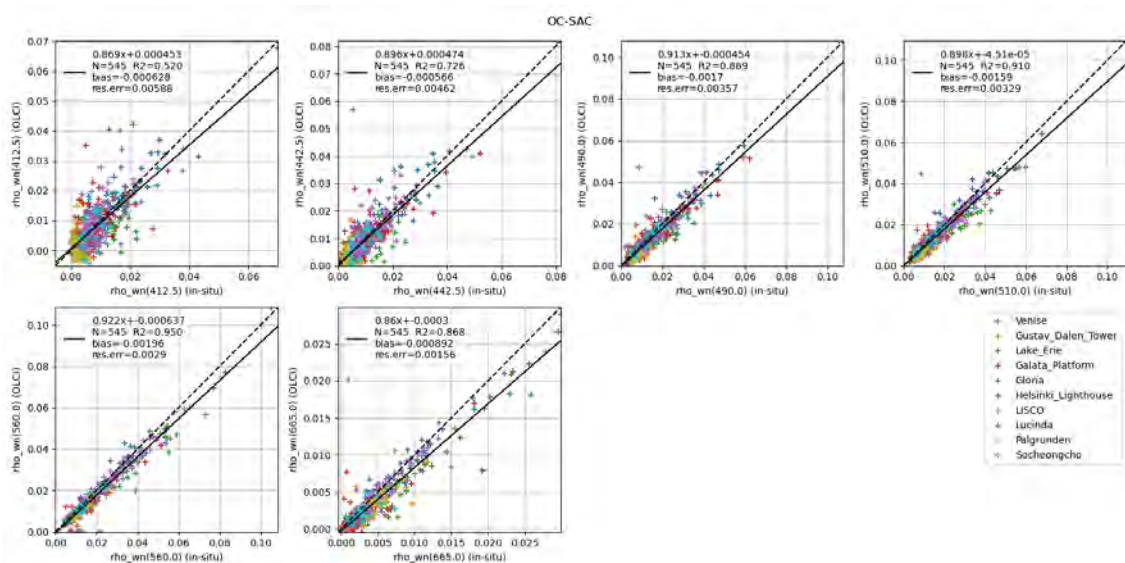
## 4.6 PERFORMANCE AND VALIDATION

Extended validation of OC-SAC on in-situ match-ups, scenes, global maps and time-series is given in [AD-2]. A summary is given in next subsection. An extended validation, notably on internal OC-SAC component listed below, is planned for a future version of the document. Note that all results were generated with OC-SAC-SACSO prototype (with SVC gains of section 7), which is known to have some limitations in the cloud detection.

As in [AD-2], results were generated with a fixed input RH of 90%.

### 4.6.1 PERFORMANCE SUMMARY

Validation of OC-SAC marine reflectance against AERONET-OC in-situ data is given on Figure 30. Except at 412 nm, the robustness is demonstrated with relatively large correlation coefficient and small residual. Indeed, in comparison with standard IPF, it was found in [AD-2] that OC-SAC significantly reduces residual error and mean absolute deviation; however, it presents a slightly higher bias that has to be investigated with more robust statistics, data screening and possibly revised SVC gains.



**Figure 30 Validation of OC-SAC marine reflectance on AERONET-OC database (OLCI-A). From [AD-2].**

In term of aerosol retrieval, OC-SAC provides systematically higher Angstrom and lower AOT (Figure 32) while Collection 3 is known to underestimate Angstrom and overestimate AOT.

Qualitatively, less noise, more homogenous data, and less anomalous and flagged data are achieved with the new OC-SAC module, as illustrated on Figure 32 over the Baltic Sea.

On global maps, a negative shift with respect to air mass is observed against nominal IPF, which could also compensate the known bias of this latter (Figure 33).

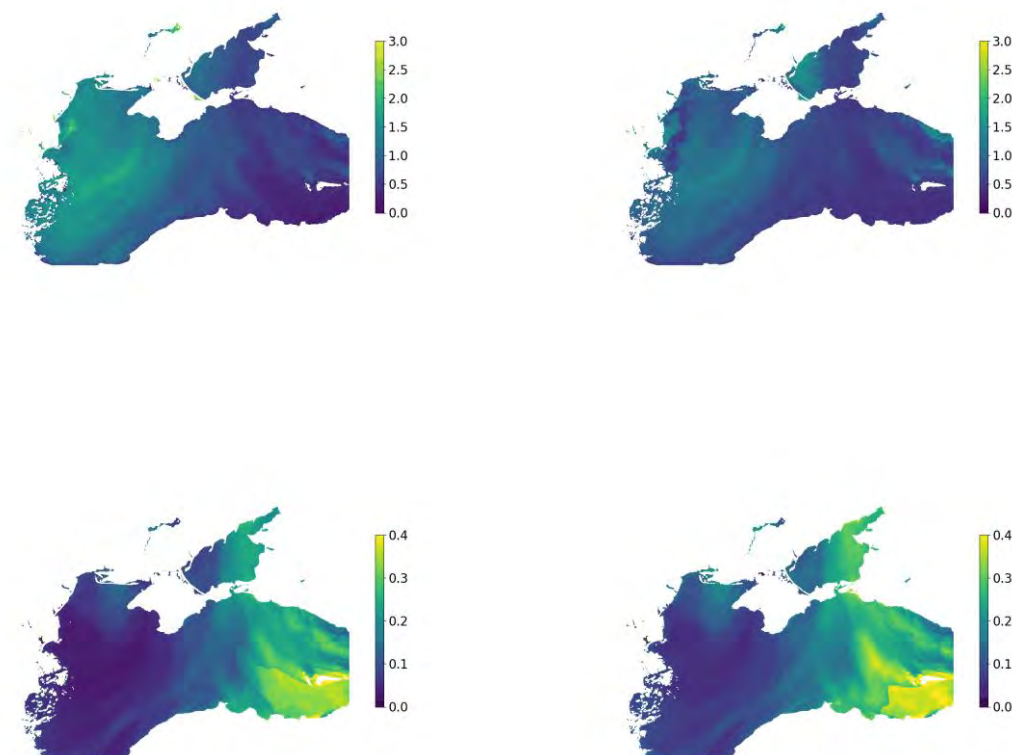


Figure 31 Angstrom exponent (top) and AOT (bottom) retrieved by OC-SAC (left) and Collection 3 IPF (right) over the Black Sea (OLCI-A 2017-09-13)

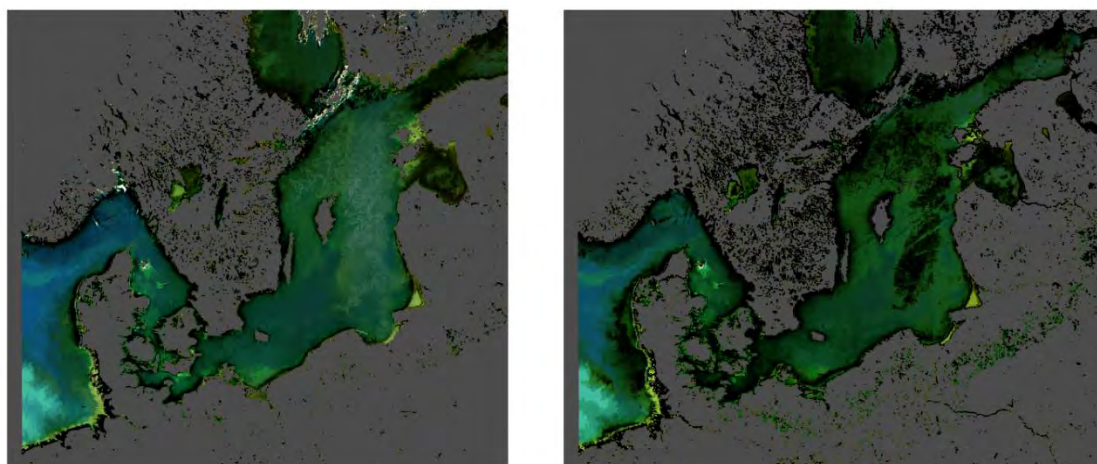
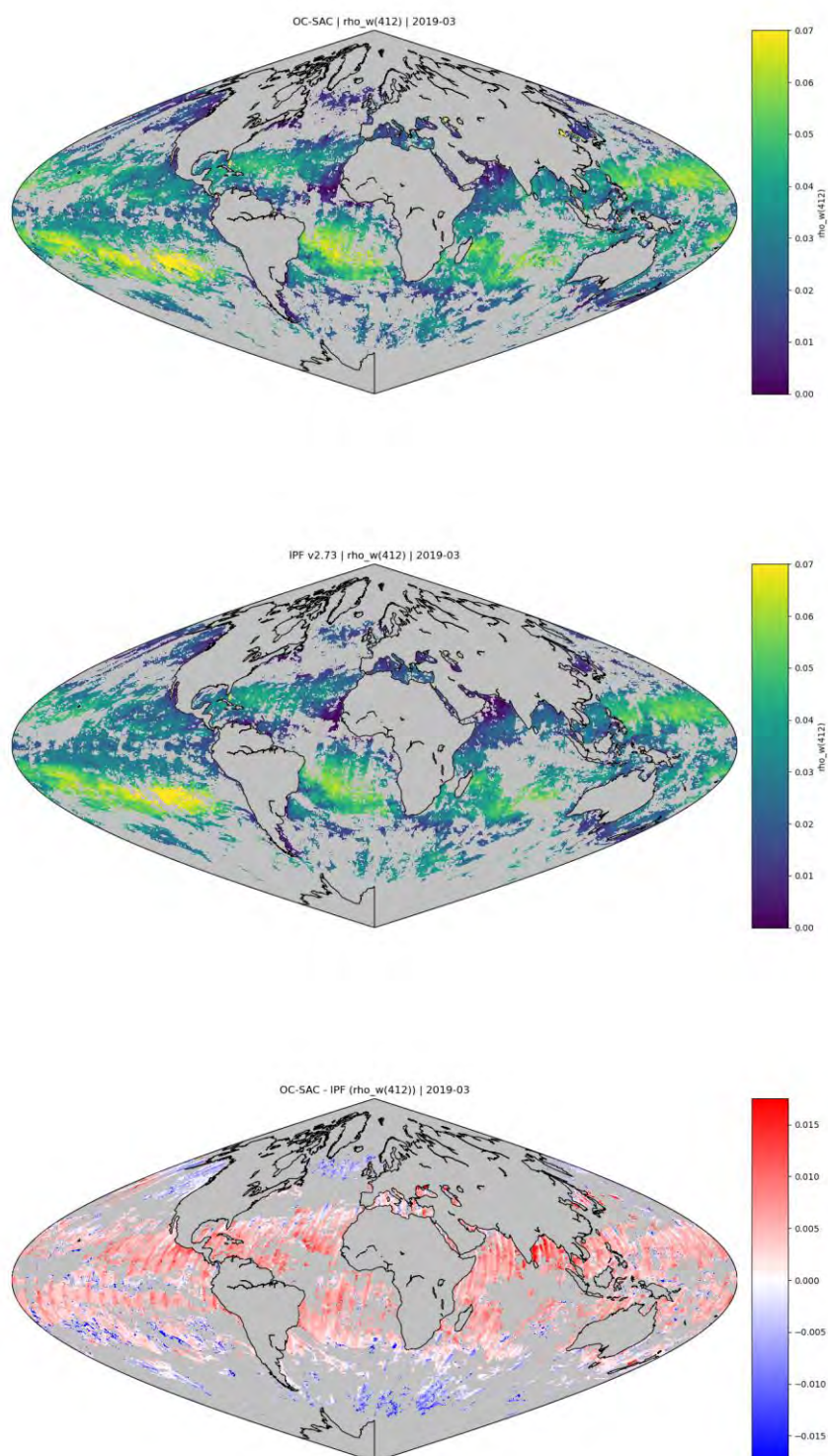


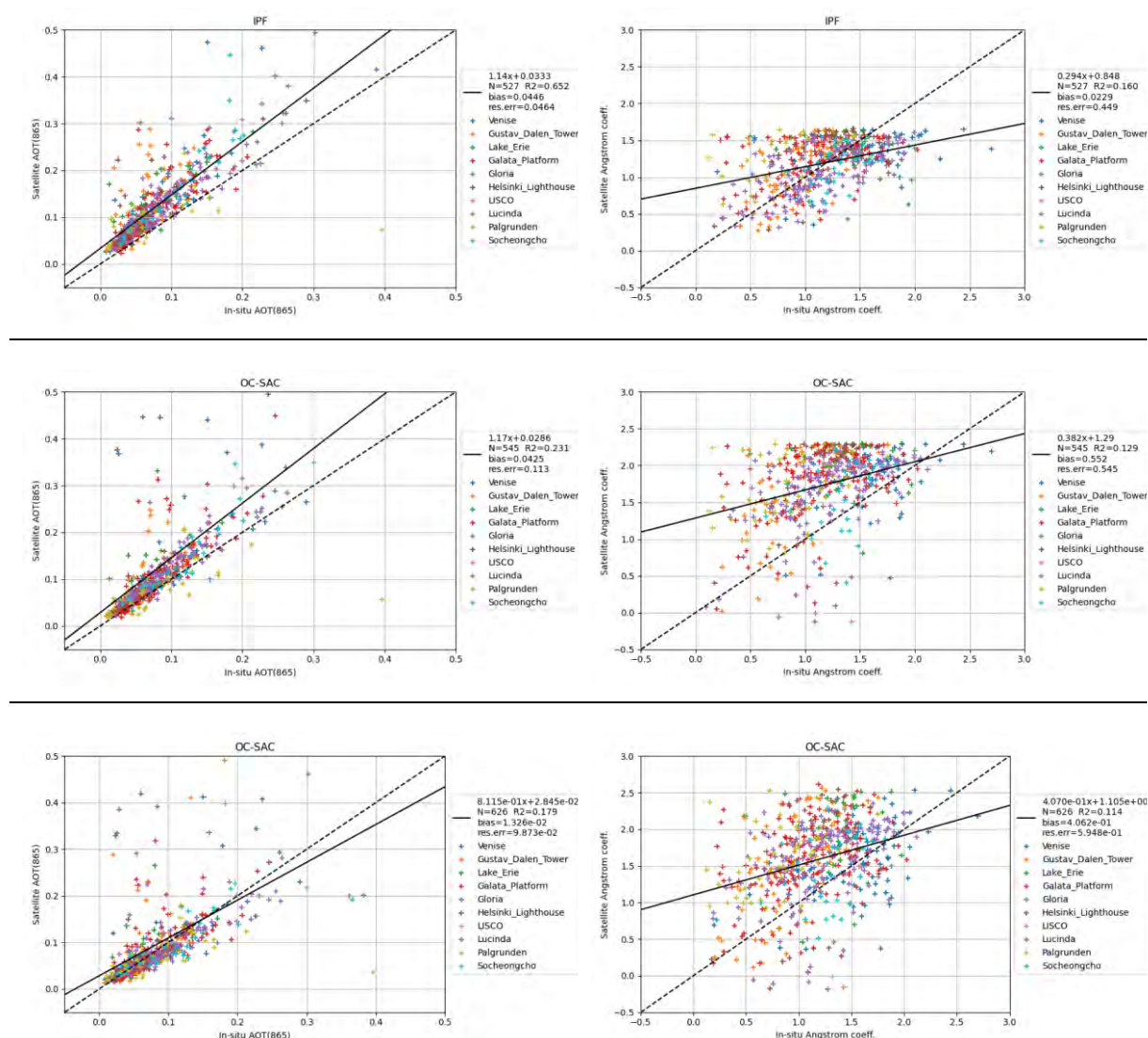
Figure 32. Natural colour composite of OLCI-A marine reflectance over the Baltic Sea (2018-05-07), left with new OC-SAC module and right as of OLCI Collection 3. RGB composite uses R=665, G=560 and B=443 nm.



**Figure 33 Global map of marine reflectance at 412 nm over 4 days in March 2019 with OC-SAC (top) and nominal IPF (middle). Bottom: difference between OC-SAC and IPF. Note that some orbits are missing in OC-SAC processing.**

#### 4.6.2 AOT AND ANGSTROM

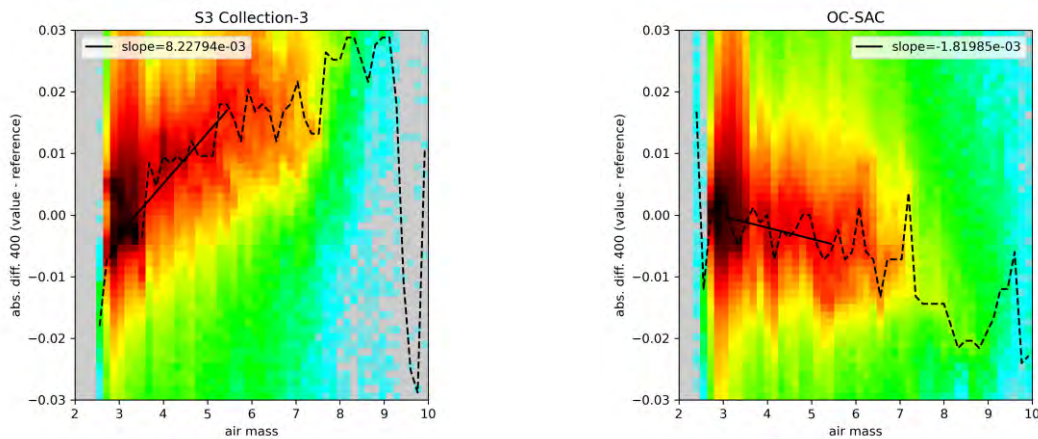
Validation of AOT and Angstrom exponent is done against AERONET measurements, and compared to IPF (Figure 34, top and middle rows). The present configuration of OC-SAC with an input RH fixed to 90% does not reduce the bias on AOT and overestimate the Angstrom, while it was found to give better retrieval of marine reflectance in the blue. For comparison, results on AOT and Angstrom are improved with the RH provided by ECMWF (currently at 850 hPa), as shown in Figure 34 bottom. Providing more realistic RH to OC-SAC shall be attempted in future version of the algorithm.



**Figure 34 Validation of AOT (left) and Angstrom exponent (right) for IPF (top), OC-SAC and fixed RH=90% (middle) and OC-SAC with RH given by ECMWF (bottom), over AERONET sites, for OLCI-A.**

#### 4.6.3 SENSORS EFFECTS

A methodology has been developed in [AD-2] to investigate the air mass dependence of marine reflectance over the Arctic region in Summer, observed various times per day with different geometries. It is found that the dependency is reduced at 400 nm (Figure 35). Results are overall similar at other bands.



**Figure 35 Density graphs of the air mass self-consistency analysis, for IPF (left) and OC-SAC (right), at 400 nm.**

*Geometric effects investigated during/outside the tandem phase will be reported in next version when results from [AD-2] will be consolidated.*

#### 4.6.4 ITERATIVE TRANSMITTANCE

Section 4.3.2.3 has introduced an option to iterate the OC-SAC process for improving aerosol transmittance in Sun glint correction and BPC. Adding one iteration has been tested on a scene impacted by Sun glint and presenting coastal waters (Black Sea test case, 20170913, Figure 36). Overall, the impact seems very marginal. Some small effects on marine reflectance are visible over the most turbid waters of the Danube Delta. However, the iteration does not help to reduce the Sun glint overcorrection in the eastern part of the scene. Adding one iteration obviously multiplies by two the CPU time spent in Sun glint correction, BPC and CWAC. With our prototype, on this scene, the total processing time (including i/o) increases by about 40 %. Some optimization could be attempted, like not recomputing interpolation coefficients which depend only on geometry and ancillary data. Still, the gain seems marginal versus CPU cost. More advanced tests could be done on match-ups. If confirmed, these results suggest to rather improve other modelling aspects, like Sun glint computation at sea level, possibly BPC marine model, etc.

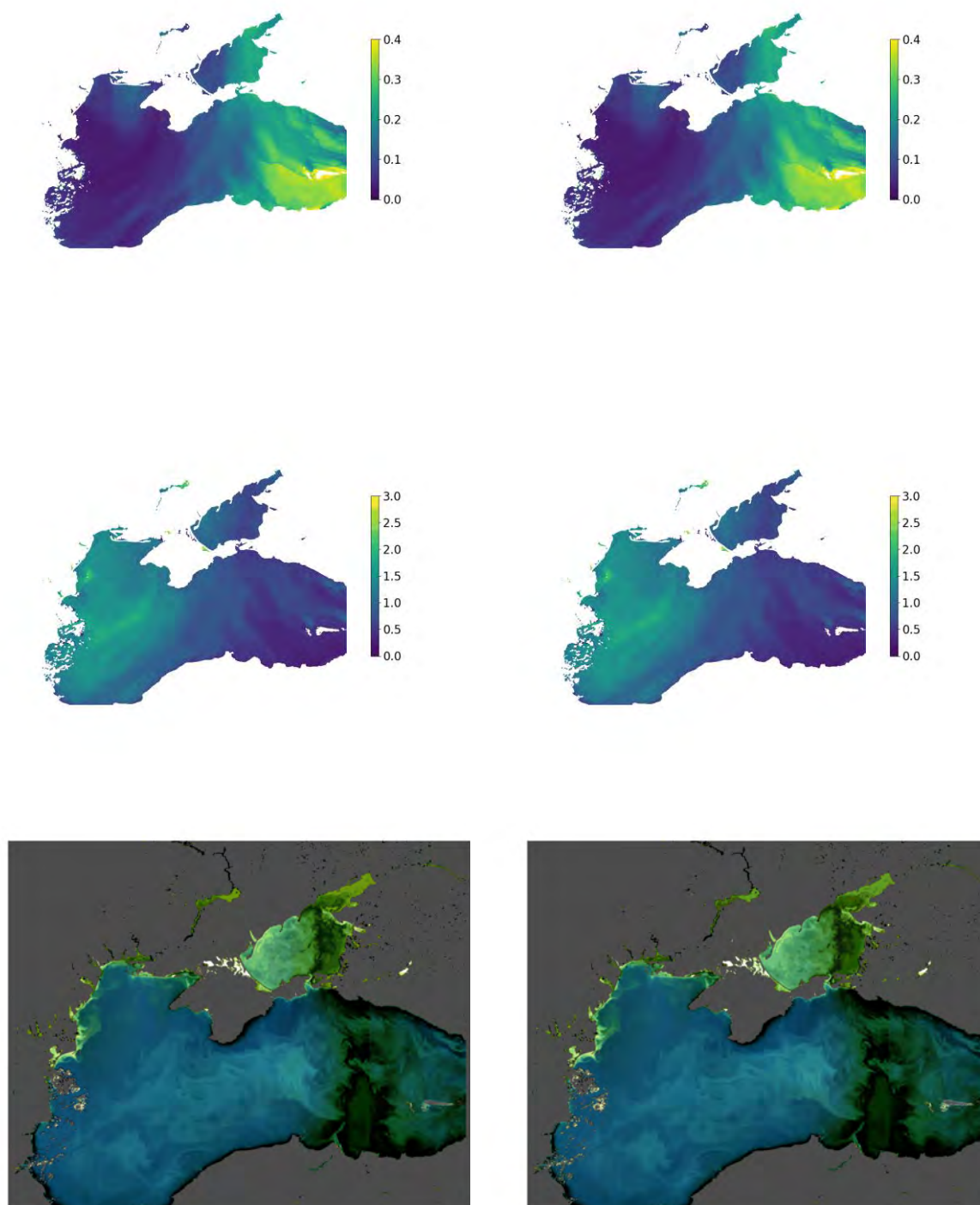


Figure 36 OC-SAC retrieval over the Black Sea (20170913), left with nominal algorithm and right with a second iteration for CWAC. From top to bottom: AOT, Angstrom coefficient, RGB of marine reflectance.

