

Inherent Optical Properties

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Abstract

This algorithm returns near-surface spectral inherent optical properties (IOPs) using a semianalytical inverse model. The spectral products derived are the total absorption coefficient, $a(\lambda)$ [units: m^{-1}], phytoplankton absorption coefficient, $a_{ph}(\lambda)$ [units: m^{-1}], the absorption coefficient of non-algal particles and chromophoric dissolved organic matter, $a_{dg}(\lambda)$ [units: m^{-1}], the total backscattering coefficient, $b_b(\lambda)$ [units: m^{-1}], and the particulate backscattering coefficient, $b_{bp}(\lambda)$ [units: m^{-1}]. The spectral slope of the absorption coefficient of non-algal particles and chromophoric dissolved organic matter, S_{dg} [units: nm^{-1}], and the spectral slope of the particle backscattering coefficient, S_{bp} [unitless], are also derived.

IOP data products are derived using the default configuration of the Generalized Inherent Optical Properties (GIOP) algorithm framework model (Werdell et al., 2013). The implementation is contingent on valid remote sensing reflectances, $R_{rs}(\lambda)$ [units: sr^{-1}], in the visible (400 - 700 nm) spectral range. The algorithm is applicable to all current ocean color sensors supported by NASA. The IOP products are distributed as part of the NASA standard Level-2 IOP product suite and the Level-3 IOP product suite.

Plain Language Summary

We use this algorithm to derive inherent optical properties (IOPs) which help us understand how different wavelengths (colors) of light are scattered and absorbed by materials present in natural waters such as lakes, coastal waters, and the ocean. The different constituents in natural waters - including the water itself, phytoplankton, dissolved matter, and non-algal particulate matter - absorb and scatter light in different ways due to factors such as shape, size, and pigmentation. Consequently, the types and relative concentrations of constituent matter drive the character of the light reflected from the water. The algorithm we use is based on a scientific understanding of the physics of light in water and relates IOPs to the light reflected from the ocean that is observed by space-borne sensors.

1. Introduction

Inherent optical properties (IOPs; spectral absorption and backscattering coefficients) are key parameters used to understand marine biogeochemical processes and the characteristics of the under-water light field. A range of algorithms have been developed to derive IOPs from satellite-observed water-leaving reflectances Werdell et al., 2018. The algorithm described here returns the spectral inherent optical properties (IOPs) of near-surface waters using a physics-based semianalytical inverse model. The spectral products derived are the total absorption coefficient, $a(\lambda)$ [units: m⁻¹], phytoplankton absorption coefficient, $a_{ph}(\lambda)$ [units: m⁻¹], the absorption coefficient of non-algal particulate matter and chromophoric dissolved organic matter, $a_{dg}(\lambda)$ [units: m⁻¹], the total backscattering coefficient, $b_b(\lambda)$ [units: m⁻¹], and the particulate backscattering coefficient, $b_{bp}(\lambda)$ [units: m⁻¹].

The IOP data products are derived using the default configuration of the Generalized Inherent Optical Properties (GIOP-DC) algorithm framework model Werdell et al., 2013. The implementation is contingent on valid remote sensing reflectances (R_{rs}) the visible (400 - 700 nm) spectral range used as model inputs. The algorithm is applicable to supported ocean color sensors. The IOP products are included as part of the NASA standard Level-2 (L2) IOP product suite and the Level-3 (L3) IOP product suite.

The current implementation for the standard IOP products, as applied in version R2022 of NASA's multi-mission ocean color processing, is the GIOP-DC algorithm with reflectances that have been corrected for inelastic Raman scattering effects McKinna et al., 2016 Westberry et al., 2013. Standard uncertainties in derived IOPs are estimated per McKinna et al., 2019.