#### 4.6.5 ALH

*To be completed in a future version of the document*

#### 4.6.6 STRONGLY ABSORBING AEROSOLS

*To be completed in a future version of the document*

#### 4.6.7 UNCERTAINTY ESTIMATES

*To be completed in a future version of the document*

## 5 LIMITATIONS AND POTENTIAL FUTURE EVOLUTIONS

### 5.1 PERFORMANCE ASSUMPTIONS

The OC-SAC module is based on following assumptions and limitations:

- The coupling between gaseous absorption and aerosol scattering is assumed to be negligible.
- The ocean surface is assumed Lambertian.
- The aerosol reflectance (including multiple scattering with Rayleigh) at any band is assumed to be represented by a polynomial function of  $\rho_{a0}$ , for AOT up to 0.4 at 865 nm, with 2<sup>nd</sup> order polynomial in the NIR and 4<sup>th</sup> order at all other bands.
- The aerosol reflectance is interpolated linearly with respect to other dimensions (RH,  $\mu_s$ ,  $\mu_v$ ,  $\Delta\varphi$ ,  $w_s$ ).
- The aerosol reflectance comes from radiative transfer simulations at only one central wavelength per band, from averaged sensor SRF (i.e. not per detector), and are interpolated by high order polynomial at any wavelength.
- Radiometry at 865 nm, corrected for BPC and Rayleigh, is used to define  $\rho_{a0}$ .
- ALH is assumed to not impact the aerosol signal at 865 nm (lower node for  $z_a$  is taken in the first guess estimate of  $\rho_{a0}$ , hence AOT).
- The ratio of TOA radiometry between band 760 to 753 nm is assumed to be represented by a 2<sup>nd</sup> order polynomial versus ALH.
- The linear mixing ratio between two bracketing fine mode fraction is assumed to be spectrally flat.
- Given two successive fine mode fractions, the  $\chi^2$  measuring the discrepancy between modelled and observed aerosol reflectance in the NIR is assumed to have a unique minimum with respect to AOT and mixing ratio.
- The  $\chi^2$  for standard aerosol model detection is unweighted and not normalized (same weights as those already used for absorbing aerosol detection could be used, for the NIR bands, i.e. weights from BPC).
- The logarithm of atmospheric transmittance is interpolated linearly with respect to all non-spectral dimensions (AOT, ROT, ALH, RH,  $\mu_s$ ,  $\mu_v$ ,  $\Delta\varphi$ ,  $w_s$ ).
- The selection of aerosol models relies strongly on the input RH, provided by ECMWF. Current value of RH given at 850 hPa is not optimal (generally too low). A fixed value of 90% was forced in present results and gains generation, but is not optimal either for the validation of atmospheric products over AERONET sites.

### 5.2 POTENTIAL IMPROVEMENTS

The following improvements have been identified for further improvement of OC-SAC, in term of extended validation and algorithm tuning:

- Re-investigate the NIR gains methodology following Ahmad et al. (2011), i.e. without forcing the model to MAR-90, and recompute VIS gains as necessary.
- Compare S3-A and S3-B aerosol product during and outside the tandem phase, to detect possible issue with geometry

- Better address the benefit of CWAC from the ALH module (e.g. by comparison with a fixed ALH) and further validate ALH with Sentinel-5P data.
- Investigate on few case studies the benefit of using CAMS data for ALH and default AOT (first guess)
- Further validate the detection and correction of strongly absorbing aerosol models on case studies of the Diagnostic Dataset; tune the IOPs of the models as necessary.
- Investigate the performance of standard aerosol identification when using input uncertainties in the aerosol retrieval.
- Investigate the benefit of OC-SAC iterative process for improved aerosol transmittance in Sun glint and BPC correction.
- Investigate a better handling of BRDF effect in the OC-SAC inversion to go beyond the Lambertian assumption.
- Assess the improvement gained by adding a climatological content of gas in atmospheric LUT generation and adjusting only for residual in the upstream gaseous correction.
- Assess the impact of background tropospheric and stratospheric aerosols with RT simulations in typical conditions.
- Assess impact of per-pixel spectral variation of the aerosol transmittance.
- Provide OC-SAC more realistic values of RH.
- Keep investigating the multi-band optimization for aerosol load computation.

## 6 APPENDIX 1: LUT GRID OPTIMISATION

### 6.1 RAYLEIGH REFLECTANCE LUT

This optimization is performed in PPA for CPU reason to speed up the analyses, although the final Rayleigh LUT used in OC-SAC is generated in SSA. We work on  $\rho_R$  with  $\rho_R = \rho_{TOA}(\tau_a = 0) - T(\tau_a = 0)\rho_g$  where  $\rho_g$  is the glitter reflectance at sea level and  $T$  the direct transmission. Rayleigh LUT does not depend on OLCI band or wavelength. Wavelength is implicitly accounted for through  $\tau_R$ . We have thus  $\rho_R = f(\mu_S, \mu_V, \Delta\varphi, w_s, \tau_R)$ .

In order to evaluate interpolation error related to LUTs sampling/interpolation choice, we compute higher resolution LUT for each axis successively. When considering a given axis, the other axes are restricted to only a few representative “test” values (due to CPU demand). This “test” sampling is defined as follow:

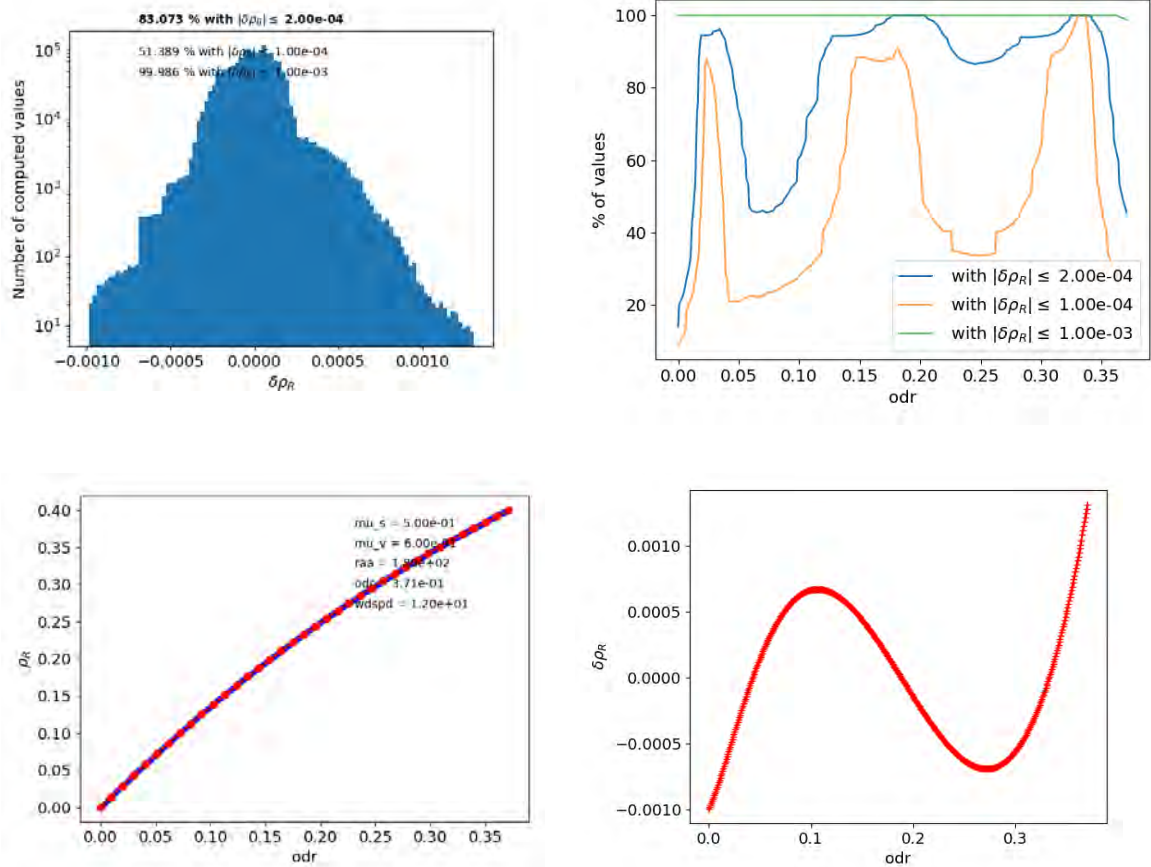
- The relative azimuth ( $\Delta\varphi$ ): 181 values linearly sampled between 0 and 180 deg. Note that  $\Delta\varphi$  is always kept at relatively high resolution since it does not impact the CPU demand. Also, note that in this chapter the convention of  $\Delta\varphi$  is opposite as that in OLCI.
- The cosine of view zenith angles ( $\mu_V$ ): 0.6, 0.8, 1.0
- The cosine of solar zenith angles ( $\mu_S$ ): 0.5, 0.65, 0.8
- Rayleigh Optical Depth,  $\tau_R$  : 0.05 and 0.3
- wind speed ( $w_s$ ): 4 and 12 m/s

#### 6.1.1 AXIS $\tau_R$

The first studied axis is  $\tau_R$ . To lower the size of the LUT, this axis will be fitted as a polynomial and coefficients will be stored in LUT for each  $(\mu_S, \mu_V, \Delta\varphi, w_s)$  nodes. We first consider a 2<sup>nd</sup> order polynomial,  $\rho_R = a * \tau_R^2 + b * \tau_R + c$ . For each  $(\mu_S, \mu_V, \Delta\varphi, w_s)$  nodes (with “test” sampling), we compute  $\rho_R$  for 500 values of  $\tau_R$  between 0 and 0.3706. We compare fitted polynomials to the actual  $\rho_R$  for all  $(\mu_S, \mu_V, \Delta\varphi, w_s)$  nodes x 500  $\tau_R$  values to obtain a statistical error due to the polynomial representation in LUT.

Note that the selection of a subset of  $\tau_R$  for the fit is necessary because we could not produce  $\rho_R$  for 500 values of  $\tau_R$  for the final  $(\mu_S, \mu_V, \Delta\varphi, w_s)$  sampling. The selection of this subset of values is optimized to lower the statistical error given a polynomial order. We simply iterate on the number of equally spaced values (taken among the 500) until the expected accuracy is matched in terms of the fraction of points having an error  $\leq 2 \cdot 10^{-4}$ . If the accuracy between two iterations is not enhanced, it stops.

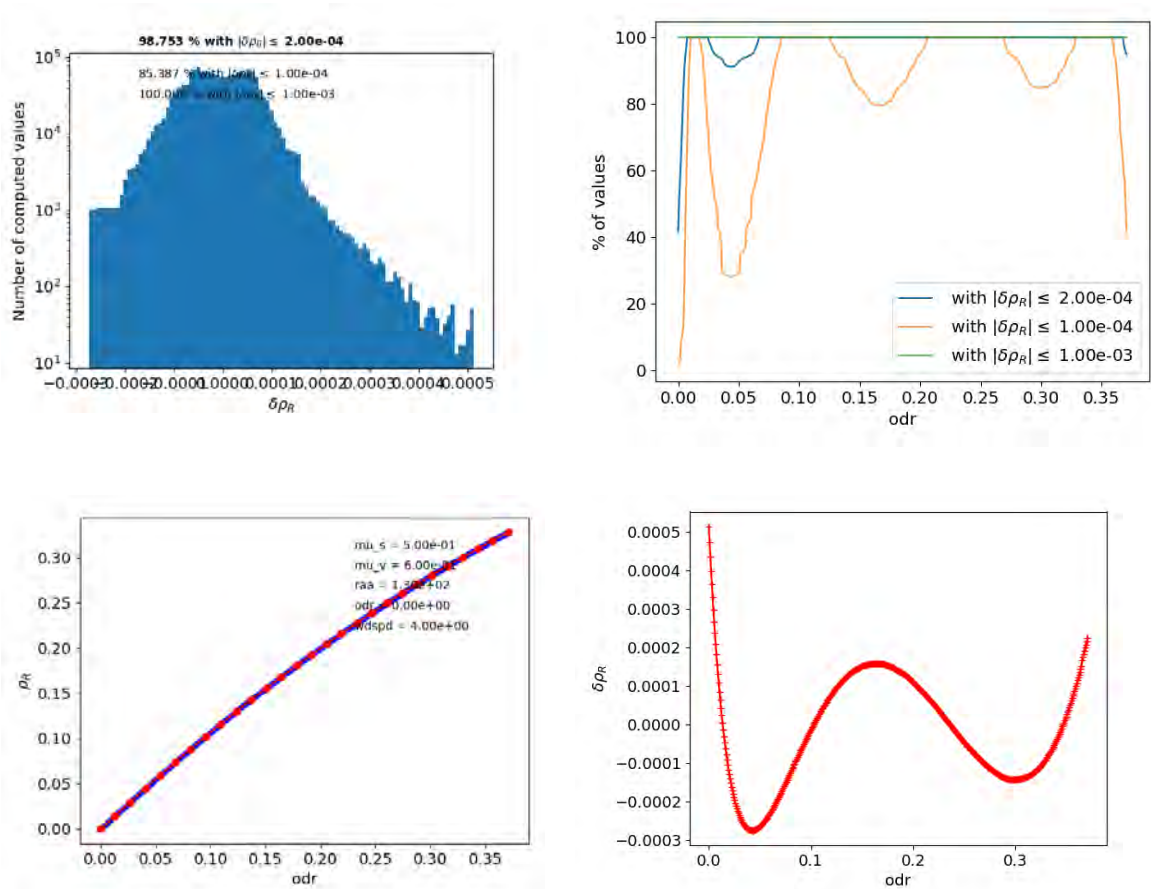
Figure 37 shows results obtained when fitting  $\rho_R = a * \tau_R^2 + b * \tau_R + c$ .



**Figure 37. Accuracy of  $\rho_R = f(\tau_R)$  when fitting,  $\rho_R = a * \tau_R^2 + b * \tau_R + c$  for each  $(\mu_S, \mu_V, \Delta\phi, w_s)$  nodes. Upper left panel: Histogram of the error for all  $(\mu_S, \mu_V, \Delta\phi, w_s)$  nodes x 500  $\tau_R$  values. Upper right panel: Fraction of pixels satisfying a given error as a function of  $\tau_R$ . Lower left panel:  $\rho_R = f(\tau_R)$  for the  $(\mu_S, \mu_V, \Delta\phi, w_s)$  node having the largest error encountered. Red dots are the points used for the fit while the red line is the fit. Lower right panel:  $\delta\rho_R = f(\tau_R)$  for the  $(\mu_S, \mu_V, \Delta\phi, w_s)$  node having the largest error encountered. Red dots are the points used for the fit while the red line is the fit.**

The same exercise can be performed fitting a 3<sup>rd</sup> order polynomial. We then fit successively function  $\rho_R = a * \tau_R^3 + b * \tau_R^2 + c * \tau_R + d$ . The corresponding results are shown on Figure 38.

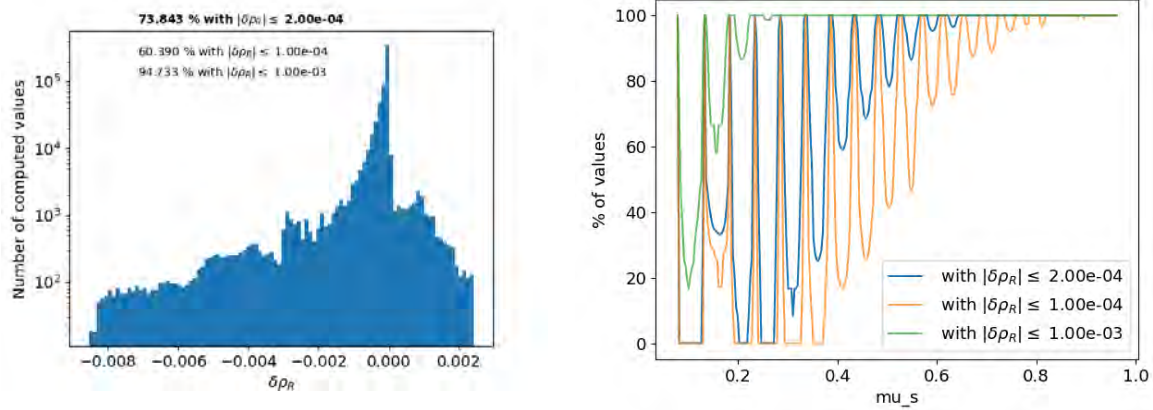
We see that to fit  $\rho_R = a * \tau_R^3 + b * \tau_R^2 + c * \tau_R + d$  clearly offers the better accuracy with 98.7% of LUT values having an error better the  $2 * 10^{-4}$ .



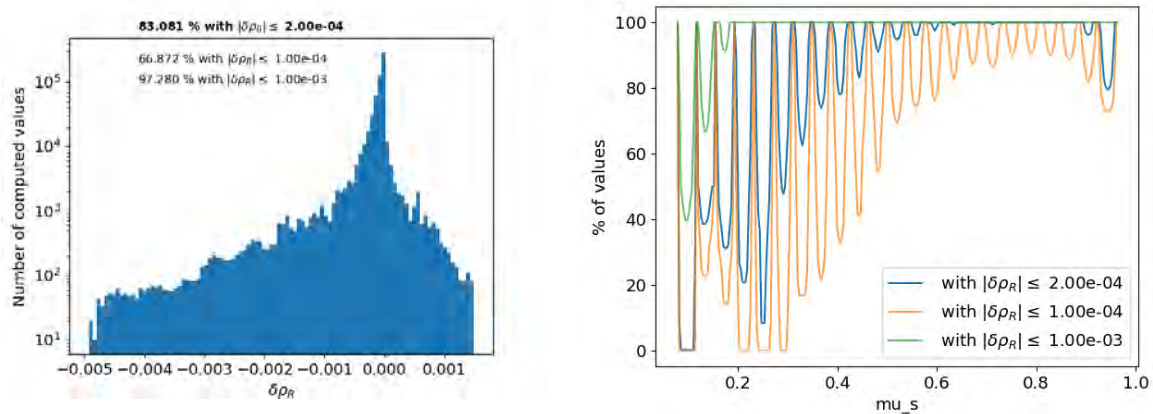
**Figure 38. Accuracy of  $\rho_R = f(\tau_R)$  when fitting  $\rho_R = a * \tau_R^3 + b * \tau_R^2 + c * \tau_R + d$  for each  $(\mu_S, \mu_V, \Delta\phi, w_s)$  nodes. Upper left panel: Histogram of the error for all  $(\mu_S, \mu_V, \Delta\phi, w_s)$  nodes x 500  $\tau_R$  values. Upper right panel: Fraction of pixels satisfying a given error as a function of  $\tau_R$ . Lower left panel:  $\rho_R = f(\tau_R)$  for the  $(\mu_S, \mu_V, \Delta\phi, w_s)$  node having the largest error encountered. Red dots are the points used for the fit while the red line is the fit. Lower right panel:  $\delta\rho_R = f(\tau_R)$  for the  $(\mu_S, \mu_V, \Delta\phi, w_s)$  node having the largest error encountered. Red dots are the points used for the fit while the red line is the fit.**

### 6.1.2 AXIS $\mu_s$

For the other  $\mu_s$  axis, we do not fit  $\rho_R$ . We simply select a sample of values to be stored in LUT. To evaluate interpolation error related to LUTs sampling/interpolation of  $\mu_s$ , we compute  $\rho_R$  for all  $(\mu_v, \Delta\phi, w_s, \tau_R)$  nodes (with “test” sampling) and for 300 values of  $\mu_s$  between 0.05 and 1.0. Figure 39 shows the accuracy obtained using the OLCI standard AC LUT sampling for the  $\mu_s$ , which is in fact based on a regular sampling on  $\theta_s$ . As seen on Figure 40, using the same number of samples (24) but with a regular sampling in  $\mu_s$  brings the fraction of points having an error less or equal to  $2 \cdot 10^{-4}$  to 83% as compared with 73.8% for the OLCI standard sampling.



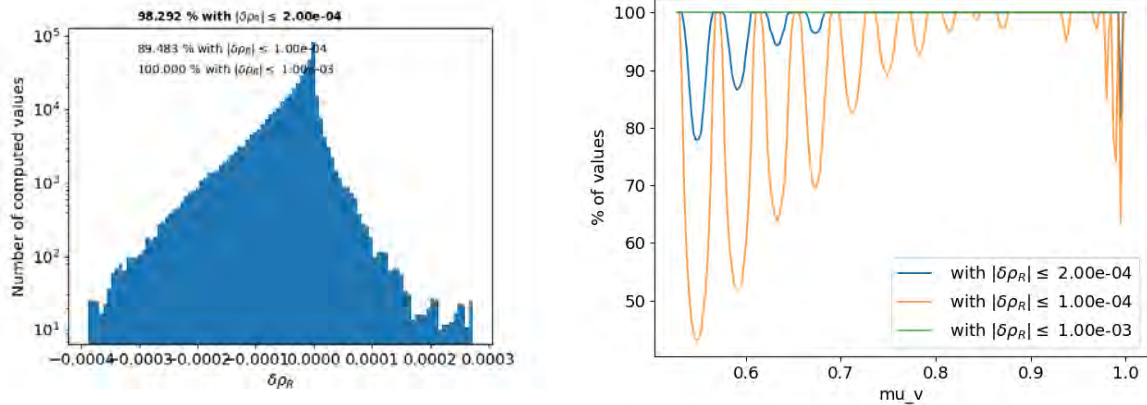
**Figure 39. Accuracy of  $\rho_R = f(\mu_s)$  LUT interpolation for OLCI standard sampling. Left panel: Histogram of the error for all  $(\mu_v, \Delta\phi, w_s, \tau_R)$  nodes x 300  $\mu_s$  values. Right panel: Fraction of pixels satisfying a given error as a function of  $\mu_s$ .**



**Figure 40. Accuracy of  $\rho_R = f(\mu_s)$  LUT interpolation, for a LUT with the same boundaries and number of samples as OLCI standard LUT, but with a regular sampling in  $\mu_s$ . Left panel: Histogram of the error for all  $(\mu_v, \Delta\phi, w_s, \tau_R)$  nodes x 300  $\mu_s$  values. Right panel: Fraction of pixels satisfying a given error as a function of  $\mu_s$ .**

### 6.1.3 AXIS $\mu_V$

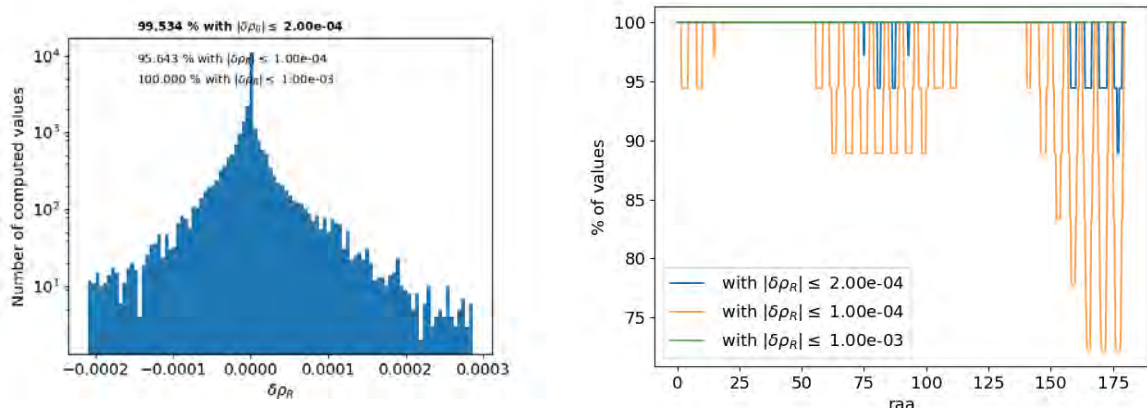
To evaluate interpolation error related to LUTs sampling/interpolation of  $\mu_V$ , we compute  $\rho_R$  for all  $(\mu_S, RAA, w_S, \tau_R)$  nodes (with “test” sampling) and for 200 values of  $\mu_V$  between 0.5 and 1.0. We see on Figure 41 that the OLCI standard sampling allows one to have 98.3 % of the points having an error less or equal to  $2 \cdot 10^{-4}$ .



**Figure 41. Accuracy of  $\rho_R = f(\mu_V)$  LUT interpolation, for a LUT with OLCI standard sampling. Left panel: Histogram of the error for all  $(\mu_S, \Delta\varphi, w_S, \tau_R)$  nodes x 200  $\mu_V$  values. Right panel: Fraction of pixels satisfying a given error as a function of  $\mu_V$ .**

### 6.1.4 AXIS $\Delta\varphi$

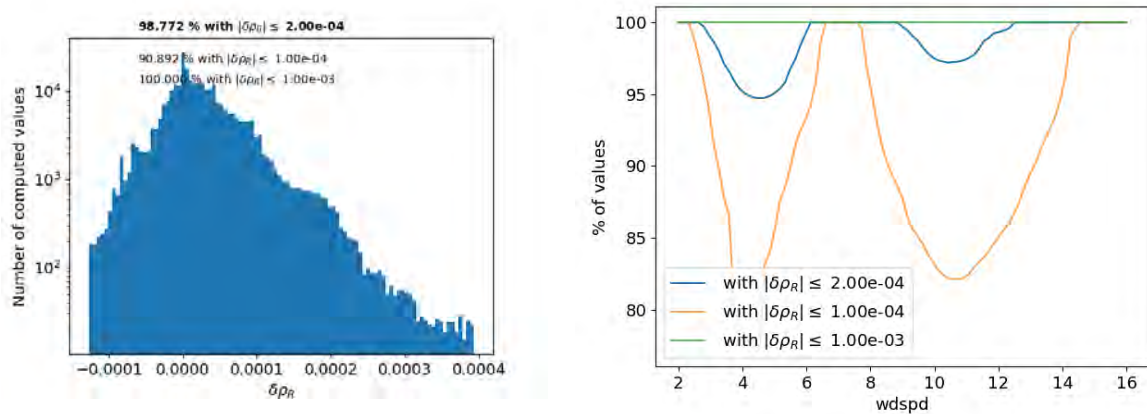
For  $\Delta\varphi$  axis study, we compute  $\rho_R$  for all  $(\mu_S, \mu_V, w_S, \tau_R)$  nodes (with “test” sampling) and for 721 values of  $\Delta\varphi$  between 0 and  $180^\circ$ . We see on Figure 42 that the OLCI standard sampling allows one to have 99.5 % of the points having an error less or equal to  $2 \cdot 10^{-4}$ .



**Figure 42. Accuracy of  $\rho_R = f(\Delta\varphi)$  LUT interpolation, for a LUT with OLCI standard sampling. Left panel: Histogram of the error for all  $(\mu_S, \mu_V, w_S, \tau_R)$  nodes x 721  $\Delta\varphi$  values. Right panel: Fraction of pixels satisfying a given error as a function of  $\Delta\varphi$ .**

### 6.1.5 AXIS $w_s$

Finally, to study  $w_s$  sampling, we compute  $\rho_R$  for all  $(\mu_s, \mu_v, \Delta\varphi, \tau_R)$  nodes (with “test” sampling) and for 100 values of  $w_s$  between 0.25 and 16 m/s. A sampling using only 3 values (2, 7, 16 m/s) allows one to have 98.7% of the points having an error less or equal to  $2 \cdot 10^{-4}$  (see Figure 43).



**Figure 43. Accuracy of  $\rho_R = f(w_s)$  LUT interpolation, for a LUT with 3 wind speeds. Left panel: Histogram of the error for all  $(\mu_s, \mu_v, \Delta\varphi, \tau_R)$  nodes x 100  $w_s$  values. Right panel: Fraction of pixels satisfying a given error as a function of  $w_s$ .**

## 6.2 AEROSOL REFLECTANCE LUT

This LUT is computed in PPA. We consider  $\rho_a = \rho_{path} - \rho_R$  where  $\rho_{path}$  is corrected for Sun glint, i.e.  $\rho_{path} = \rho_t - T\rho_g$ . We have  $\rho_a = f(\mu_s, \mu_v, \Delta\varphi, w_s, \tau_R, FMF, R_H, z_a, \tau_a)$ .

When optimizing a given axis, the other axes are restricted to only a few representative “test” values (due to CPU demand). This “test” sampling is defined as follow:

- The relative azimuth ( $\Delta\varphi$ ): 181 values linearly sampled between 0 and 180 deg. Note that  $\Delta\varphi$  is always kept at relatively high resolution since it does not impact the CPU demand. Also, note that in this chapter the convention of  $\Delta\varphi$  is opposite as that in OLCI.
- The cosine of view zenith angles ( $\mu_v$ ): 0.6, 0.8, 1.0
- The cosine of solar zenith angles ( $\mu_s$ ): 0.5, 0.65, 0.8
- Rayleigh Optical Depth,  $\tau_R$ : 4 equally spaced values between the maximum and minimum expected values (accounting for smile and a minimum/maximum pressure of 830/1040 hPa) for each band, e.g. for band 1: 0.2894, 0.3177, 0.3459, 0.3741. This restricts the impact of aerosol/Rayleigh coupling on  $\rho_a$  to relevant values to be fitted or sampled
- Wind speed ( $w_s$ ): 4 and 12 m/s
- Aerosol optical depth,  $\tau_a$ : 0, 0.05, 0.13, 0.2
- Aerosol altitude,  $z_a$ : 0.5 and 2 km
- Aerosol fine mode fraction, FMF : 0., 0.5, 1.0
- Aerosol relative humidity,  $R_H$ : 70 and 90 %

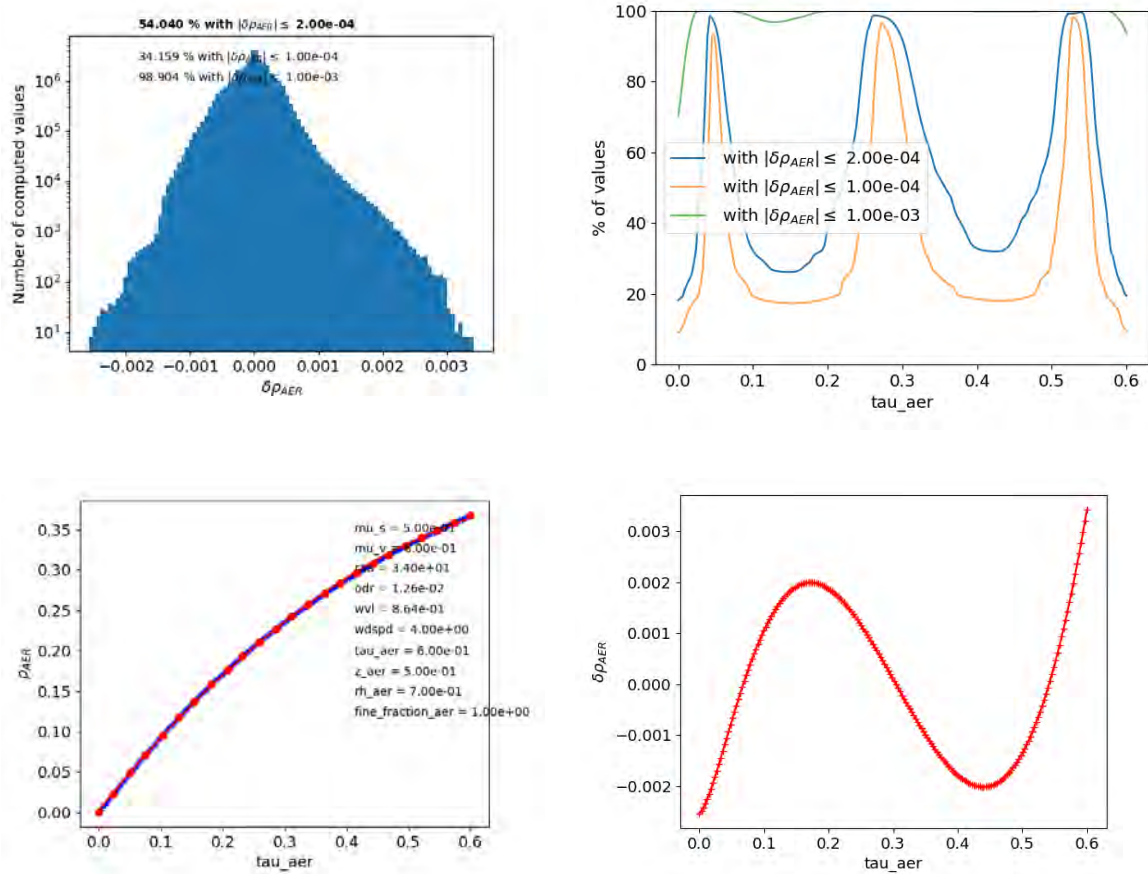
For  $\rho_a$ , despite the glitter subtraction ( $-T\rho_g$ ), geometries toward the glitter can have greater “LUT” error (probably related to the aerosol/Rayleigh/glitter coupling). Since these geometries are flagged in the OC-SAC treatment, we mask “test” nodes ( $\Delta\varphi, \mu_v, \mu_s, w_s$ ) for which the glitter reflectance at sea level has a reflectance greater than  $5 \cdot 10^{-4}$  for the present error analysis (OLCI MEDIUM\_GLINT threshold).

### 6.2.1 AXIS $\tau_a$

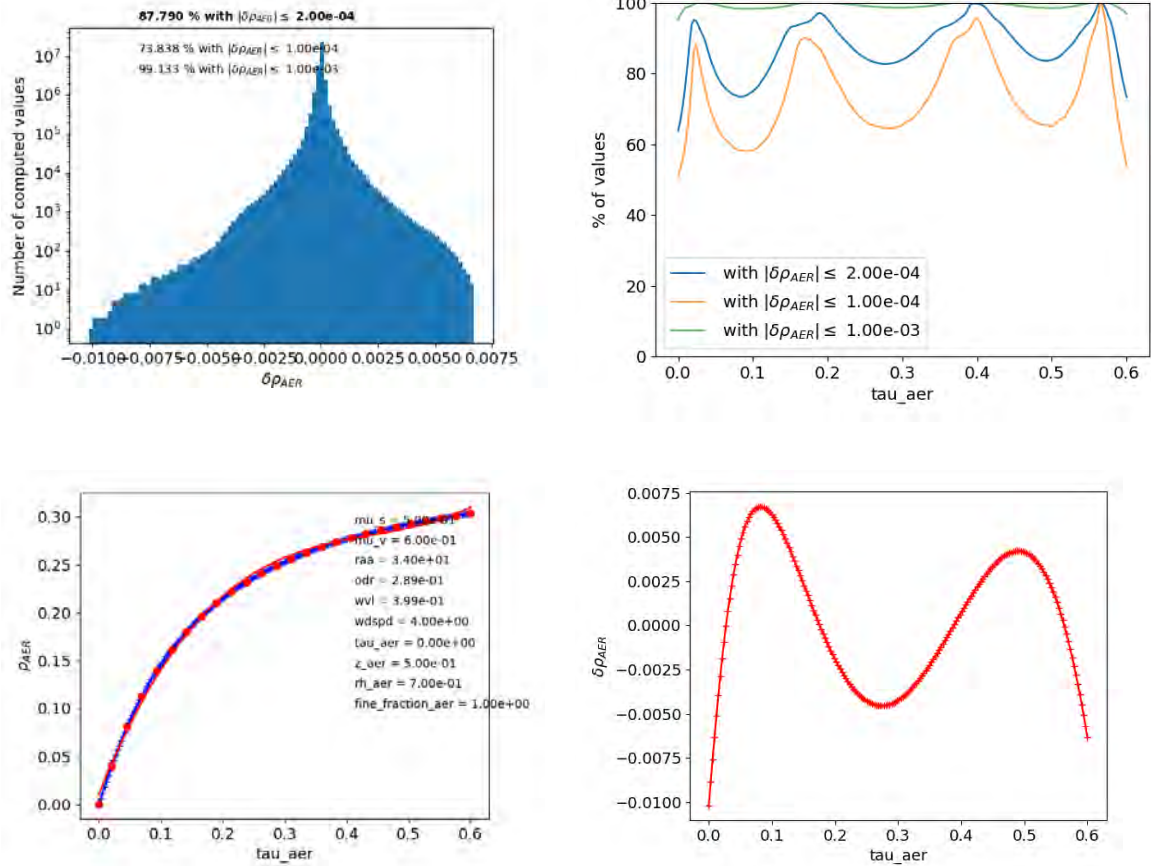
We fit  $\rho_a = f(\tau_a)$  with polynomials and coefficients are stored in LUT for each  $(\mu_s, \mu_v, \Delta\varphi, w_s, \tau_R, FMF, R_H, z_a)$  nodes. We first consider a 2<sup>nd</sup> order polynomial,  $\rho_a = \tau_a^2 a + \tau_a b + c$ . For all  $(\mu_s, \mu_v, \Delta\varphi, w_s, \tau_R, FMF, R_H, z_a)$  nodes (with “test” sampling), we compute  $\rho_a$  for 200 values of  $\tau_a$  between 0 and 0.6. We select a restricted number of  $\tau_a$  for the fit. The selection of the subset of  $\tau_a$  values is optimized to lower the statistical error given the polynomial order. We simply iterate on the number of equally spaced values until the expected accuracy is matched in terms of the fraction of points having an error  $\leq 2 \cdot 10^{-4}$ . If the accuracy between two iterations is not enhanced, the iterations stop.

Band 17 (865 nm) is used for the inversion of  $\tau_{a0}$  and it is crucial for the algorithm to have only a 2<sup>nd</sup> order polynomial representation. There is, however, no specification in term of accuracy at 865 nm. Figure 44 shows that about 54% only of the points reach an error  $\leq 2 \cdot 10^{-4}$ . However, around 98% of the points reach an error  $\leq 1 \cdot 10^{-3}$  and the maximum error is less than around  $3 \cdot 10^{-3}$ . Hence, we use a 2<sup>nd</sup> order polynomial for this band.

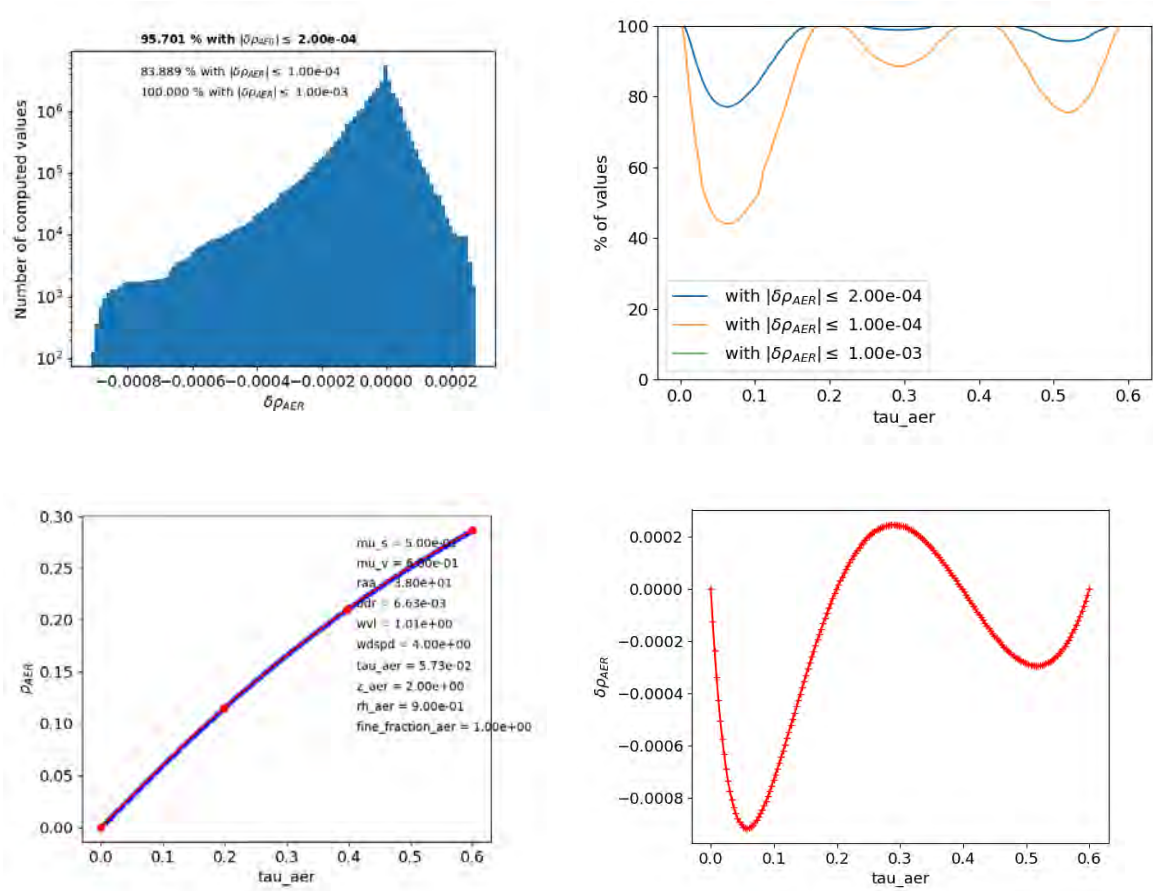
For the other bands, we can use a 3<sup>rd</sup> order polynomial fitting,  $\rho_a = a * \tau_a^3 + b * \tau_a^2 + c * \tau_a + d$ , because it implies no problem to the algorithm implementation. We see on Figure 45 and Figure 46 the result obtained for band 1 and band 21 respectively. For band 1, 87.7% of the points have an error  $\leq 2 * 10^{-4}$  and 99% an error  $\leq 1 * 10^{-3}$ . For band 21, 95.7% of the points have an error  $\leq 2 * 10^{-4}$  and 100% an error  $\leq 1 * 10^{-3}$ .