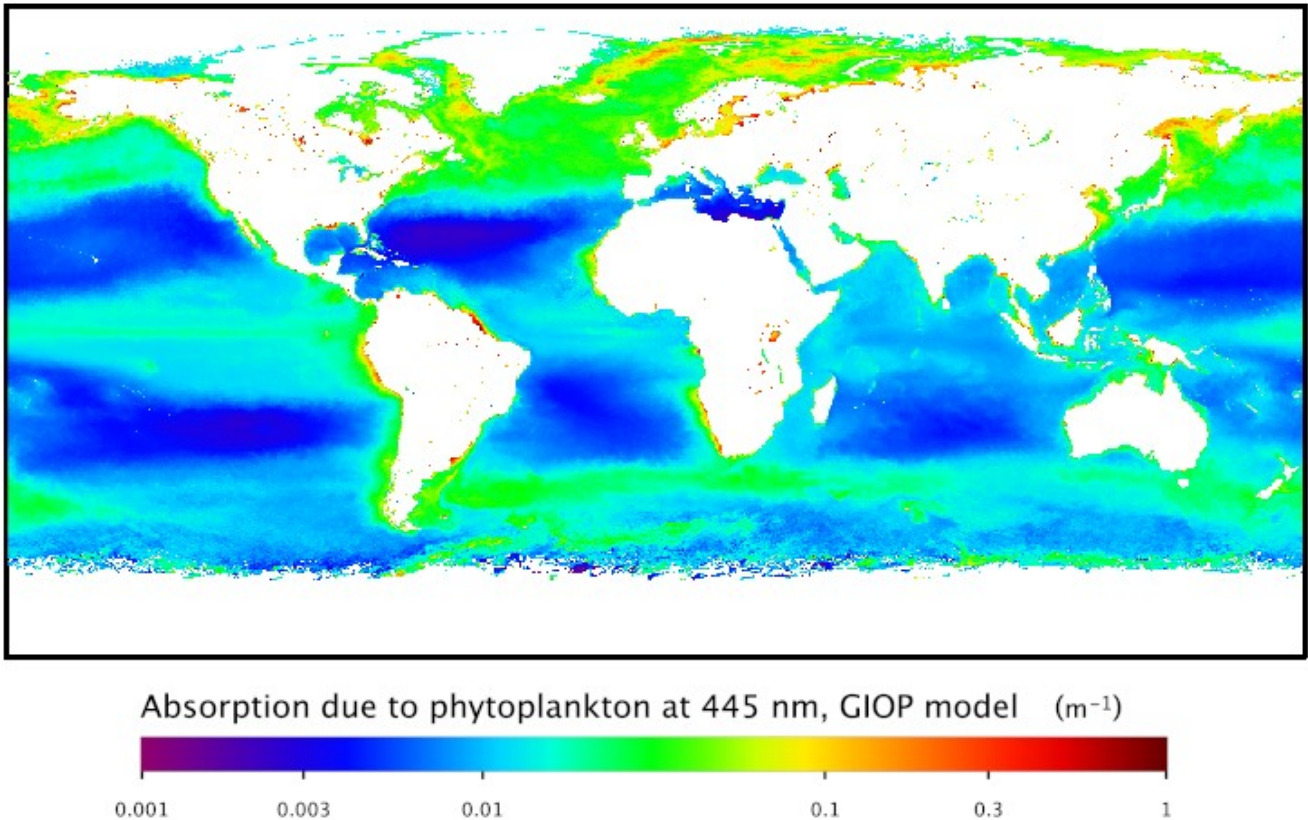


Figure 1: **Figure 1:** Example IOP level-3 data spatiotemporal mapped product derived from NOAA20-VIIRS data. Phytoplankton absorption coefficient at 445 nm. Entire mission (2018-2023) for the northern hemisphere spring.

2. Context / Background

2.1. Historical Perspective

An Inherent Optical Properties Algorithm Workshop was convened at the Ocean Optics XIX Conference in Barga, Italy 3-4 October 2008. The IOP workshop followed eight months of collaboration between twenty-three international researchers Werdell, 2009. One objective of the workshop, amongst others, was to achieve a community-wide consensus on a unified semi-analytical algorithm (SAA) for deriving IOPs from global ocean color observations. As a result, NASA developed a generic modular SAA to facilitate the testing of multiple SAA configurations within a consistent software environment Werdell, 2009.

The modular SAA became known as the Generalized Inherent Optical Properties Framework Algorithm (GIOP) Werdell et al., 2013 with a default configuration (-DC)

determined per consensus reached at the IOP Workshop. The GIOP-DC has been used to produce OB.DAAC's distributed IOP data product suite and is embedded within NASA's Ocean Color Software Suite ([OCSSW](#)).

2.2. Additional information

The GIOP is modular in structure with a range of possible model configurations based on a range of existing methodologies. While the default configuration is used for deriving standard OB.DAAC IOP products, other model configurations (discussed in detail in Werdell et al., 2013) are available for end-user research. These other model configurations are freely distributed as part of OCSSW for those wishing to customize and experiment with ocean color data processing.