**Figure 44. Accuracy of  $\rho_a = f(\tau_a)$  when fitting  $\rho_a = \tau_a^2 a + \tau_a b + c$  for each  $(\mu_s, \mu_v, \Delta\varphi, w_s, \tau_R, FMF, R_H, z_a)$  node for band 17 (865 nm). Upper left panel: Histogram of the error for all nodes x 500  $\tau_a$  values. Upper right panel: Fraction of pixels satisfying a given error as a function of  $\tau_a$ . Lower left panel:  $\rho_a = f(\tau_a)$  for the  $(\mu_s, \mu_v, \Delta\varphi, w_s, \tau_R, FMF, R_H, z_a)$  node having the largest error encountered. Red dots are the points used for the fit while the red line is the fit. Lower right panel:  $\delta\rho_a = f(\tau_a)$  for the node having the largest error encountered. Red dots are the points used for the fit while the red line is the fit.**



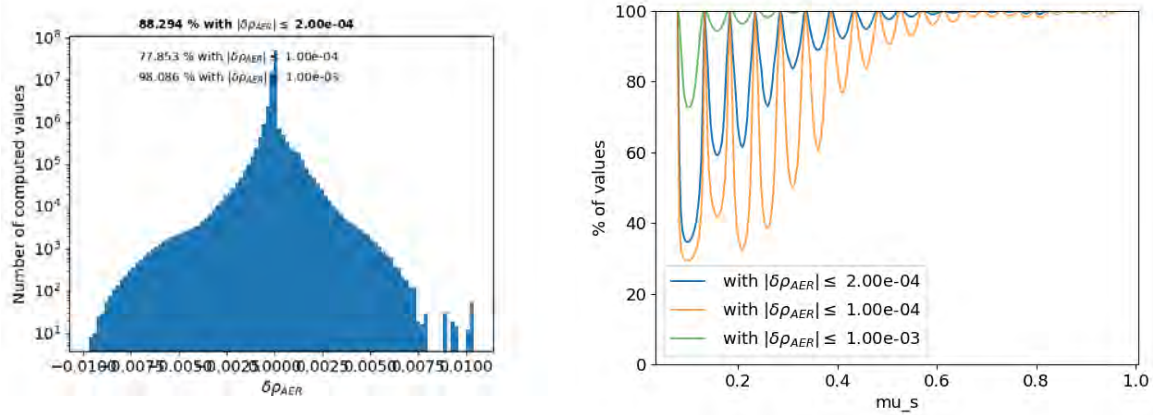
**Figure 45. Accuracy of  $\rho_a = f(\tau_a)$  when fitting  $\rho_a = a * \tau_a^3 + b * \tau_a^2 + c * \tau_a + d$  for each  $(\mu_s, \mu_v, \Delta\phi, w_s, \tau_R, FMF, R_H, z_a)$  node for band 1. Upper left panel: Histogram of the error for all nodes x 500  $\tau_a$  values. Upper right panel: Fraction of pixels satisfying a given error as a function of  $\tau_a$ . Lower left panel:  $\rho_a = f(\tau_a)$  for the  $(\mu_s, \mu_v, \Delta\phi, w_s, \tau_R, FMF, R_H, z_a)$  node having the largest error encountered. Red dots are the points used for the fit while the red line is the fit. Lower right panel:  $\delta\rho_a = f(\tau_a)$  for the node having the largest error encountered. Red dots are the points used for the fit while the red line is the fit.**



**Figure 46 . Accuracy of  $\rho_a = f(\tau_a)$  when fitting  $\rho_a = a * \tau_a^3 + b * \tau_a^2 + c * \tau_a + d$  for each  $(\mu_s, \mu_v, \Delta\phi, w_s, \tau_R, FMF, R_H, z_a)$  node for band 21. Upper left panel: Histogram of the error for all nodes  $\times 500 \tau_a$  values. Upper right panel: Fraction of pixels satisfying a given error as a function of  $\tau_a$ . Lower left panel:  $\rho_a = f(\tau_a)$  for the  $(\mu_s, \mu_v, \Delta\phi, w_s, \tau_R, FMF, R_H, z_a)$  node having the largest error encountered. Red dots are the points used for the fit while the red line is the fit. Lower right panel:  $\delta\rho_a = f(\tau_a)$  for the node having the largest error encountered. Red dots are the points used for the fit while the red line is the fit.**

### 6.2.2 AXIS $\mu_s$

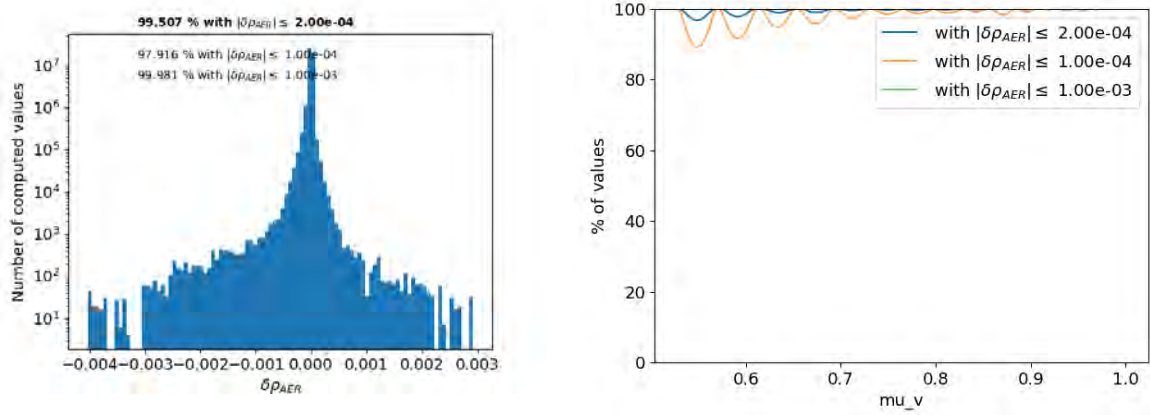
For the other axis, we do not fit  $\rho_a$ . We simply select a sample of values to be stored in LUT. To evaluate interpolation error related to LUTs sampling/interpolation of  $\mu_s$ , we compute  $\rho_a$  for all  $(\mu_v, \Delta\phi, w_s, \tau_R, \tau_a, FMF, R_H, z_a)$  nodes (with “test” sampling) and for 300 values of  $\mu_s$  between 0.05 and 1.0. Figure 47 shows the accuracy obtained using the OLCI standard AC LUT sampling for  $\mu_s$ , which is in fact based on a regular sampling of  $\theta_s$ . Using the same number of samples (24) but with a regular sampling in  $\mu_s$  does not significantly improve the accuracy.



**Figure 47. Accuracy of  $\rho_a = f(\mu_s)$  LUT interpolation (band 17) for OLCI standard sampling. Left panel: Histogram of the error for all  $(\mu_v, \Delta\phi, w_s, \tau_R, \tau_a, FMF, R_H, z_a)$  nodes x 300  $\mu_s$  values. Right panel: Fraction of pixels satisfying a given error as a function of  $\mu_s$ .**

### 6.2.3 AXIS $\mu_v$

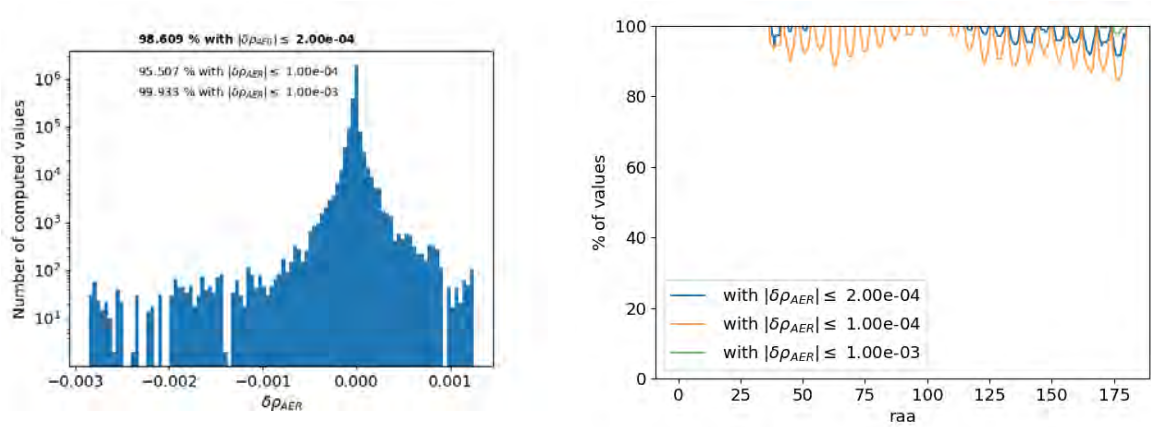
To evaluate interpolation error related to LUTs sampling/interpolation of  $\mu_v$ , we compute  $\rho_a$  for all  $(\mu_s, \Delta\varphi, w_s, \tau_R, \tau_a, FMF, R_H, z_a)$  nodes (with “test” sampling) and for 200 values of  $\mu_v$  between 0.5 and 1.0. Figure 48 shows the accuracy obtained using the OLCI standard AC LUT sampling for  $\mu_v$ . OLCI LUT is in fact based on a regular sampling on  $\theta_v$ . Using the same number of samples (24) but with a regular sampling in  $\mu_v$  does not significantly improve the accuracy.



**Figure 48. Accuracy of  $\rho_a = f(\mu_v)$  LUT interpolation (band 17) for OLCI standard sampling. Left panel: Histogram of the error for all  $(\mu_s, \Delta\varphi, w_s, \tau_R, \tau_a, FMF, R_H, z_a)$  nodes x 300  $\mu_v$  values. Right panel: Fraction of pixels satisfying a given error as a function of  $\mu_v$ .**

#### 6.2.4 AXIS $\Delta\varphi$

For  $\Delta\varphi$  axis study, we compute  $\rho_a$  for all  $(\mu_s, \mu_v, w_s, \tau_R, \tau_a, FMF, R_H, z_a)$  nodes (with “test” sampling) and for 721 values of  $\Delta\varphi$  between 0 and 180°. Figure 49 shows very good performance with the OLCI standard grid.

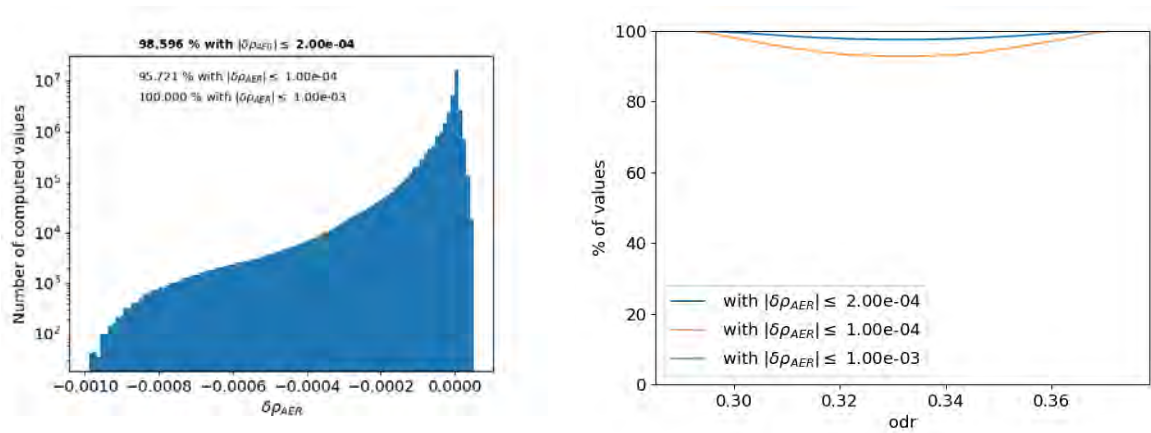


**Figure 49. Accuracy of  $\rho_a = f(\Delta\varphi)$  LUT interpolation (band 17) for OLCI standard sampling. Left panel: Histogram of the error for all  $(\mu_s, \mu_v, w_s, \tau_R, \tau_a, FMF, R_H, z_a)$  nodes x 721  $\Delta\varphi$  values. Right panel: Fraction of pixels satisfying a given error as a function of  $\Delta\varphi$ .**

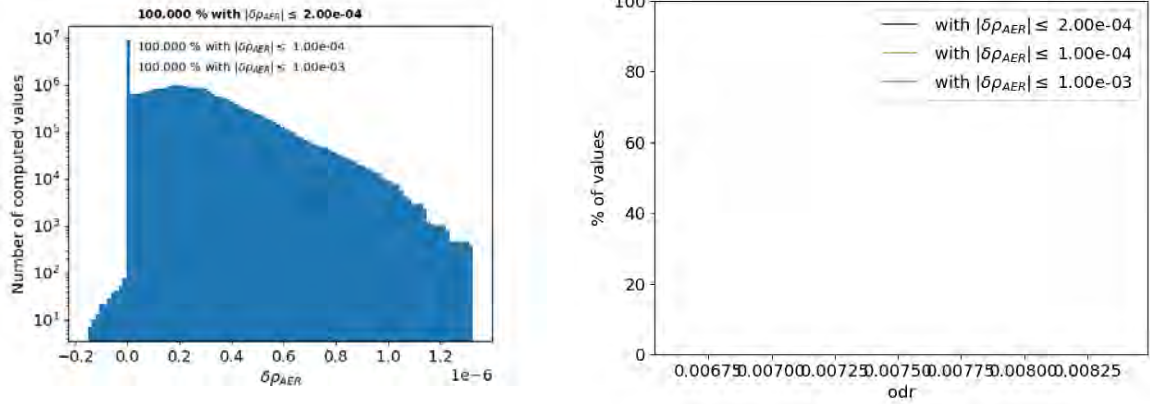
### 6.2.5 AXIS $\tau_R$

To evaluate error related to LUTs sampling/interpolation of  $\tau_R$ , we compute  $\rho_a$  for all  $(\mu_s, \mu_v, \Delta\varphi, w_s, \tau_a, FMF, R_H, z_a)$  nodes (with “test” sampling) and for 200 values of  $\tau_R$  between the maximum and minimum expected values (accounting for smile and a minimum/maximum pressure of 830/1040 hPa) for each band, e.g. for band 1: 0.2894 and 0.3741. This restricts the impact of aerosol/Rayleigh coupling on  $\rho_a$  to relevant values to be fitted or sampled.

Figure 50 and Figure 51 show the result obtained for band 1 and band 21. We see that thanks to the restricted  $\tau_R$  range, only 2 sampled values (the minimum and maximum) are required to have 98.6% of the points with an error  $\leq 2 \cdot 10^{-4}$  for band 1 and 100% of the points with an error  $\leq 2 \cdot 10^{-4}$  for band 21.



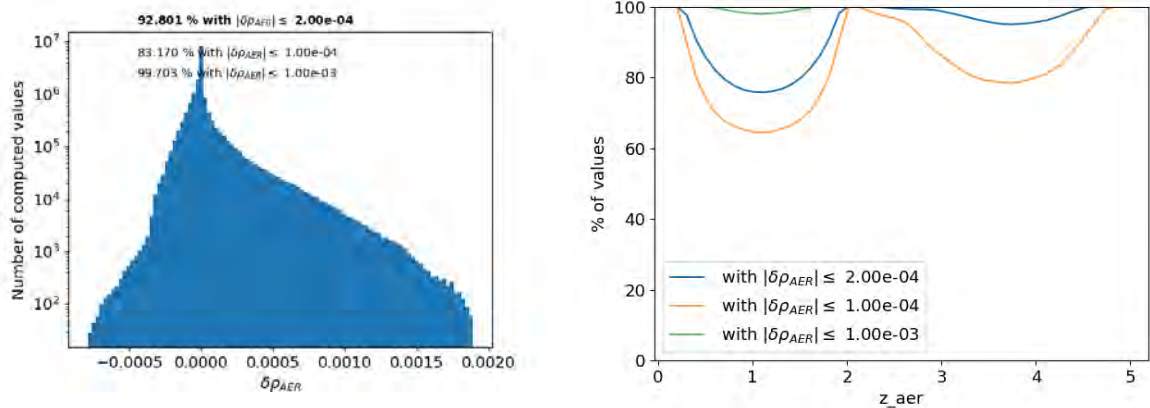
**Figure 50. Accuracy of  $\rho_a = f(\tau_R)$  LUT (band 1) interpolation for only two sample grid (the minimum and maximum values 0.2894 and 0.3741). Left panel: Histogram of the error for all  $(\mu_s, \mu_v, \Delta\varphi, w_s, \tau_a, FMF, R_H, z_a)$  nodes x 200  $\tau_R$  values. Right panel: Fraction of pixels satisfying a given error as a function of  $\tau_R$ .**



**Figure 51.** Accuracy of  $\rho_a = f(\tau_R)$  LUT (band 21) interpolation for only two sample grid (the minimum and maximum values 0.0066 and 0.0084). Left panel: Histogram of the error for all  $(\mu_s, \mu_v, \Delta\phi, w_s, \tau_a, FMF, R_H, z_a)$  nodes x 200  $\tau_R$  values. Right panel: Fraction of pixels satisfying a given error as a function of  $\tau_R$ .

#### 6.2.6 AXIS $z_a$

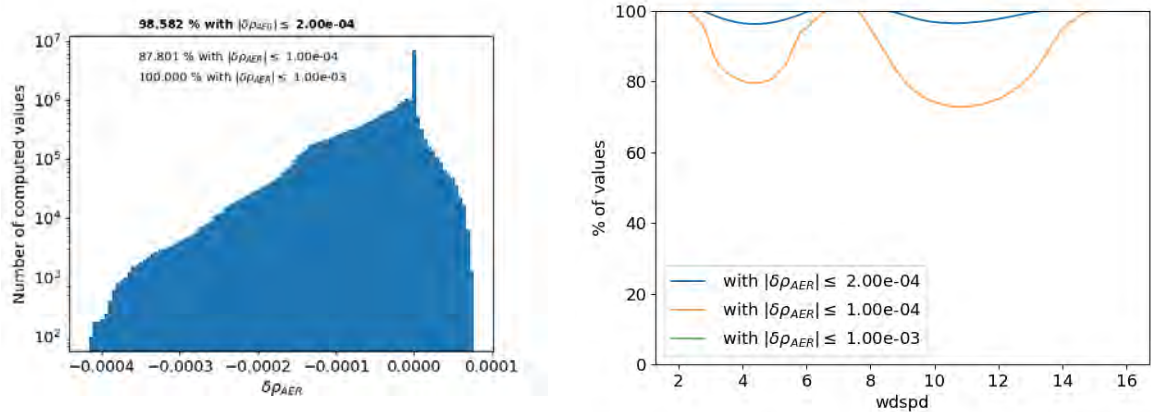
To evaluate error related to LUTs sampling/interpolation of  $z_a$ , we compute  $\rho_a$  for all  $(\mu_s, \mu_v, \Delta\phi, w_s, \tau_R, \tau_a, FMF, R_H)$  nodes (with “test” sampling) and for 100 values of  $z_a$  between 0.0 and 10 km. We study band 1 because the aerosol/Rayleigh coupling is more important for this band and produce more variability of  $\rho_a = f(z_a)$ . We see that with only 3 points at 0.2, 2.0 and 5.0 km 92.8% of the points have an error  $\leq 2 \cdot 10^{-4}$ .



**Figure 52.** Accuracy of  $\rho_a = f(z_a)$  LUT interpolation for grid [0.2, 2.0 and 5.0 km] for band 1. Left panel: Histogram of the error for all  $(\mu_s, \mu_v, \Delta\phi, w_s, \tau_R, \tau_a, FMF, R_H)$  nodes x 100  $z_a$  values. Right panel: Fraction of pixels satisfying a given error as a function of  $z_a$ .

### 6.2.7 AXIS $w_s$

To evaluate error related to LUTs sampling/interpolation of  $w_s$ , we compute  $\rho_a$  for all  $(\mu_s, \mu_v, \Delta\phi, \tau_R, \tau_a, FMF, R_H, z_a)$  nodes (with “test” sampling) and for 100 values of  $w_s$  between 0.25 and 16 m/s. We see on Figure 53 that with only 3 points at 2, 7 and 16 m/s, 98.5% of the points have an error  $\leq 2 \cdot 10^{-4}$  for band 1. For band 17, we obtain 99.7% of the points with an error  $\leq 2 \cdot 10^{-4}$  with the same grid sampling.

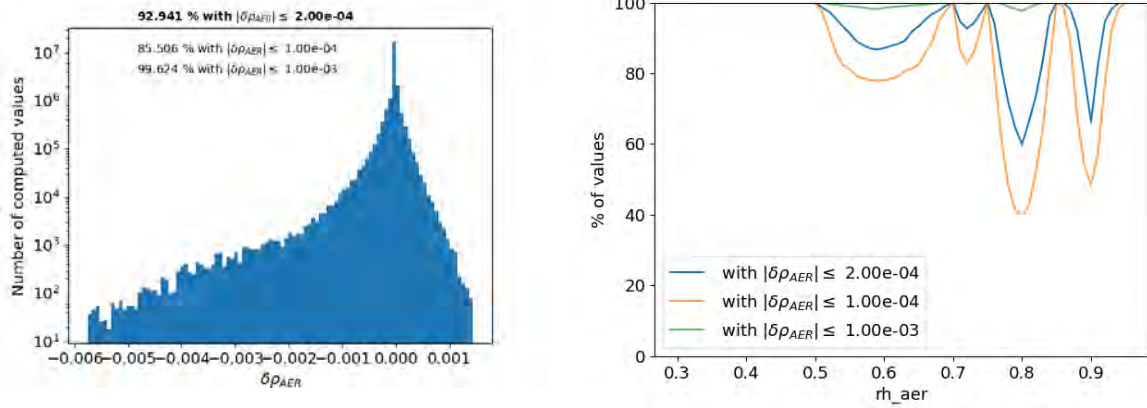


**Figure 53. Accuracy of  $\rho_a = f(w_s)$  LUT interpolation for grid [ 2, 7 and 16 m/s] for band 1. Left panel: Histogram of the error for all  $(\mu_s, \mu_v, \Delta\phi, \tau_R, \tau_a, FMF, R_H, z_a)$  nodes x 100  $w_s$  values. Right panel: Fraction of pixels satisfying a given error as a function of  $w_s$ .**

### 6.2.8 AXIS $R_H$

To evaluate error related to LUTs sampling/interpolation of  $R_H$ , we compute  $\rho_a$  for all  $(\mu_s, \mu_v, \Delta\phi, \tau_R, \tau_a, FMF, w_s, z_a)$  nodes (with “test” sampling) and for 95 values of  $R_H$  between 0 and 0.95.

We see on Figure 54 that with the grid [0.3, 0.5, 0.7, 0.75, 0.85, 0.95], 92.9% of the points have an error  $\leq 2 \cdot 10^{-4}$  for band 17. For band 1, we obtain 93.6% of the points with an error  $\leq 2 \cdot 10^{-4}$  with the same grid sampling.

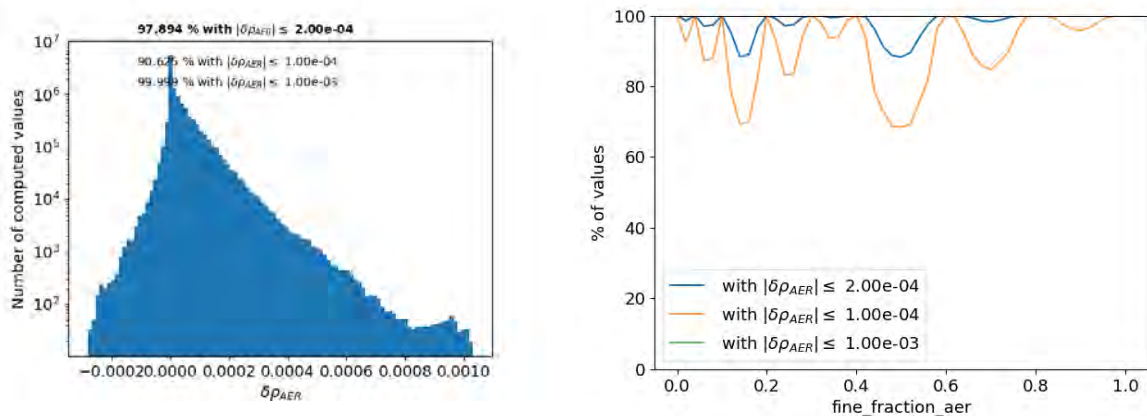


**Figure 54. Accuracy of  $\rho_a = f(R_H)$  LUT interpolation for grid [0.3, 0.5, 0.7, 0.75, 0.85, 0.95] for band 17. Left panel: Histogram of the error for all  $(\mu_s, \mu_v, \Delta\phi, \tau_R, \tau_a, FMF, w_s, z_a)$  nodes x 100  $R_H$  values. Right panel: Fraction of pixels satisfying a given error as a function of  $R_H$ .**

### 6.2.9 AXIS FMF

To evaluate error related to LUTs sampling/interpolation of FMF, we compute  $\rho_a$  for all  $(\mu_s, \mu_v, \Delta\phi, \tau_R, \tau_a, R_H, w_s, z_a)$  nodes (with “test” sampling) and for 50 values of FMF between 0 and 1.

We see on Figure 55 that with the grid [0, 0.04, 0.1, 0.2, 0.3, 0.4, 0.6, 0.8, 1.0], 97.9% of the points have an error  $\leq 2 \cdot 10^{-4}$  for band 17. For band 1, we obtain 82.5% of the points with an error  $\leq 2 \cdot 10^{-4}$  with the same grid sampling.



**Figure 55. Accuracy of  $\rho_a = f(FMF)$  LUT interpolation for grid [0, 0.04, 0.1, 0.2, 0.3, 0.4, 0.6, 0.8, 1.0] for band 17. Left panel: Histogram of the error for all  $(\mu_s, \mu_v, \Delta\phi, \tau_R, \tau_a, R_H, w_s, z_a)$  nodes x 50 FMF values. Right panel: Fraction of pixels satisfying a given error as a function of FMF.**

## 7 APPENDIX 2: OC-SAC SVC GAINS COMPUTATION

### 7.1 DATA AND METHOD

Dedicated SVC gains have been generated for with EUMETSAT OC-SVC-TOOL (Mazéran and Ruescas, 2020), for both OLCI-A and OLCI-B., with OC-SAC launched with OC-SAC-SACSO prototype [AD-1].

The datasets and overall approach follow exactly that used for IPF of Collection 3 (Mazéran and Ruescas, 2020): MDB at SPG for NIR gains and MOBY for VIS gains, screening criteria, configuration. This means the OC-SAC gains can be directly compared to those of Collection 3; the only limitation resides in some flags, in particular cloud screening, done outside the OC-SAC module and less restrictive in OC-SAC-SACSO than IPF.

In particular, for NIR SVC, the standard protocol is as follows (Franz et al., 2007):

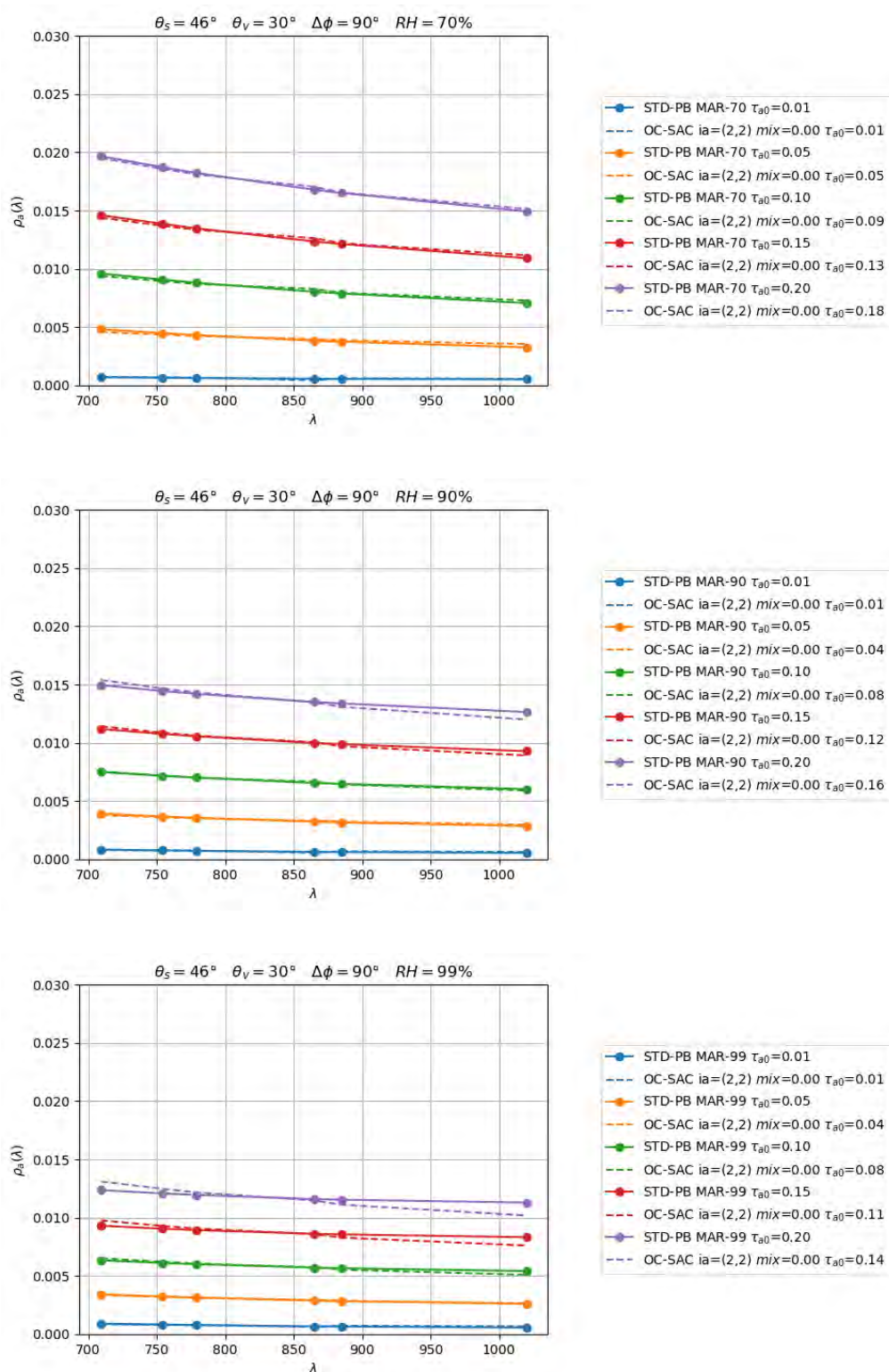
- Gains are computed over SPG where marine signal in the NIR is zero:  $\rho_w(\lambda) = 0$ , for  $\lambda \geq 708.75$ .
- BPC is deactivated
- Marine reflectance in the NIR is the output of CWAC and not BPC (by default in OC-SAC)
- Gain at 865 nm is fixed:  $g(865) = 0.986$  for OLCI-A,  $g(865) = 1$  for OLCI-B.
- Aerosol model is fixed, classically to a MAR-90 (Shettle and Fenn, 1979).

This latter condition on MAR-90, however, cannot strictly be applied, since OC-SAC aerosol models are different in their inherent optical properties, and also in the way they depend on ancillary relative humidity and are selected thanks to five (possibly six) bands in the NIR instead of two. Current CWAC determines  $\rho_{a0}$  at 865 nm, which has a fixed gain, so there is no coupling between SVC and  $\rho_{a0}$ . Fixing the aerosol model in OC-SAC means that only one model is allowed in the ADF (through the list of aerosol models) and that the mixing ratio is also fixed to zero. The loop on aerosol models is thus limited to one pass, and the  $\chi^2_{iaer}$  computation plays no role. The question is then to find a FMF that best match a MAR-90 model, when RH is 90%. Our methodology has consisted in:

- i. Simulating aerosol reflectance in the NIR for a MAR-90 model, as done with OLCI previous LUTs (Collection 3), for different geometries and AOTs. In fact, simulations were also carried out for other RHs, since in OC-SAC RH is pixel dependent: MAR-50, MAR-70 and MAR-99.
- ii. Run the CWAC in nominal mode (5 bands, free list of aerosol models) to inverse these aerosol spectra, and identify which bracketing FMFs are retrieved and select that most representative (upper FMF if mixing ratio above 0.5, lower FMF otherwise).
- iii. Finally, inverse again these spectra with this fixed FMF only (single model mode, implying mixing ratio = 0) and check relevance.

Results of this exercise is that a FMF of 0.1 (ia=2 in OC-SAC LUT) allows to best match the standard maritime model, for different RH and AOT (Figure 56). We see that the AOT retrieved by OC-SAC is consistent but always lower than the original AOT used with the Shettle and Fenn (1979) models, what is perfectly in line with findings of Ahmad et al. (2010).

Because there is currently an uncertainty in the input ECMWF RH (always given at 850 hPa), it is also decided to fix input RH to 90% for the whole SVC process, what completely fixes the aerosol model.



**Figure 56** Aerosol reflectance in the NIR simulated for three standard models (LUT of Collection 3, solid line, top=MAR-70, middle = MAR-90, bottom=MAR-99) for various AOTs (colours) and their inversion with OC-SAC when fixing FMF=0.1 (dashed line, corresponding to  $ia=2$  in OC-SAC LUT).

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## 7.2 OLCI-A GAINS

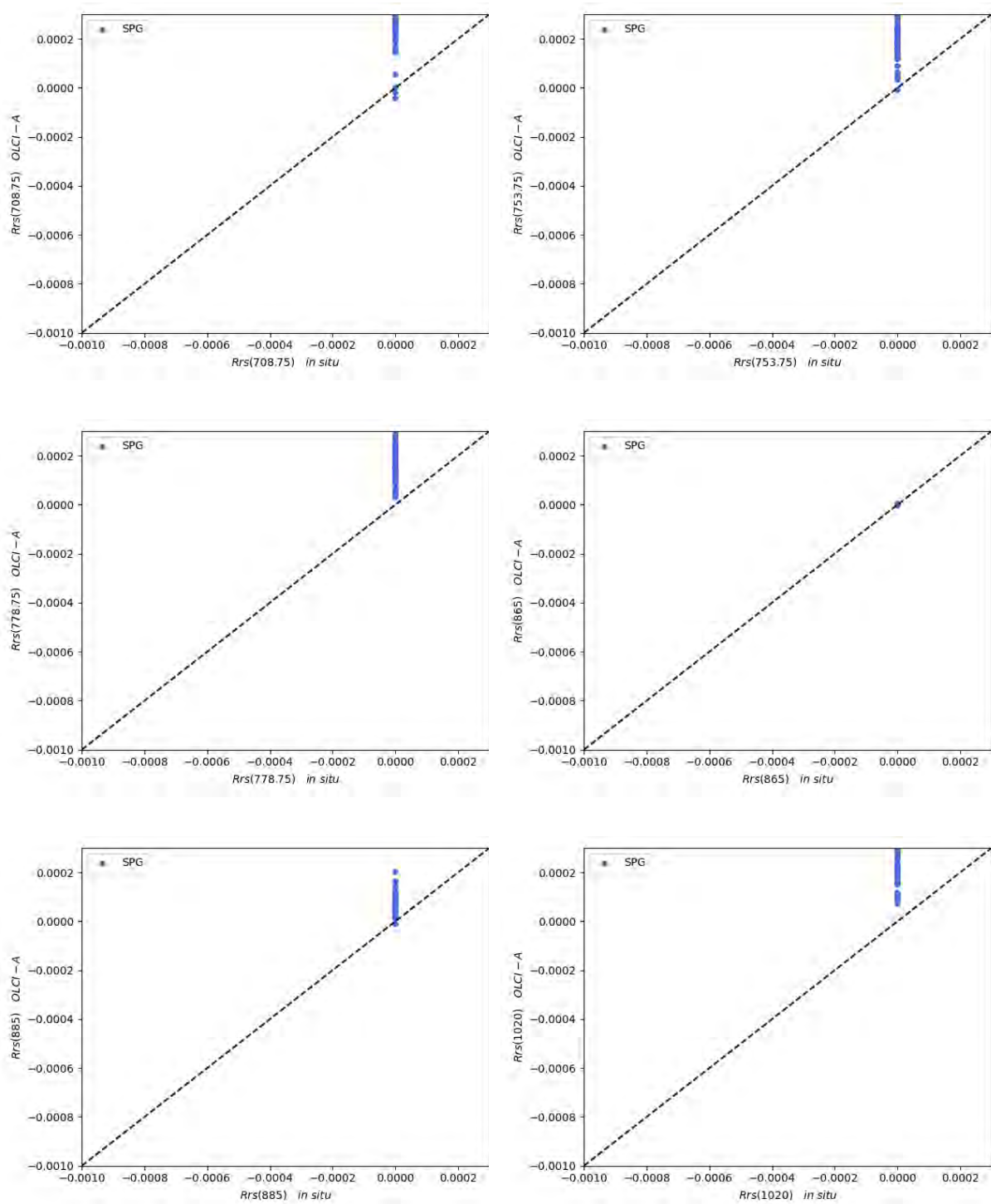
### 7.2.1 NIR GAINS

Reminder: results are generated with a fixed input RH=90%.

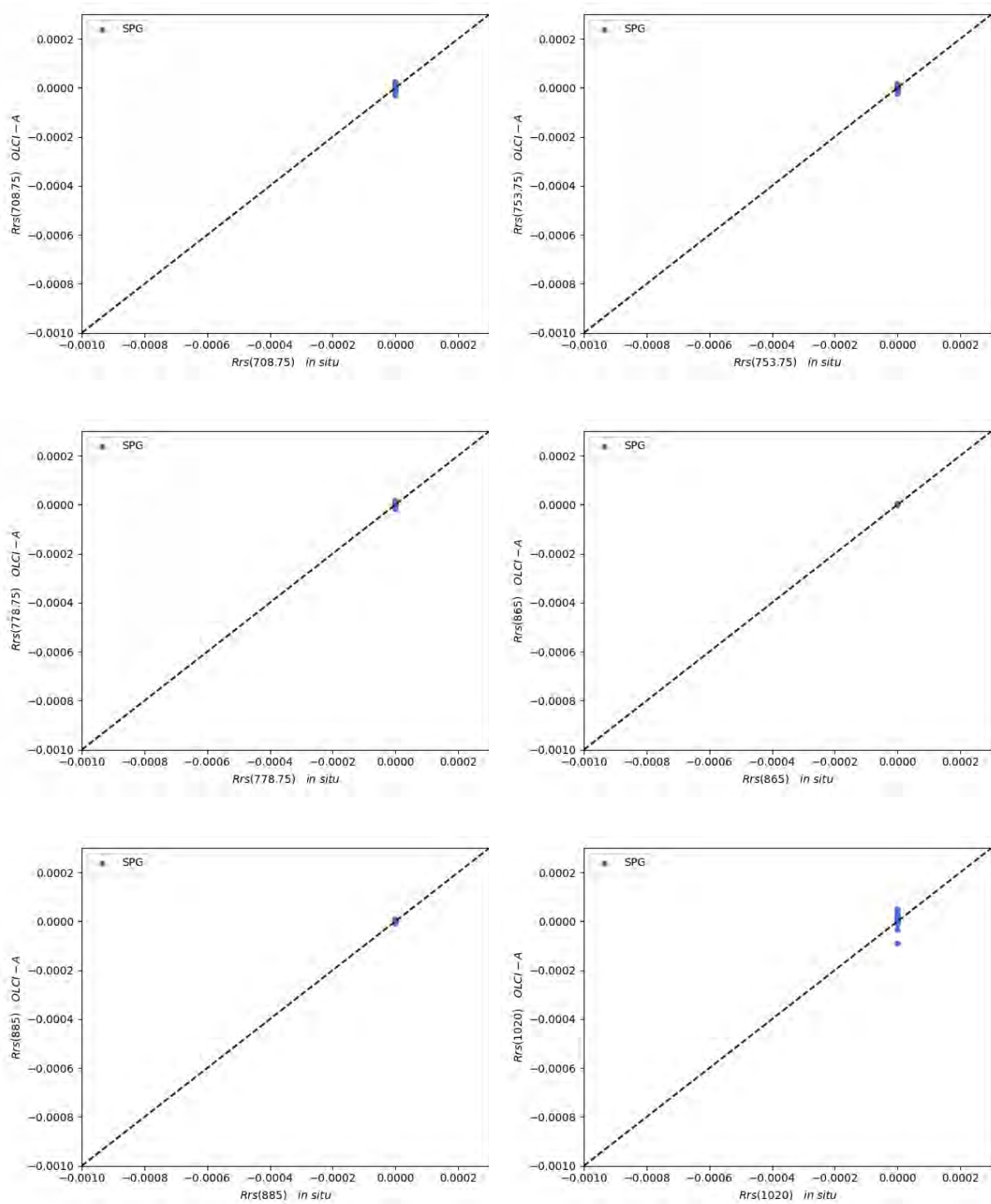
The comparison between the targeted marine reflectance (fixed to zero) and OC-SAC reflectance in the NIR is shown on Figure 57 and Figure 58 for respectively the default gains (unity except 0.986 at 865 nm) and the computed gains per match-up. A nearly perfect retrieval is achieved after applying the individual gains, considering the very low level of the signal (see scale on the figures).

The averaged NIR gains (Table 10 and Figure 59, right) are relatively consistent with those of Collection 3 (Figure 59, left), however with an amplitude noticeably increasing towards 709 nm (gain of about -3.2% at this band). This shape is much less pronounced with former processor. Fixing a FMF of 0.1 at SPG can be questioned; Ahmad et al. (2010) actually adapted the original method, by targeting the Angstrom exponent to the value measured at the closest AERONET station, i.e. Tahiti. They targeted and Angstrom between 440 and 865 of 0.68. This value can also be reached with our chosen model (FMF=0.1) but with a RH of 50% ( $\alpha_{440} = 0.672$ ). An attempt was made to fix RH to 50%, but the shape did not improve (not shown).

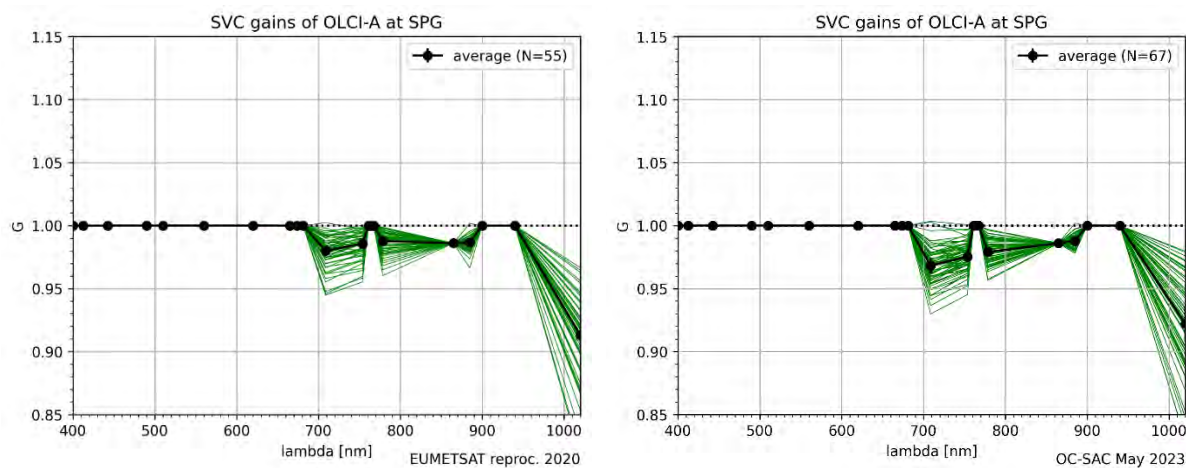
Robustness versus time, geometry and detector remains excellent (Figure 60 to Figure 64).