3. Algorithm Description

3.1. Scientific Theory

The spectral remote-sensing reflectance, $R_{rs}(\lambda)$ [units: sr^{-1}], is a fundamental radiometric quantity measured by ocean color spectroradiometers. $R_{rs}(\lambda)$ is the ratio of the spectral water leaving radiances just above the water surface, $L_w(\lambda, 0+)$ [units: $\text{W sr}^{-1} \text{m}^{-2}$], to the spectral downwelling irradiance at the surface, $E_d(\lambda, 0+)$ [units: W m^{-2}]. The spectral shape and magnitude of $R_{rs}(\lambda)$ is directly related to the IOPs. The objective of the GIOP-DC is to derive IOPs from sensor-observed $R_{rs}(\lambda)$.

The GIOP-DC is a spectral matching algorithm. It uses a semianalytical relationship, referred to as the "forward model", to simulate the spectral subsurface remote-sensing reflectance, $r_{rs}(\lambda)$, defined as the ratio of upwelling radiance just beneath the surface, $L_w(\lambda, 0-)$ [units: $\text{W sr}^{-1} \text{m}^{-2}$], to downwelling irradiance just beneath the surface $E_d(\lambda, 0-)$ [units: W m^{-2}]. The forward model is a function of the IOPs Gordon et al., 1988. The GIOP-DC forward model is parameterized with realistic spectral IOPs.

For each valid sensor-observed $R_{rs}(\lambda)$, a subsurface remote sensing reflectance spectrum, $r_{rs,obs}(\lambda)$ [units: sr^{-1}] is computed:

$$r_{rs,obs}(\lambda) = \frac{R_{rs,obs}(\lambda)}{0.52 + 1.7R_{rs,obs}(\lambda)}. \quad (1)$$

GIOP-DC then attempts to model a closely matching sub-surface remote sensing reflectance spectrum, $r_{rs,mod}(\lambda)$ [units: sr^{-1}]. This matching process is done by iteratively adjusting the shape and magnitude of the IOPs within the forward model until $r_{rs,mod}(\lambda)$ agrees with $r_{rs,obs}(\lambda)$ to within a predefined tolerance. At this stage the algorithm stops and the IOPs associated with the best match are returned as the solution.

3.1.1. Assumptions

No content available.

3.2. Mathematical Theory

The GIOP-DC is a semianalytical algorithm (SAA) and can be split into three components: (i) the forward reflectance model, (ii) spectral IOP shape models, and (iii) the inverse solution method. Each component of GIOP-DC are described below.

The forward reflectance model

The forward reflectance model simulates $r_{rs,mod}(\lambda)$ as a function of IOPs. GIOP-DC uses the quasi-single scattering approximation of Gordon et al., 1988 to model the subsurface remote-sensing reflectance, $r_{rs,mod}(\lambda)$, as a function of IOPs:

$$r_{rs}(\lambda) = \sum_{i=1}^2 g_i \left[\frac{b_b(\lambda)}{a(\lambda) + b_b(\lambda)} \right]^i. \quad (2)$$

Where $a(\lambda)$ [units: m^{-1}] is the total spectral absorption coefficient, $b_b(\lambda)$ [units: m^{-1}] is the total spectral backscattering coefficient, and g_1 and g_2 are scalar constants with default values of 0.0949 and 0.0794, respectively.

Spectral IOP models

In GIOP-DC, the coefficient $a(\lambda)$ is expressed as the sum of absorbing sub-components present in the medium

$$a(\lambda) = a_w(\lambda) + M_{ph}a_{ph}^*(\lambda) + M_{dg}a_{dg}^*(\lambda) \quad (3)$$

where the subcomponents are water, phytoplankton, and non-algal particles plus chromophoric dissolved organic matter denoted in Eq.3 by the subscripts w , ph , and dg , respectively. Each non-water subcomponent absorption coefficient is expressed as the product of a normalized spectral absorption coefficient (denoted by $*$) and its magnitude (M). Similarly, $b_b(\lambda)$ is expressed as

$$b_b(\lambda) = b_{bw}(\lambda) + M_p b_{bp}^*(\lambda) \quad (4)$$

where the subcomponents water and particulate matter are denoted by the subscripts w and p , respectively.

The parameterization of IOP spectral shapes is given in further detail below.

Spectral shape of pure water absorption and backscattering coefficients

GIOP-DC uses a spectral constant for the pure water absorption coefficient, $a_w(\lambda)$ [units: m^{-1}]. Spectral $a_w(\lambda)$ used in OCSSW spans 200 – 2450 nm and is derived from Pope & Fry, 1997 and Kou et al., 1993. Temperature-salinity dependent seawater backscattering coefficients, $b_{bw}(\lambda)$ [units: m^{-1}], are computed on a per-pixel basis using ancillary sea surface temperature (SSS; units: PSU) and sea surface temperature (SST; units: $^{\circ}C$) data. The method for computing $b_{bw}(\lambda)$ follows Zhang et al., 2009.