**Figure 57 Validation of OLCI-A  $R_{rs}$  at SPG with nominal gains (see text) at 708.75, 753.75, 778.75, 865, 885 and 1020 nm.**



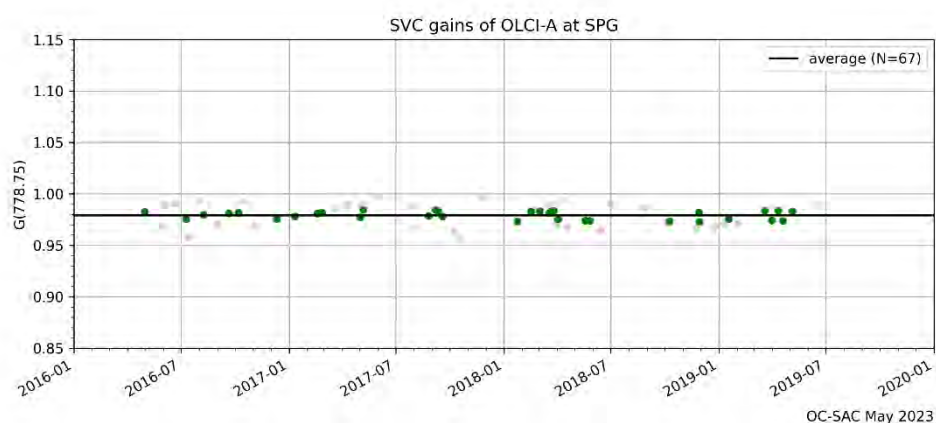
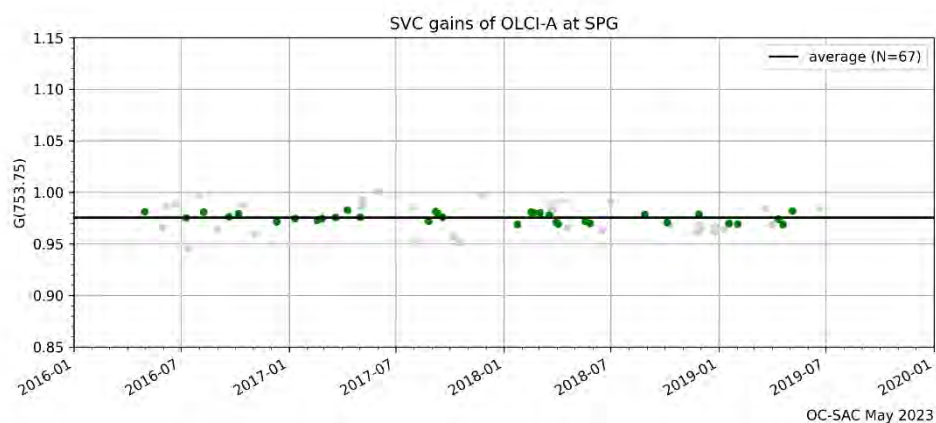
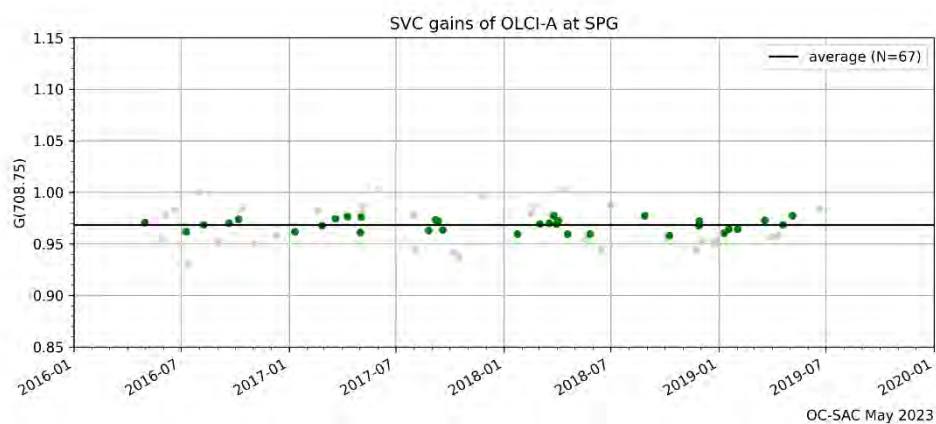
**Figure 58 Validation of OLCI-A  $R_{rs}$  at SPG after calibration by individual gains (see text) at 708.75, 753.75, 778.75, 865, 885 and 1020 nm.**



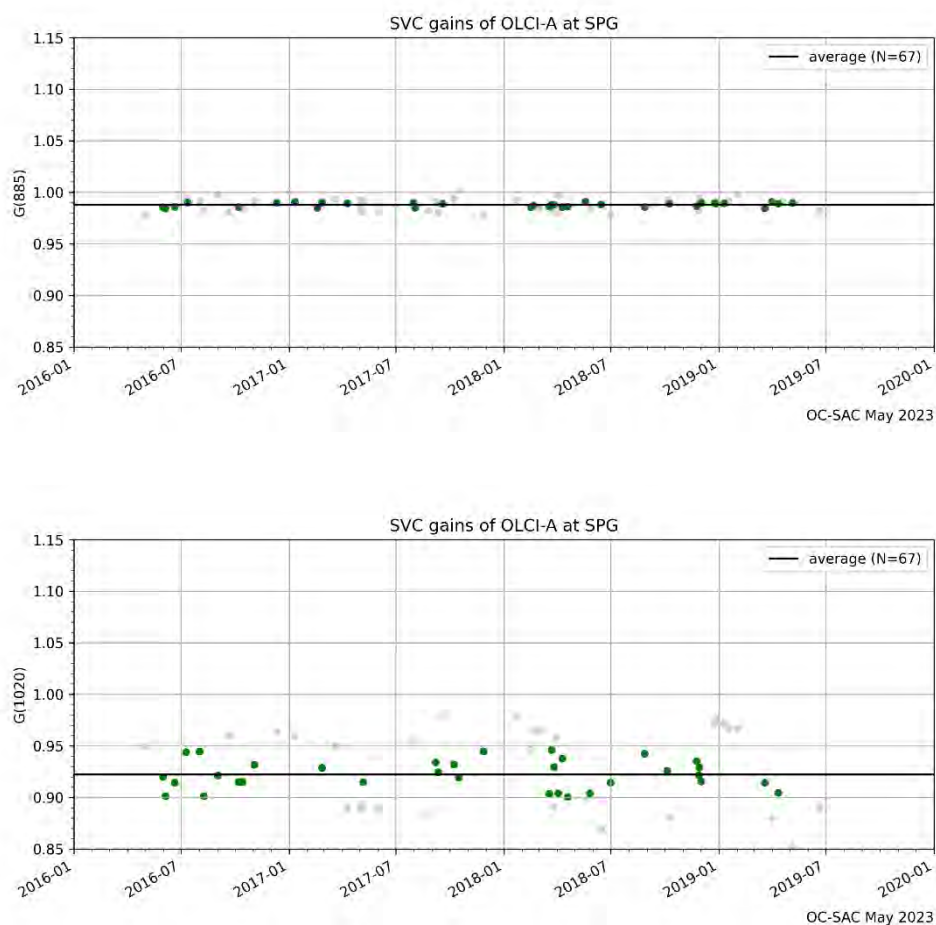
**Figure 59 Individual spectral gains of OLCI-A at SPG, before MSIQR screening, left for Collection 3, right for present OC-SAC processor.**

**Table 10 Statistics of OLCI-A averaged gains at SPG, after MSIQR filtering**

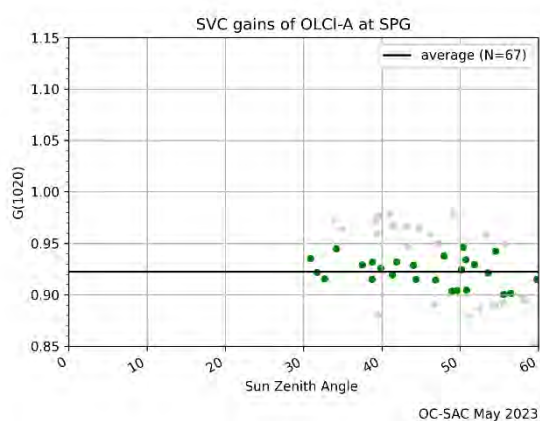
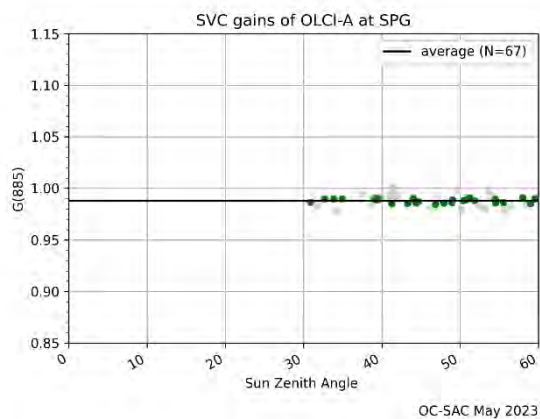
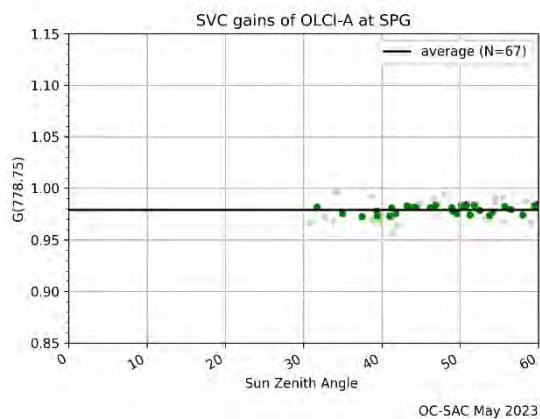
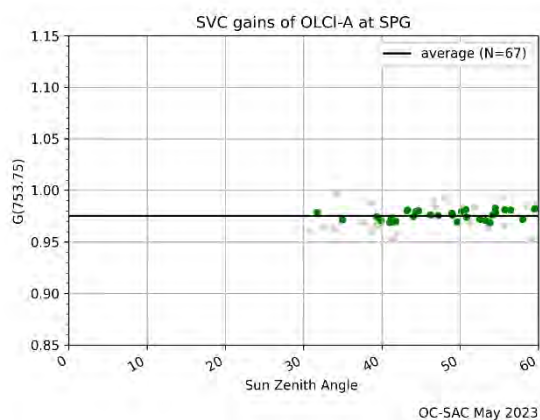
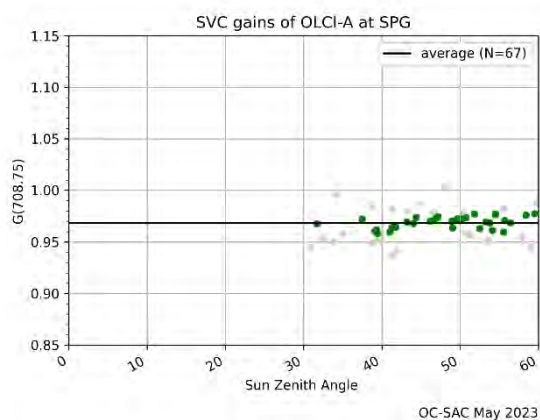
| Wavelength | Number | Average gain | Standard-deviation |
|------------|--------|--------------|--------------------|
| 708.75     | 33     | 0.968208     | 0.005692           |
| 753.75     | 33     | 0.975404     | 0.003392           |
| 778.75     | 32     | 0.977003     | 0.003001           |
| 865        |        | 0.986        |                    |
| 885        | 33     | 0.987786     | 0.002065           |
| 1020       | 33     | 0.922184     | 0.013944           |



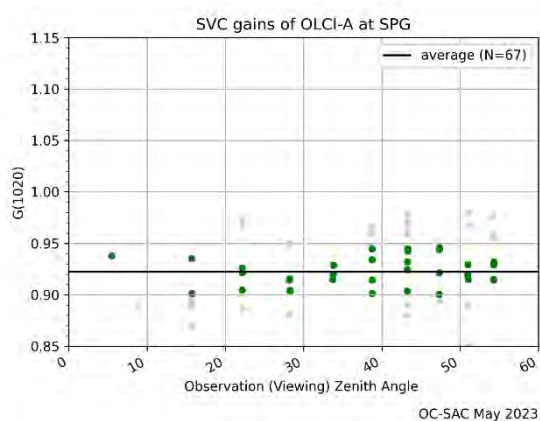
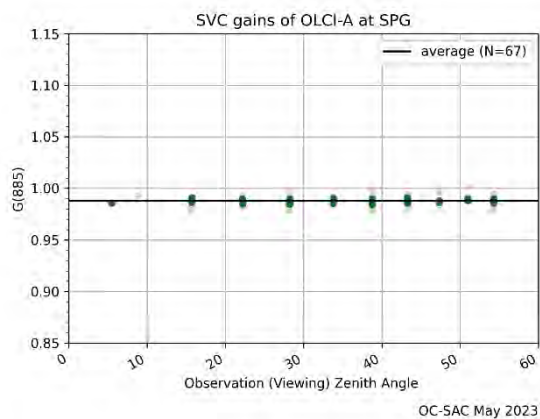
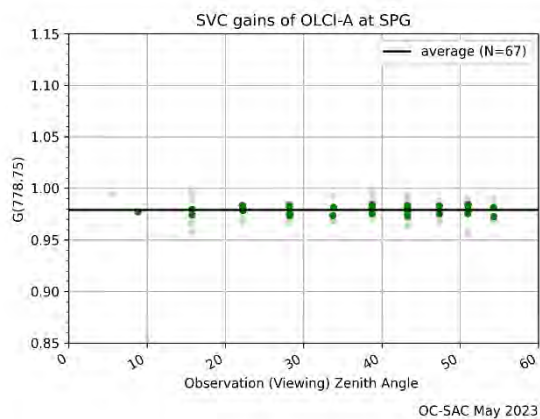
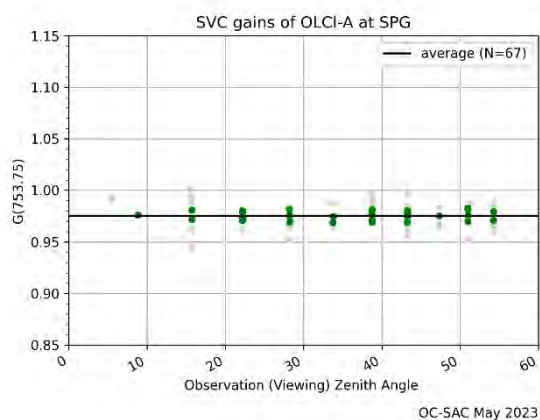
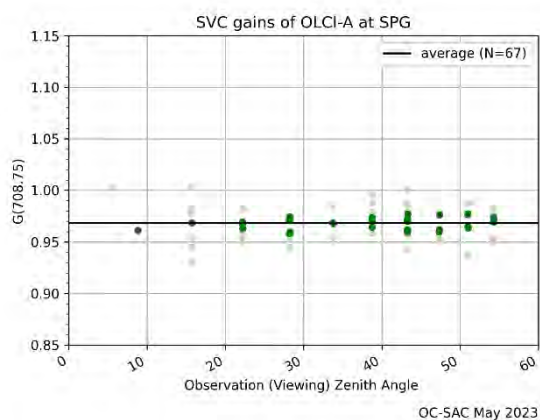
**Figure 60 Time-series of OLCI-A gains at SPG at 708.75, 753.75 and 778.75 nm. Gains in green fall within the semi-interquartile range used in final averaging.**



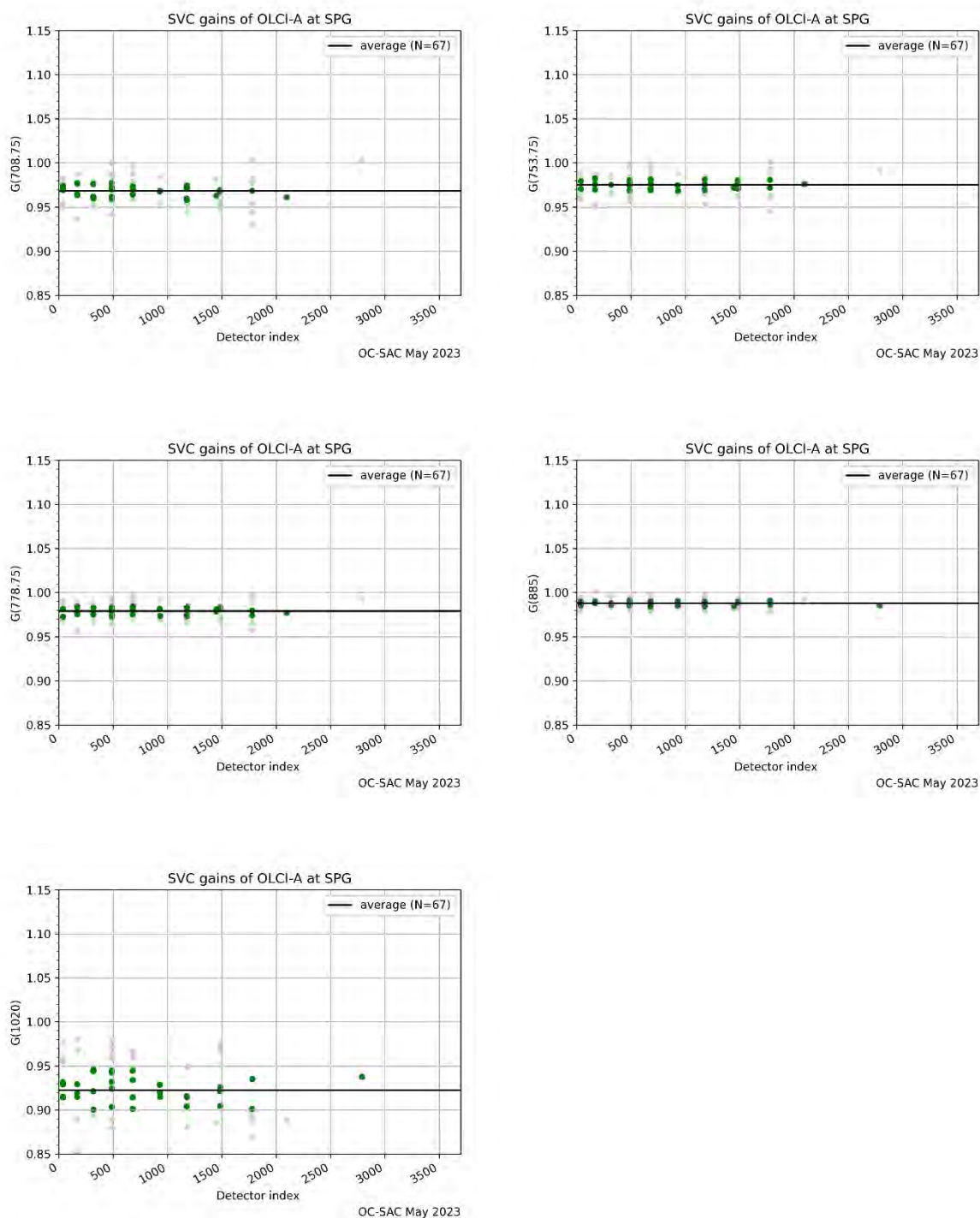
**Figure 61 Time-series of OLCI-A gains at SPG at 885 and 1020 nm. Gains in green fall within the semi-interquartile range used in final averaging.**



**Figure 62 OLCI-A gains at SPG at 708.75, 753.75, 778.75, 885 and 1020 nm as a function of sun zenith angle. Gains in green fall within the semi-interquartile range used in final averaging.**



**Figure 63 OLCI-A gains at SPG at 708.75, 753.75, 778.75, 885 and 1020 nm as a function of view zenith angle. Gains in green fall within the semi-interquartile range used in final averaging.**



**Figure 64 OLCI-A gains at SPG at 708.75, 753.75, 778.75, 885 and 1020 nm as a function of detector index. Gains in green fall within the semi-interquartile range used in final averaging.**

### 7.2.2 VIS GAINS

**Reminder: results are generated with a fixed input RH=90%.**

The comparison between the MOBY  $R_{rs}^t$  and satellite  $R_{rs}$  in the VIS is shown on Figure 65 and Figure 66 for respectively the default gains (unit gain in the VIS, new gains in the NIR) and the computed VIS gains per match-up. This demonstrates the relevance of the individual gains in the VIS.

The averaged gains (Table 11 and Figure 67) shows a similar pattern to those of Collection 3, with a relatively flat shape from 400 to 665 nm. We see clearly on Figure 67 some outliers, likely due to some erroneous cloud filtering in OC-SAC-SACSO; these dubious spectra are removed in the computation of the mean gains thanks to statistical filtering, although they impact the standard-deviation. The amplitude is, again, higher (-3.6% at 400 nm, -4.2% at 510 nm) what is consistent with the OC-SAC gains in the NIR. Probably a change of the NIR gains (reduced values) would affect the amplitude of the VIS gains while keeping the relatively flat shape, as expected from Level-1 calibration. Values of RSEM, scalded over a decade (Table 11) reach nearly the requirements of see Zibordi et al. (2015), with value of 0.07% in the blue and nearly 0.05% at 560 nm; this is slightly worse than Collection 3, but again a revision of NIR gains and cloud filtering should improve the results. RSEM decreases in the red toward 0.017%, however without reaching the target of 0.005% that seems unachievable over clear waters (as for Collection 3).

Robustness versus time, geometry and detector remains again excellent (Figure 68 to Figure 73).

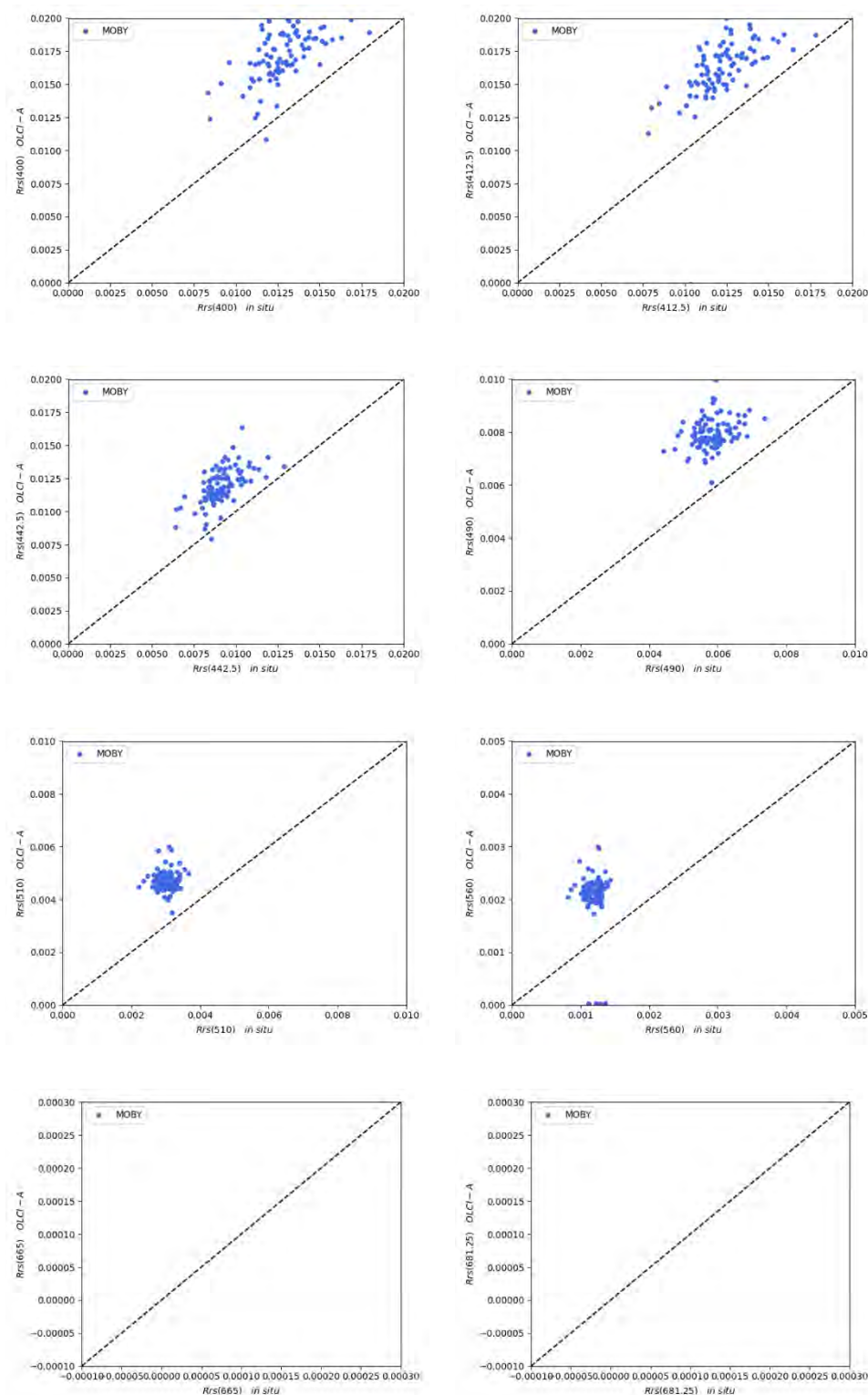
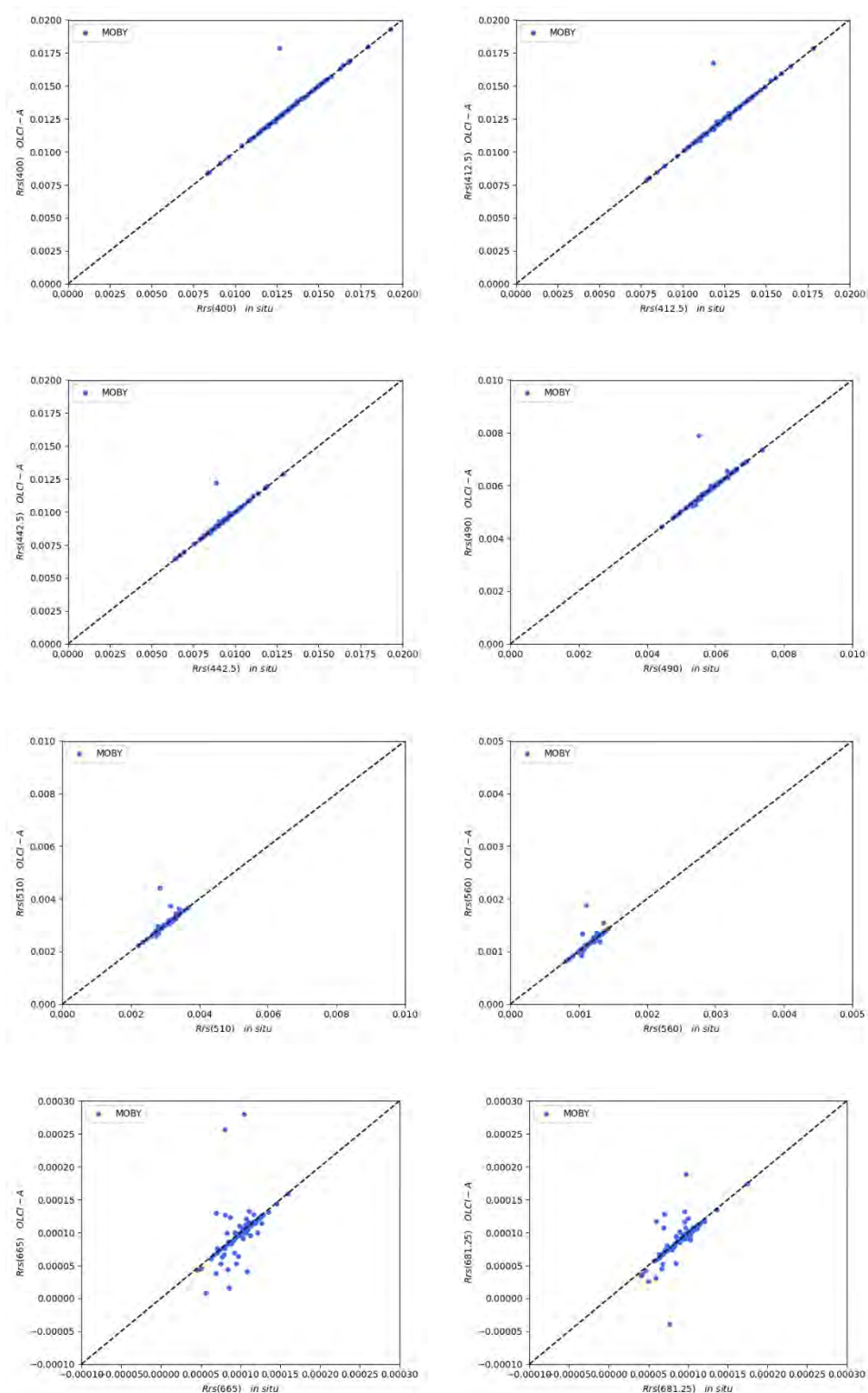
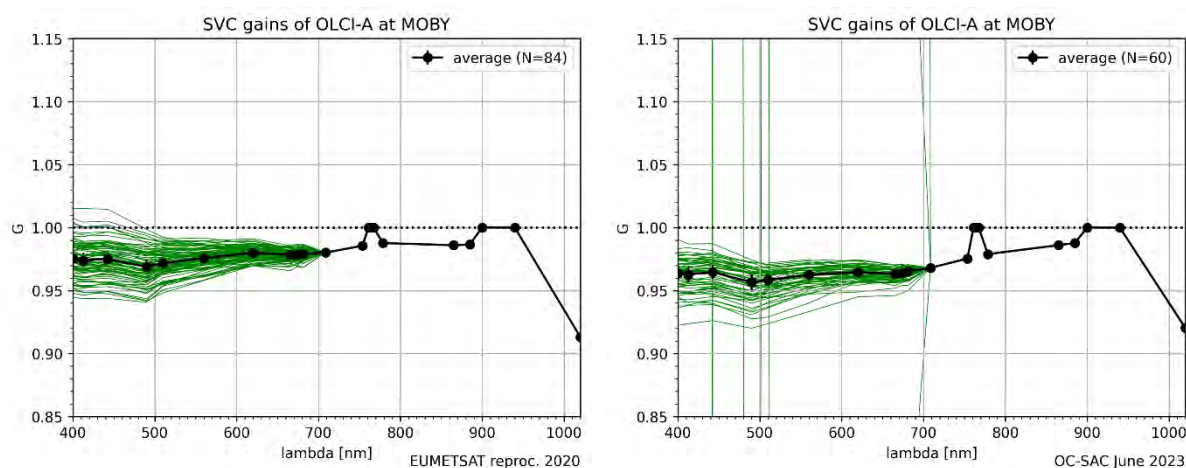


Figure 65 Validation of OLCI-A  $R_{rs}$  at MOBY with nominal gains (see text) at 400, 412.5, 442.5, 490, 510, 560, 665 and 681.25 nm.



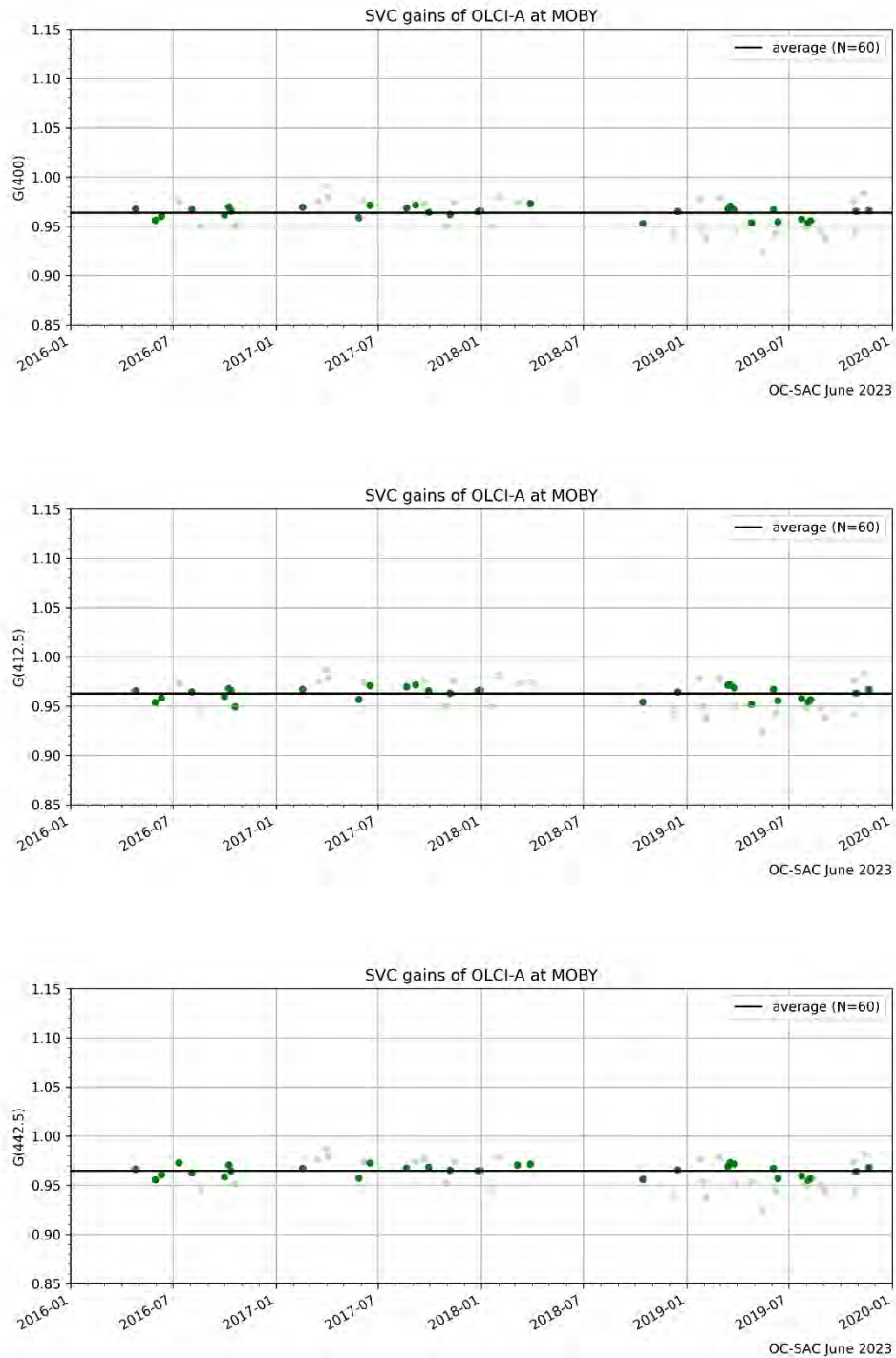
**Figure 66 Validation of OLCI-A  $R_{rs}$  at MOBY after calibration by individual gains (see text) at 400, 412.5, 442.5, 490, 510, 560, 665 and 681.25 nm.**



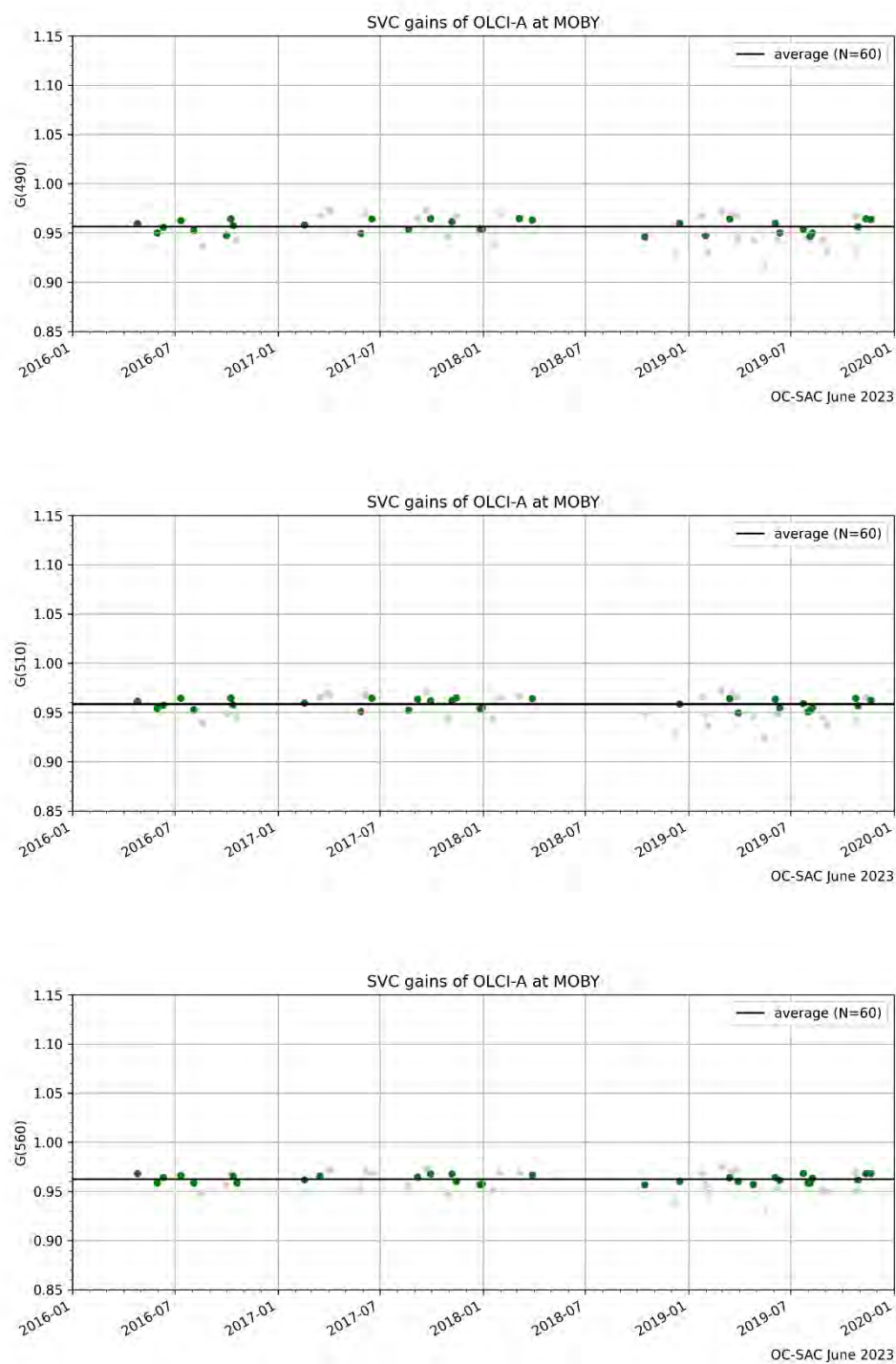
**Figure 67 Individual spectral gains of OLCI-A at MOBY, before MSIQR screening, left for Collection 3, right for present OC-SAC processor.**

**Table 11 Statistics of OLCI-A averaged gains at MOBY, after MSIQR filtering**

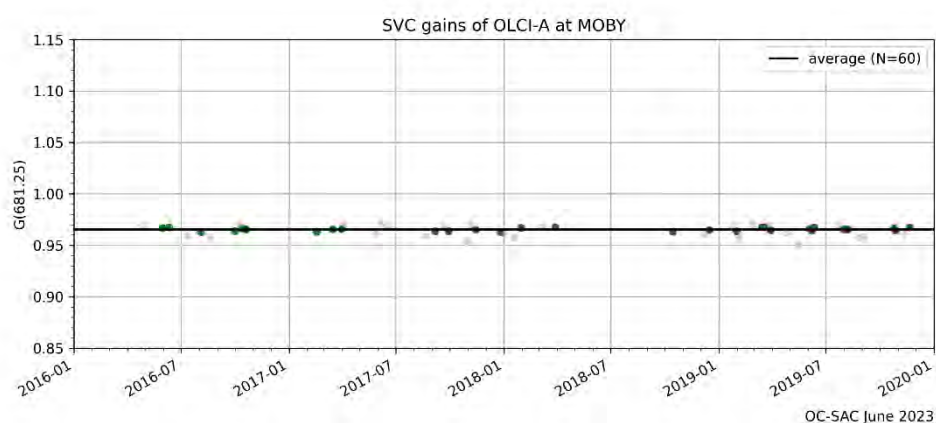
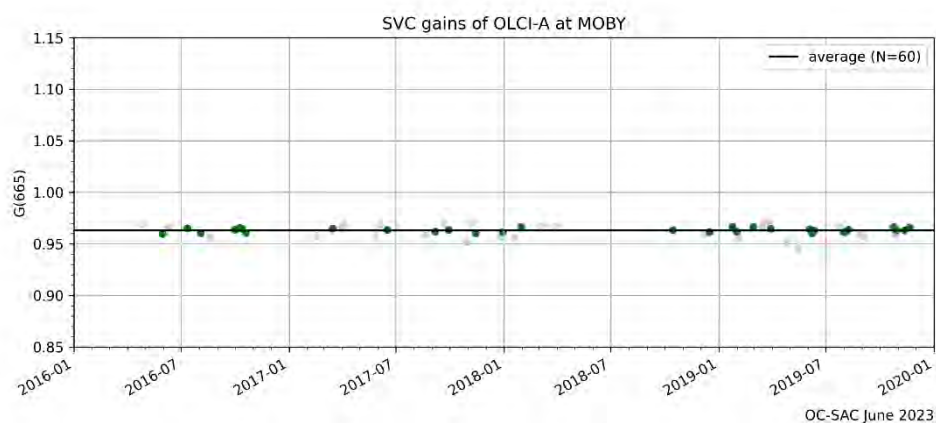
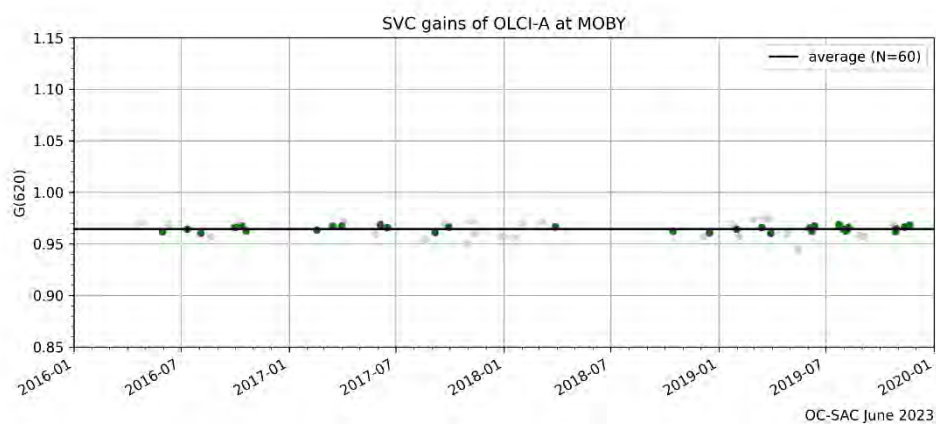
| Wavelength | Number | Average gain | Standard-deviation | RSEM [%] |
|------------|--------|--------------|--------------------|----------|
| 400        | 30     | 0.963688     | 0.005912           | 0.0669%  |
| 412.5      | 30     | 0.962709     | 0.006319           | 0.0716%  |
| 442.5      | 30     | 0.964771     | 0.005643           | 0.0638%  |
| 490        | 30     | 0.956524     | 0.006191           | 0.0706%  |
| 510        | 30     | 0.958425     | 0.004971           | 0.0566%  |
| 560        | 30     | 0.962528     | 0.003964           | 0.0449%  |
| 620        | 30     | 0.964537     | 0.002512           | 0.0284%  |
| 665        | 30     | 0.963211     | 0.002098           | 0.0238%  |
| 673.75     | 30     | 0.963768     | 0.001958           | 0.0222%  |
| 681.25     | 30     | 0.965271     | 0.001549           | 0.0175%  |