Spectral shape model for phytoplankton absorption coefficient

The normalized chlorophyll-specific spectral phytoplankton absorption coefficient, $a_{ph}^*(\lambda)$ [units: $m^2 mg^{-1}$], is parameterized on a per-pixel basis following Bricaud et al., 1998. To generate $a_{ph}^*(\lambda)$ two spectral basis vectors $A(\lambda)$ and $B(\lambda)$ are required as well as satellite-derived chlorophyll-a pigment concentration, $Chla$ [units: $mg m^{-3}$], using the following relationship:

$$a_{ph}^*(\lambda) = \frac{0.055}{\tau} A(\lambda) Chla^{B(\lambda)-1}. \quad (5)$$

The scaling factor, τ [units: $m^2 mg^{-1}$], is an estimated value of the phytoplankton chlorophyll-specific absorption coefficient at 442 nm, $a_{ph}^*(442)$, per:

$$\tau = A(442) Chl^{B(442)-1}. \quad (6)$$

The wavelength at which τ is computed for PACE OCI processing is at or near 442 nm, however, this wavelength is sensor dependent. For example, for legacy sensors such as MODIS Aqua 443 nm is used. The GIOP-DC parameterization allows $a_{ph}^*(\lambda)$ to vary in shape with trophic conditions while keeping the coefficient proportionally constant to $Chla$ by setting $a_{ph}(442) = 0.055 Chla$ Werdell et al., 2013.

Spectral shape model for non-algal particles plus chromophoric dissolved organic matter coefficient

The normalized spectral shape of non-algal particles plus chromophoric dissolved organic matter, $a_{dg}^*(\lambda)$ [unitless], is parameterized using an exponential function:

$$a_{dg}^*(\lambda) = e^{-S_{dg}(\lambda-442)} \quad (7)$$

where, the spectral slope coefficient, S_{dg} [units: nm⁻¹], is set to a constant value of 0.0183 nm⁻¹ Werdell et al., 2013. The value of $a_{dg}^*(\lambda)$ at 442 nm is 1.0.

Spectral shape model for particle backscattering coefficient

The normalized spectral shape of the particle backscattering, $b_{bp}^*(\lambda)$ [unitless], is parameterized using a power law function:

$$b_{bp}^*(\lambda) = \left(\frac{442}{\lambda}\right)^{S_{bp}} \cdot (8)$$

The value of $b_{bp}^*(\lambda)$ at 442 nm is 1.0 and the spectral slope coefficient, S_{bp} [unitless], is computed following Lee et al., 2002 as

$$S_{bbp} = 2.0 \left[1 - 1.3 \exp \left(-0.9 \left(\frac{r_{rs}(442)}{r_{rs}(550)} \right) \right) \right] \cdot (9)$$

Inverse solution method

The seawater IOPs (a_w and b_{bw}) and the IOP spectral shape models are parameterized per-pixel. Thus, the forward reflectance model can be expressed as the function of the three parameters M_{ph} , M_{dg} , and M_p :

$$r_{rs,mod}(\lambda) = f(M_{ph}, M_{dg}, M_p) \cdot (10)$$

For GIOP-DC, M_{ph} , M_{dg} , and M_p correspond to $Chla$, $a_{dg}(442)$ and $b_{bp}(442)$, respectively. GIOP-DC employs unconstrained Levenberg-Marquardt non-linear least squares optimization as the mathematical solution method. The optimization routine finds the optimal set of M_{ph} , M_{dg} , and M_p such that $r_{rs,mod}(\lambda)$ best matches $r_{rs,obs}(\lambda)$. A “best match” is achieved once the Levenberg-Marquardt convergence criteria are met.

Output IOP quality control

After solution is returned, the GIOP-DC performs a quality control test. A retrieval is considered valid if:

$$-0.05 b_{bw}(\lambda) \leq b_{bp}(\lambda) \leq 0.05 \text{ m}^{-1}, \quad (11) \quad (11)$$

$$-0.05 a_w(\lambda) \leq a_{dg}(\lambda) \leq 5 \text{ m}^{-1}, \quad (12) \quad (12)$$

$$-0.05 a_w(\lambda) \leq a_{ph}(\lambda) \leq 5 \text{ m}^{-1} \text{ and} \quad (13) \quad (13)$$

$$\Delta R_{rs} \leq 33\%. \quad (14) \quad (14)$$

The mean relative difference in the spectral remote sensing reflectance is computed as:

$$\Delta R_{rs} = \frac{100\%}{N_\lambda} \sum_{i=1}^{N_\lambda} \frac{|R_{rs,mod}(\lambda_i) - R_{rs,obs}(\lambda_i)|}{R_{rs,obs}(\lambda_i)} \quad (15) \quad (15)$$

for the spectral range $400 \leq \lambda \leq 600$ nm.

Raman scattering correction

The forward reflectance model used in GIOP-DC does not account for naturally-occurring inelastic Raman scattering contributions to $R_{rs,obs}(\lambda)$. As such, GIOP-DC utilizes a Raman scattering correction. The correction estimates the Raman scattering contribution to the above-water remote sensing reflectance, $R_{rs,Raman}(\lambda)$ [units: sr^{-1}], using a semianalytical model Westberry et al., 2013. Above-water remote sensing reflectances corrected for Raman scattering effects, $R_{rs,cor}(\lambda)$ [units: sr^{-1}], are then computed as:

$$R_{rs,cor}(\lambda) = R_{rs,ob}(\lambda) - R_{rs,Raman}(\lambda). \quad (11) \quad (16)$$

Values of $R_{rs,cor}(\lambda)$ are computed and used in the GIOP-DC inverse solution method for spectral matching with forward modelled estimates of reflectances that do not account for inelastic scattering McKinna et al., 2016.

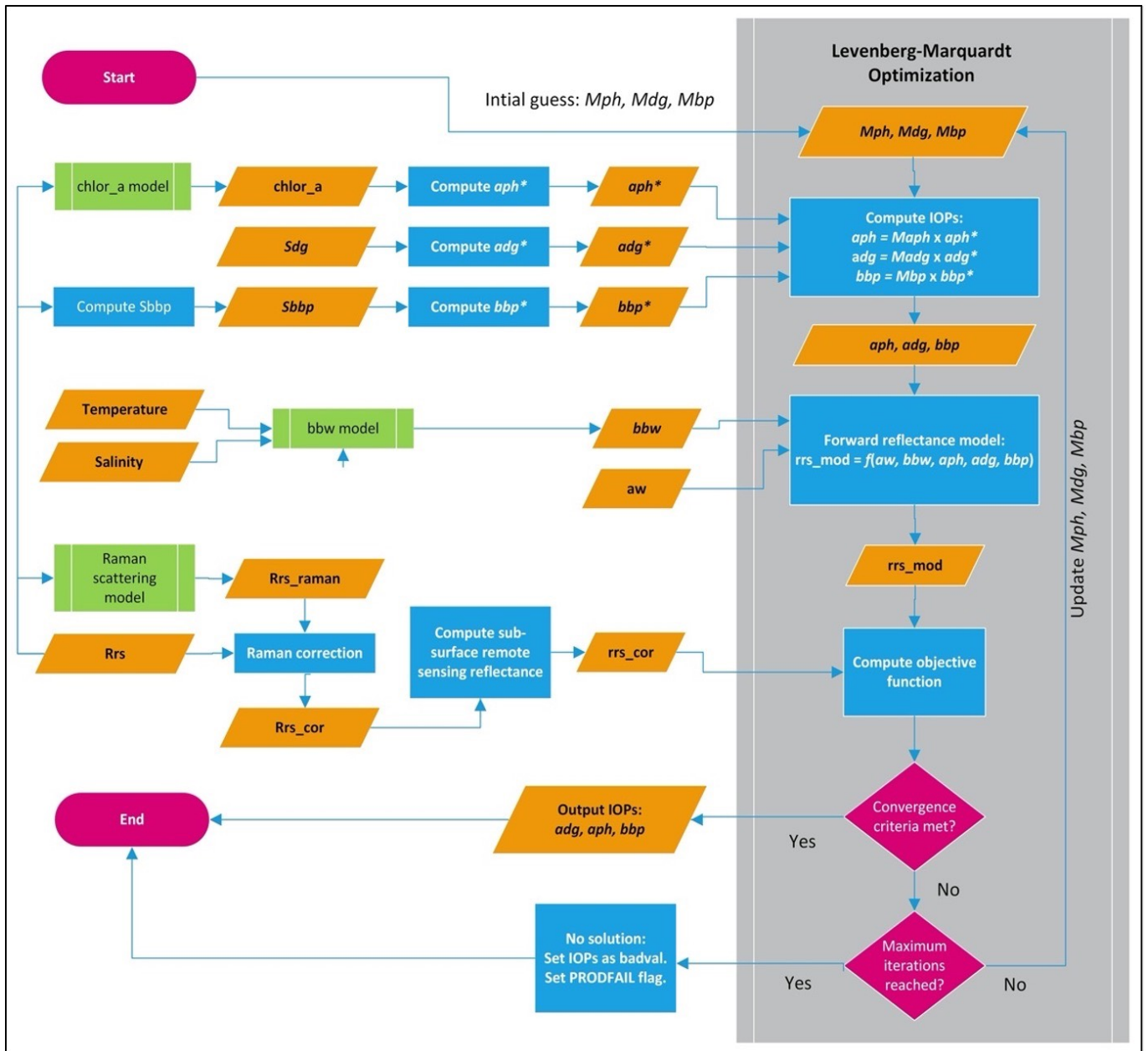


Figure 2: **Figure 2:** Schematic diagram of the GIOP-DC algorithm.

3.2.1. Assumptions

No content available.

3.3. Algorithm Input Variables

Name	Long Name	Unit
Rrs_vw	Spectral above-water sensor-observed remote sensing reflectance	sr ⁻¹
chlor_a	Derived chlorophyll-a pigment concentration	mg m ⁻³
SSS	Sea surface salinity	PSU
SST	Sea surface temperature	°C
Rrs_unc_vw	Spectral above-water sensor-observed remote sensing reflectance standard uncertainties	sr ⁻¹
chlor_a_unc	Derived chlorophyll-a pigment concentration standard uncertainty	mg m ⁻³
Rrs_raman_vw	Contribution to the spectral remote sensing reflectance due Raman scattering effects	sr ⁻¹

3.4. Algorithm Output Variables

Name	Long Name	Unit
a_vw	Spectral total absorption coefficient	m ⁻¹
bb_vw	Spectral total backscattering coefficient	m ⁻¹
aph_vw	Spectral phytoplankton absorption coefficient	m ⁻¹
adg_vw	Spectral absorption coefficient of non-algal particles and chromophoric dissolved organic matter	m ⁻¹