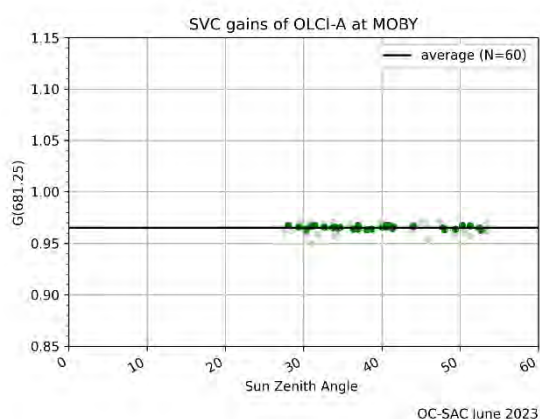
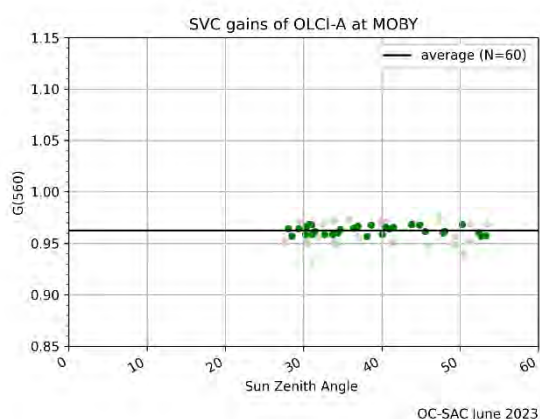
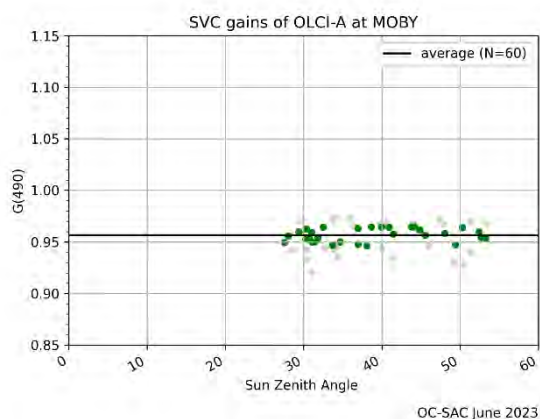
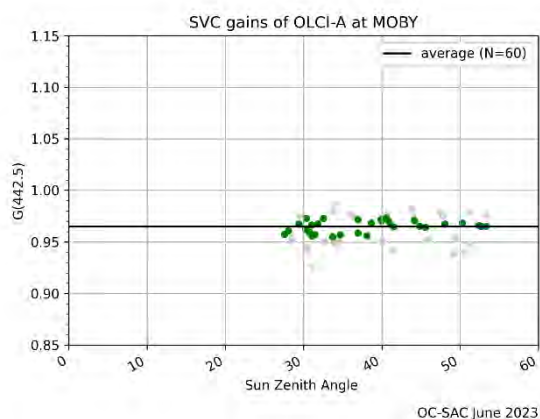
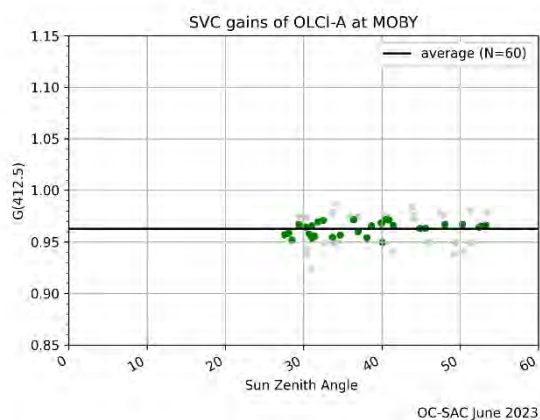
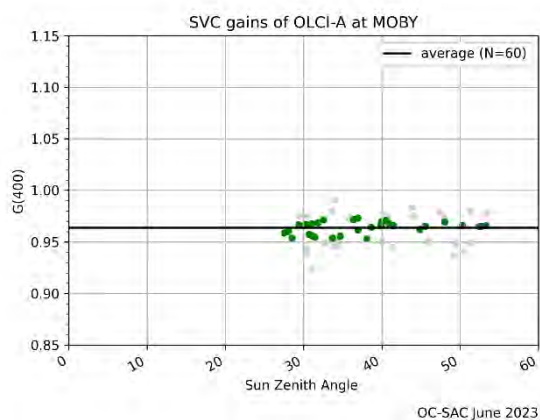
**Figure 68 Time-series of OLCI-A gains at MOBY at 400, 412.5 and 442.5 nm. Gains in green fall within the semi-interquartile range used in final averaging.**



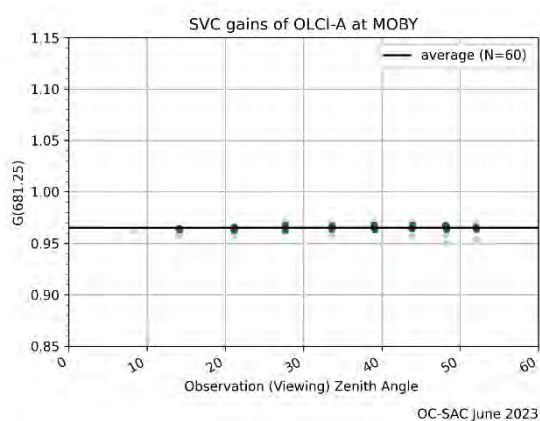
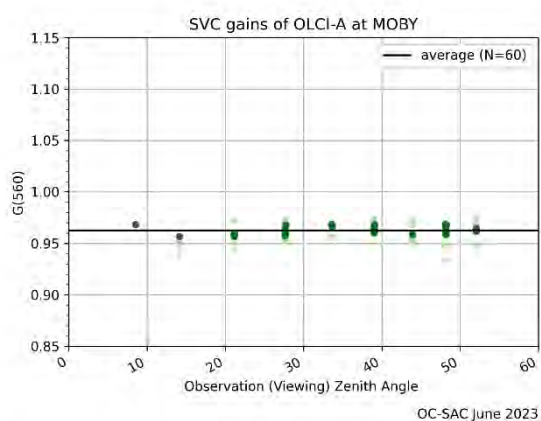
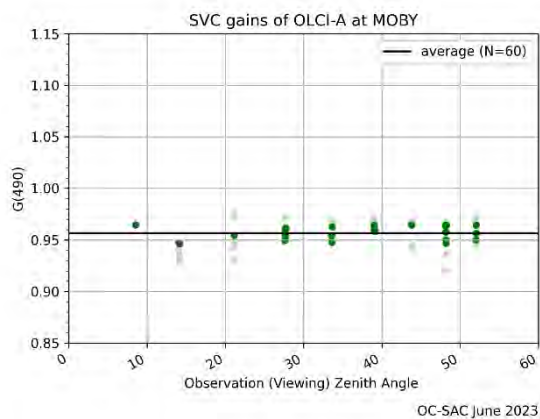
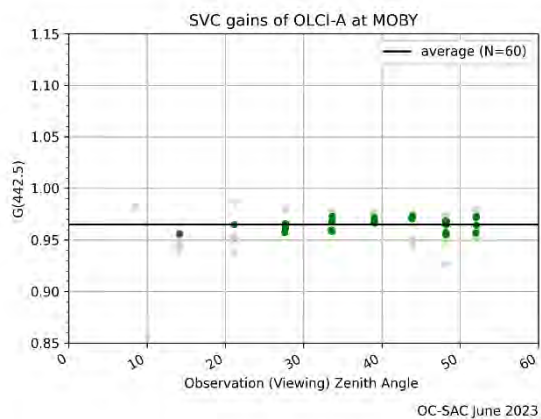
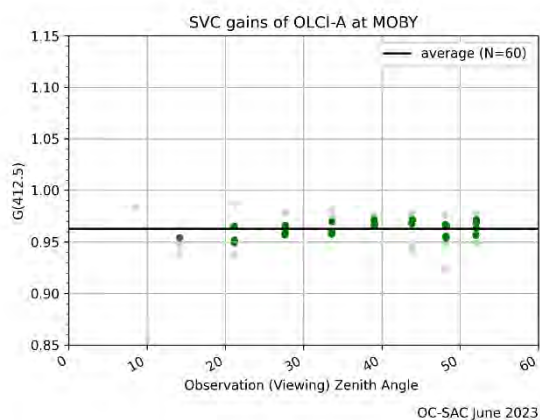
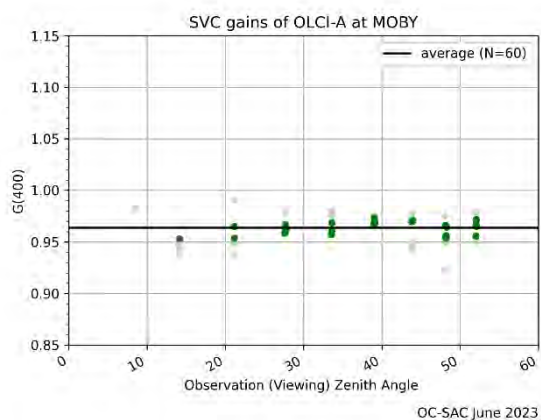
**Figure 69 Time-series of OLCI-A gains at MOBY at 490, 510 and 560 nm. Gains in green fall within the semi-interquartile range used in final averaging.**



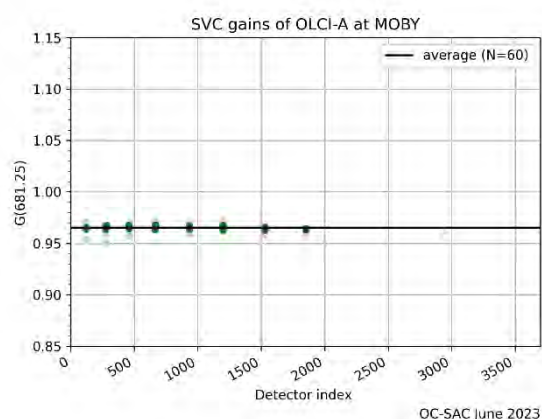
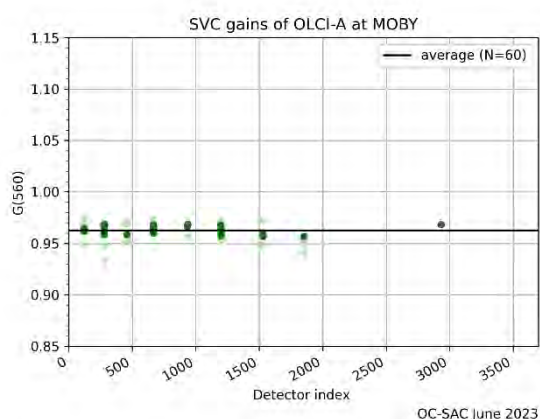
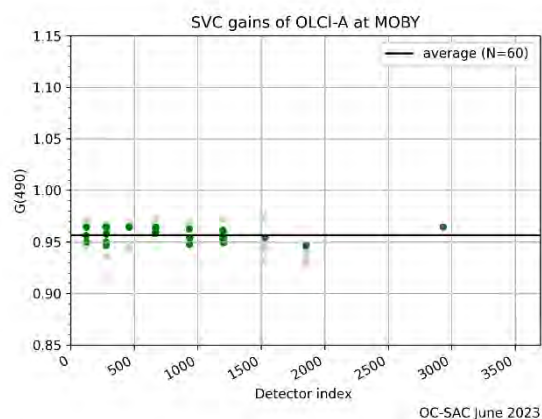
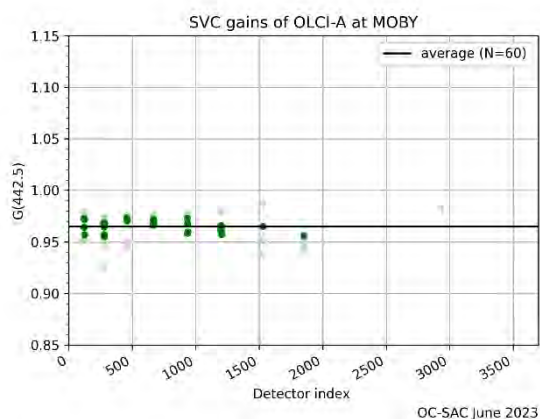
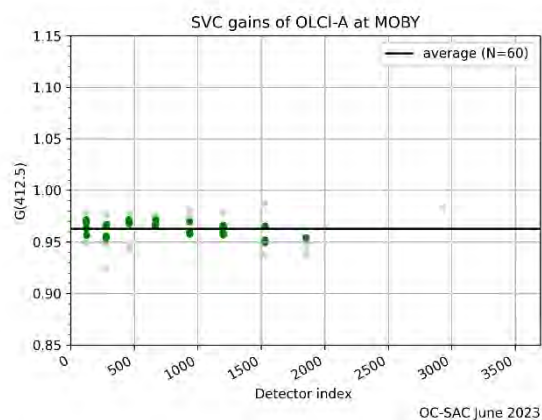
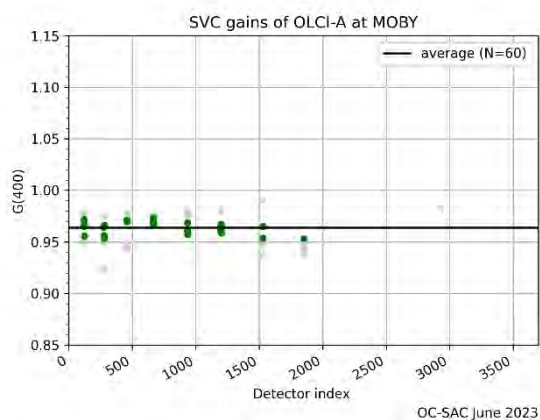
**Figure 70 Time-series of OLCI-A gains at MOBY at 620, 665 and 681.25 nm. Gains in green fall within the semi-interquartile range used in final averaging.**



**Figure 71 OLCI-A gains at MOBY at 400, 412.5, 442.5, 490, 560 and 681.25 nm as a function of sun zenith angle. Gains in green fall within the semi-interquartile range used in final averaging.**



**Figure 72 OLCI-A gains at MOBY at 400, 412.5, 442.5, 490, 560 and 681.25 nm as a function of view zenith angle. Gains in green fall within the semi-interquartile range used in final averaging.**



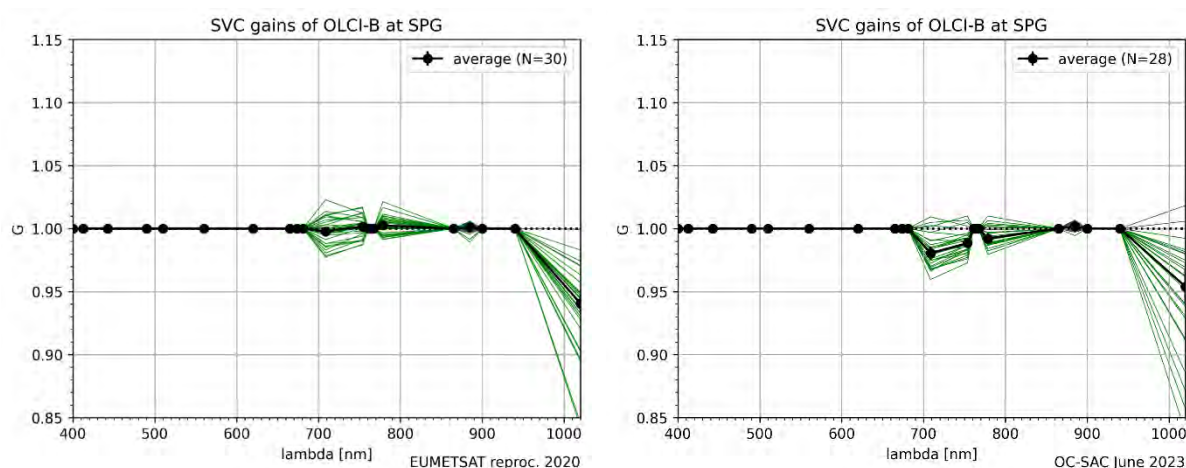
**Figure 73 OLCI-A gains at MOBY at 400, 412.5, 442.5, 490, 560 and 681.25 nm as a function of detector index. Gains in green fall within the semi-interquartile range used in final averaging.**

## 7.3 OLCI-B GAINS

### 7.3.1 NIR GAINS

Reminder: results are generated with a fixed input RH=90%.

Similarly to OLCI-A, OC-SAC NIR gains for OLCI-B presents also a spectral slope from 865 to 709 nm, which does not exist in Collection 3. Gains at 709 is of about 2%.



**Figure 74 Individual spectral gains of OLCI-B at SPG, before MSIQR screening, left for Collection 3, right for present OC-SAC processor.**

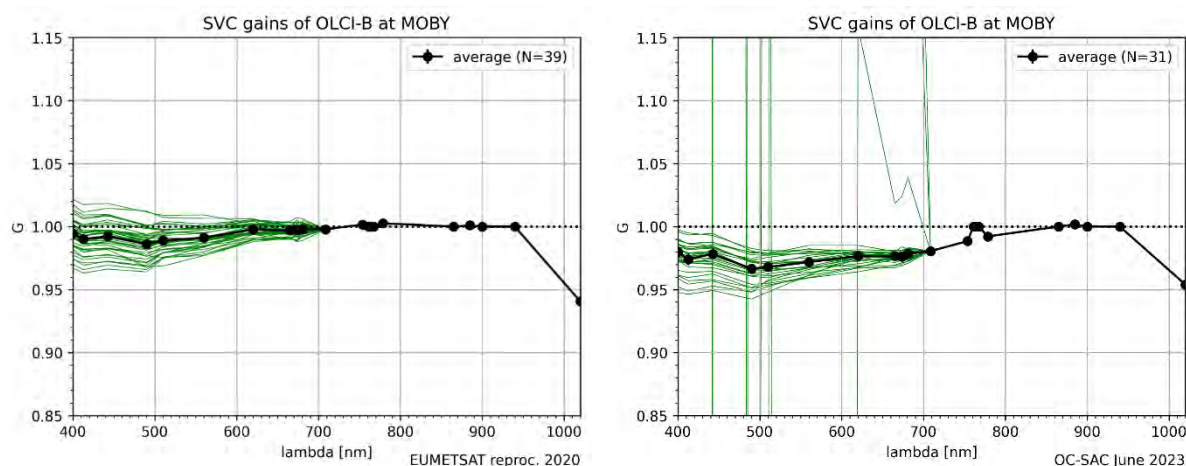
**Table 12 Statistics of OLCI-B averaged gains at SPG, after MSIQR filtering**

| Wavelength | Number | Average gain | Standard-deviation |
|------------|--------|--------------|--------------------|
| 708.75     | 14     | 0.980545     | 0.005273           |
| 753.75     | 14     | 0.988426     | 0.003581           |
| 778.75     | 14     | 0.992212     | 0.003671           |
| 865        |        | 1.000        |                    |
| 885        | 14     | 1.001781     | 0.002337           |
| 1020       | 14     | 0.954038     | 0.013962           |

### 7.3.2 VIS GAINS

Reminder: results are generated with a fixed input RH=90%.

OLCI-B gains generated for OC-SAC are also relatively flat, but again with a higher amplitude than those of Collection 3: around -3% on average in the blue and green bands, compared to -1% for Collection 3. However, the dispersion expressed by standard-deviation and RSEM is similar.



**Figure 75 Individual spectral gains of OLCI-B at MOBY, before MSIQR screening, left for Collection 3, right for present OC-SAC processor.**

**Table 13 Statistics of OLCI-B averaged gains at MOBY, after MSIQR filtering**

| Wavelength | Number | Average gain | Standard-deviation | RSEM [%] |
|------------|--------|--------------|--------------------|----------|
| 400        | 15     | 0.979979     | 0.004517           | 0.0377%  |
| 412.5      | 15     | 0.974037     | 0.004762           | 0.0400%  |
| 442.5      | 15     | 0.978373     | 0.004275           | 0.0357%  |
| 490        | 15     | 0.966521     | 0.003903           | 0.0330%  |
| 510        | 15     | 0.967896     | 0.003771           | 0.0319%  |
| 560        | 15     | 0.971806     | 0.003538           | 0.0298%  |
| 620        | 15     | 0.976704     | 0.001808           | 0.0151%  |
| 665        | 15     | 0.976548     | 0.001246           | 0.0104%  |
| 673.75     | 15     | 0.976193     | 0.001588           | 0.0133%  |
| 681.25     | 15     | 0.978527     | 0.001762           | 0.0147%  |

#### 7.4 POTENTIAL SVC FOR ABSORPTION BANDS

The amplitude and spectral shape of gains in the NIR question how could the absorption bands be vicariously calibrated. This particularly concerns the O<sub>2</sub> bands used by the ALH module. Gains are estimated at these bands by a spline interpolation of existing gains at non-absorbing bands (Figure 76). OLCI-A gains between 761 and 767 nm are of about -3.3%, but the ratio of band 760 to band 753 is only of 1.0012 (i.e. 0.1% adjustment). We thus do not expect any impact for the ALH module and gains can be safely kept to unity at these bands.

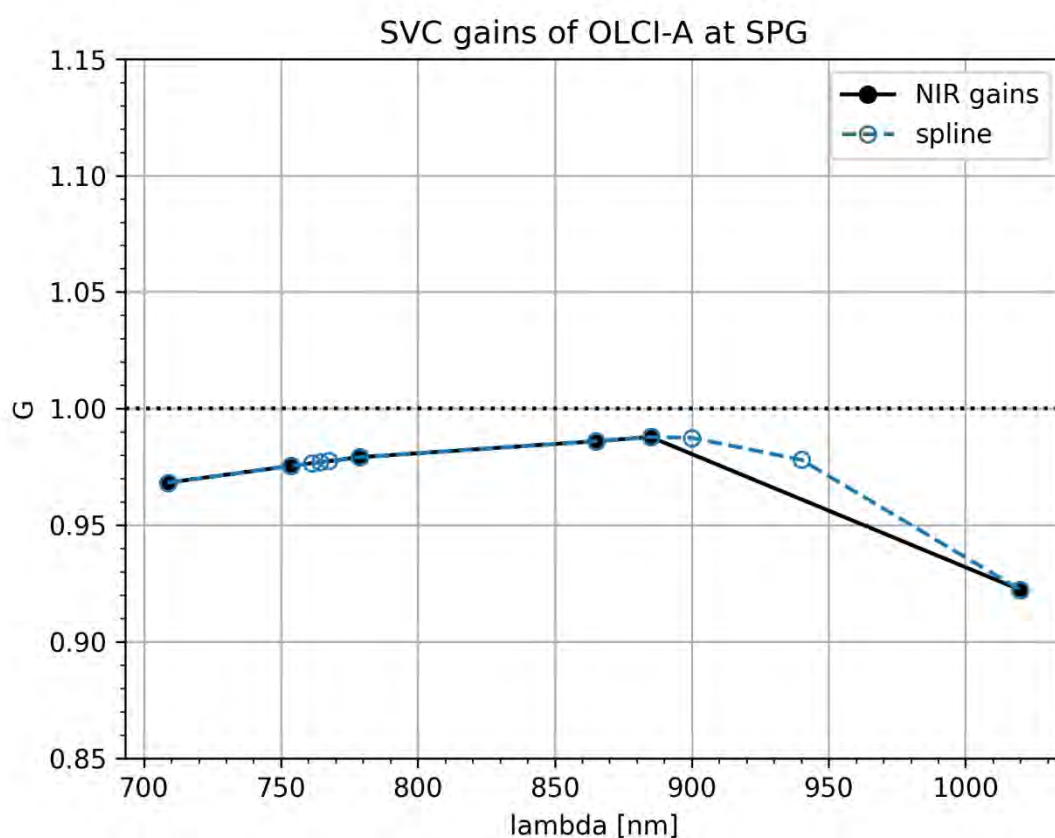


Figure 76 NIR gains for OLCI-A (black), interpolated at absorption bands (dotted blue line)