bbp_vw	Spectral particle backscattering coefficient	m ⁻¹

Name	Long Name	Unit
adg_s	Spectral slope coefficient for the absorption coefficient of non-algal particles and chromophoric dissolved organic matter	nm ⁻¹
bbp_s	Spectral slope coefficient for particle backscattering coefficient	unitless
a_unc_vwv	Total spectral absorption coefficient standard uncertainty	m ⁻¹
bb_unc_vwv	Total particle backscattering coefficient standard uncertainty	m ⁻¹
aph_unc_vwv	Spectral phytoplankton absorption coefficient standard uncertainty	m ⁻¹
adg_unc_vwv	Spectral absorption coefficient of non-algal particles and chromophoric dissolved organic matter standard uncertainty	m ⁻¹
bbp_unc_vwv	Spectral particle backscattering coefficient standard uncertainty	m ⁻¹

4. Algorithm Availability

4.1. Location of Implemented Algorithm #1

URL	https://oceancolor.gsfc.nasa.gov/docs/ocssw/giop_8c.html
DESCRIPTION	This is the source code of NASA's Ocean Color Science Software (OCSSW) for GIOP-DC. IOP products could be obtained from satellite remote sensing data via command line processing or using the graphical user interface to OCSSW known as SeaDAS (https://seadas.gsfc.nasa.gov). The following instructions provide guidance on processing data with SeaDAS: https://seadas.gsfc.nasa.gov/help-8.3.0/processors/ProcessL2gen.html#PRODUCTS_TAB.

5. Algorithm Usage Constraints

GIOP-DC has been developed for oceanic waters. End-users are advised to carefully consider the validity of IOP data products for extreme conditions such as highly turbid, optically shallow, and inland/freshwater systems.

6. Performance Assessment Validation

6.1. Performance Assessment Validation Methods

After production of IOP products using GIOP-DC, are validated using *in situ* data archived in the NASA SeaWiFS Bio-optical Archive and Storage System (SeaBASS; Werdell et al., 2003). The product validation analyses compare satellite and *in situ* measurements following the approach of Bailey & Werdell, 2006.

Using the time (T_{is}) and location (L_{is}) for an *in situ* measurement in SeaBASS, a coincident level-2 (L2) swath resolution file is selected from [OB.DAAC](#) containing targeted IOP products and associated standard uncertainties. Note, an L2 file is not always available due to orbit gaps. A window centered closest to L_{is} (5×5 pixels) is designated, from which 25 pixels are extracted. To be considered for validation, T_{is} must be within +/- 3 hours of satellite measurement, the sensor zenith angle < 60°, and solar zenith angle < 75°. Pixels

within the 5 x 5 window individual pixels are not considered valid if they are flagged during data processing (LAND, HIGLINT, HILT, STRAYLIGHT, CLDICE, ATMFAIL, LOWLW, FILTER, NAVFAIL, NAVWARN; <https://oceancolor.gsfc.nasa.gov/resources/atbd/ocl2flags/>). If more than 50% of pixels are invalid, the 5 x 5 window box is rejected as a potential validation point.

If more than 50% of pixels in the 5x5 window are valid, spatial homogeneity is evaluated. This is done by computing the median of the coefficient of variation (CV; standard deviation divided by the mean) for several ocean color products (R_{rs} between 405 and 570 nm, aerosol optical thickness at 869 nm). The median value of the CVs must be less than 15% for the 5 x 5 pixel window. We note that the center pixel of the 5 x 5 window closest to L_{is} does not have to be valid as long as there are sufficient valid pixels in the box that meet the homogeneity requirement.

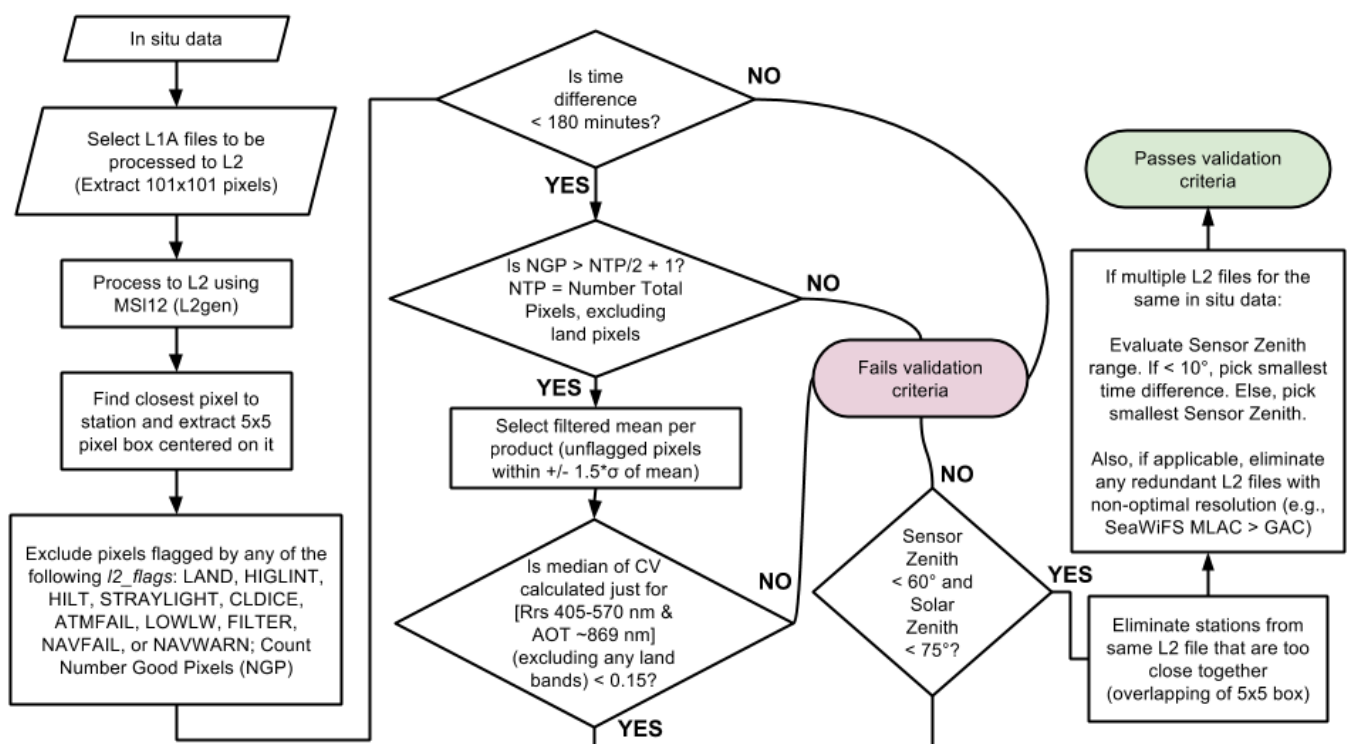


Figure 3: **Figure 3:** Flowchart of validation processing highlighting the applied exclusion criteria. Adapted and updated from Bailey and Werdell (2006).

This approach of validation is operationally applied by the OB.DAAC to most ocean color sensors. For complete details see: https://seabass.gsfc.nasa.gov/wiki/validation_description. There are a few key recommendations we make from our experience applying the described method to satellite data:

- (1) Use a consistently processed in situ data set
- (2) Eliminate suspect *in situ* data (e.g. from optically shallow waters) from the validation set
- (3) Use a narrow time window for determining coincidence (i.e. no more than ± 3 h) between T_{is} and satellite data records

- (4) Use native resolution satellite products (i.e., avoid sub-sampled data)
- (5) Use the mean of a 5×5 pixel box centered on the in situ location
- (6) Appropriately mask satellite pixels per the L2 quality flags
- (7) Use a homogeneity test (e.g. CV) to minimize the impact of geophysical variability in the 5×5 pixel box on the satellite measurement mean

Following these recommendations will aid in the analysis of the resulting validation results by minimizing the systemic uncertainties.

6.2. Performance Assessment Validation Uncertainties

Sources of uncertainty in derived IOPs include those in sensor-observed remote sensing reflectances, $u(R_{rs})$, derived chlorophyll-a pigment, $u(\text{chlor_a})$, internal model uncertainties, $u(\text{mod})$, due to assumptions and approximations, and within pixel variability due to horizontal inhomogeneity. Standard uncertainties ($1-\sigma$) are estimated for all GIOP-DC via uncertainty propagation detailed in McKinna et al. (2019). More details could be found in IOCCG report 18 IOCCG, 2019(IOCCG, 2019) and McKinna et al., 2019.

6.3. Performance Assessment Validation Errors

Based on McClain, 2009, the satellite data product accuracy goals generally accepted by the international community are $\pm 5\%$ for water-leaving radiances. The PACE mission adopted more rigorous uncertainties for R_{rs} retrieved by its Ocean Color Instrument Ahmad et al., 2019. A number of evaluations have been published, such as the global analyses by Gregg & Casey, 2004 (SeaWiFS chlor_a) and Bailey & Werdell, 2006 (SeaWiFS water-leaving radiances, chlor_a, and $K_d(490)$) to name only a very few, and the regional analysis by Zibordi et al., 2006 that compared SeaWiFS, MODIS, and MERIS water-leaving radiances to SeaPRISM observations from the Acqua Alta tower. Overall, these results indicate quite good performance. However, regional differences can be large.

Validation of IOP retrievals was performed relative to all available match-ups from SeaBASS. Statistical analysis, scatter plots and frequency distribution comparisons of the satellite to in situ match-ups are provided for each mission (SeaWiFS, MODIS Aqua/Terra, VIIRS SNPP/NOAA20, MERIS, OLCI S3A/S3B) on the following web pages:

<https://oceancolor.gsfc.nasa.gov/data/reprocessing/r2022/seawifs/>
<https://oceancolor.gsfc.nasa.gov/data/reprocessing/r2022/aqua/>
<https://oceancolor.gsfc.nasa.gov/data/reprocessing/r2022/terra/>

<https://oceancolor.gsfc.nasa.gov/data/reprocessing/r2022/snpp/>
<https://oceancolor.gsfc.nasa.gov/data/reprocessing/r2022/noaa20/>
<https://oceancolor.gsfc.nasa.gov/data/reprocessing/r2022/meris/>
<https://oceancolor.gsfc.nasa.gov/data/reprocessing/r2022/s3a/>
<https://oceancolor.gsfc.nasa.gov/data/reprocessing/r2022/s3b/>

7. Data Access

7.1. Input Data Data Access

7.1.1. Entry #1

URL	https://oceancolor.gsfc.nasa.gov/data/download_methods/
DESCRIPTION	Rrs_vvv or level 2 remote sensing reflectance and chlor_a are inputs for IOP production. They can be downloaded from the ocean color website following the different methods described in the link.

7.2. Output Data Data Access

7.2.1. Entry #1

URL	https://oceancolor.gsfc.nasa.gov/data/download_methods/
DESCRIPTION	IOPs as one of the NASA standard products can be downloaded from the ocean color website following the different methods described in the link.

7.3. Important Related URLs

7.3.1. Entry #1

URL	https://seabass.gsfc.nasa.gov/search#val
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DESCRIPTION **SeaBASS validation search provides the satellite-derived IOP products versus in situ data validation.**

Entry #2

URL <https://oceancolor.gsfc.nasa.gov/resources/atbd/giop/>

DESCRIPTION **GIOP-DC algorithm description on the NASA Ocean Color website.**

8. Contacts

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