Plymouth Marine Laboratory

EUMETSAT

Ocean Colour Multi-Mission Algorithm Prototype System (OMAPS)

Baseline Requirement Document (Ocean Colour Level 2 Algorithm and Products)

Ref: D1.2
Date: 28/02/2020
Issue: 1.2
For: EUMETSAT
ID: ID 995318

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Document Control

Version No.	Release Date	Author/Contributor	Reason for issue
0.1	10/09/2019	T Jackson	Initial structuring of document and drafting of text.
0.2	11/10/2019	T Jackson	Updates to all sections for submission to EUMETSAT.
0.3	18/10/2019	T Jackson, F Steinmetz	Updates to format of document and inclusion of content from HYGEOS.
1.1	20/11/2019	T Jackson, F Steinmetz, S Sathyendranath, C Brockmann	Major structural changes following feedback from EUMETSAT
1.2	28/02/2020	T Jackson, F Steinmetz, S Sathyendranath, C Brockmann	Updates following second round of feedback from EUMETSAT

Applicable Documents

ID	Document
AD-1	Eumetsat general SoW
AD-2	Emetsat specific SoW for ocean colour prototype
AD-3	PML proposal
AD-4	PVP
AD-5	RB offline processor
AD-6	Input Output Data Definition (IODD)
AD-7	OC-CCI Users Requirements Document (https://esa-oceancolour-cci.org/sites/esa-oceancolour-cci.org/alfresco.php?file=1d95f333-5c78-40be-a25c-8d40d0b161d8&name=Ocean%20Colour%20CCI%20-%20URD%20v4-0.pdf)
AD-8	Sentinel-3 Mission Requirements Traceability Document (MRTD)
AD-9	Algorithm Blending ATBD
AD-10	Ocean Colour in-water Algorithm ATBD

Reference Documents

ID	Document
RD-1	Carder, K. L., Chen, F. R., Lee, Z. P., Hawes, S. K., and Kamykowski, D. (1999), Semianalytic Moderate-Resolution Imaging Spectrometer algorithms for chlorophyll *a* and absorption with bio-optical domains based on nitrate-depletion temperatures, *J. Geophys. Res.*, 104(C3), 5403– 5421, doi:10.1029/1998JC900082.
RD-2	Franz, B. A., Werdell, P. J., 2010. A Generalized Framework for Modeling of Inherent Optical Properties in Ocean Remote Sensing Applications. In: Ocean Optics XX, Anchorage, Alaska, 27th Sept.-1st Oct. 2010.
RD-3	Guide to the Expression of Uncertainty in Measurement JCGM100: (2008) – GUM 1995 with minor corrections. Published by the JCGM in the name of the BIPM, IEC, IFCC, ILAC, ISO, IUPAC, IUPAP, and OIML.
RD-4	GCOS, W., 2011. Systematic Observation Requirements for Satellite–BASED Data Products for Climate, 154 Document.
RD-5	GCOS 2016. *The Global Observing System for Climate: Implementation Needs - GCOS200.* Bonn: United Nations Framework Convention on Climate Change (UNFCCC).
RD-6	Hu, C., Lee, Z., Franz, B., 2012. Chlorophyll-a algorithms for oligotrophic oceans: A novel approach based on three-band reflectance difference. Journal of Geophysical Research 117, C01011.
	IOCCG (2012). Mission Requirements for Future Ocean-Colour Sensors. McClain, C. R. and Meister, G. (eds.), Reports of the International Ocean-Colour Coordinating Group, No. 13, IOCCG, Dartmouth, Canada.
	IOCCG (2013). In-flight Calibration of Satellite Ocean-Colour Sensors. Frouin, R. (ed.), Reports of the International Ocean-Colour Coordinating Group, No. 14, IOCCG, Dartmouth, Canada.
	IOCCG (2019). Uncertainties in Ocean Colour Remote Sensing. Mélin F. (ed.), IOCCG Report Series, No. 18, International Ocean Colour Coordinating Group, Dartmouth, Canada. http://dx.doi.org/10.25607/OBP- 696
RD-7	Jackson Thomas, Sathyendranath Shubha, Mélin Frédéric, (2017) An improved optical classification scheme for the Ocean Colour Essential Climate Variable and its applications, Remote Sensing of Environment, Volume 203, Pages 152-161, doi:10.1016/j.rse.2017.03.036.
RD-8	Lee, Z., Carder, K. L., Arnone, R. A., 2002. Deriving inherent optical properties from water color: a multiband quasi-analytical algorithm for optically deep waters. Applied Optics 41 (27), 5755–5772.
RD-9	Lee, Z., Carder, K. L., Mobley, C. D., Steward, R. G., Patch, J. S., 1998. Hyperspectral remote sensing for shallow waters. 1. A semianalytical model. Applied Optics 37 (27), 6329–6338.
RD-10	Lee, Z., Carder, K. L., Mobley, C. D., Steward, R. G., Patch, J. S., 1999. Hyperspectral remote sensing for shallow waters. 2. Deriving bottom depths and water properties by optimization. Applied Optics 38, 3831–3843. Page 59
RD-11	Lee, Z., Du, K., Arnone, R., 2005. A model for the diffuse attenuation coefficient of downwelling irradiance. Journal of Geophysical Research 110, C02016.

RD-12	Lee, Z., Lubac, B., Werdell, P. J., Arnone, R., 2009. An Update of the Quasi-Analytical Algorithm (QAA_v5). Tech. rep., International Ocean Colour Coordinating Group (IOCCG) Online: http://www.ioccg.org/groups/software.html (assessed 10/02/2012).
RD-13	Maritorena, S., Siegel, D. A., Peterson, A. R., 2002. Optimization of a semi analytical ocean color model for global-scale applications. Applied Optics 41 (15), 2705–2714.
RD-14	André Morel and Bernard Gentili, "Diffuse reflectance of oceanic waters. III. Implication of bidirectionality for the remote-sensing problem," Appl. Opt. 35, 4850-4862 (1996)
RD-15	Morel, A., Huot, Y., Gentili, B., Werdell, P.J., Hooker, S.B. and B.A. Franz (2007). Examining the consistency of products derived from various ocean color sensors in open ocean (Case 1) waters in the perspective of a multi-sensor approach. Remote Sensing of Environment, 111, 69-88 O'Reilly, J.E. and Werdell, P.J., 2019. Chlorophyll algorithms for ocean color sensors-OC4, OC5 & OC6. *Remote Sensing of Environment*, *229*, pp.32-47.
RD-16	Steinmetz, F., Deschamps, P-Y., and Ramon, D. (2011) "Atmospheric correction in presence of sun glint: application to MERIS," Opt. Express 19, 9783-9800 https://doi.org/10.1364/OE.19.009783 Steinmetz, F., and Ramon, D. (2018) "Sentinel-2 MSI and Sentinel-3 OLCI consistent ocean colour products using POLYMER", Proc. SPIE 10778, Remote Sensing of the Open and Coastal Ocean and Inland Waters, 107780E; https://doi.org/10.1117/12.2500232
RD-17	Xue, K., Ma, R., Duan, H., Shen, M., Boss, E. and Cao, Z., 2019. Inversion of inherent optical properties in optically complex waters using sentinel-3A/OLCI images: A case study using China's three largest freshwater lakes. *Remote sensing of environment*, *225*, pp.328-346.

List of Acronyms

Acronym	**Description**
ATBD	Algorithm Theoretical Baseline Document
BRDF	Bidirectional Reflectance Distribution Function
CCI	Climate Change Initiative
CMEMS	Copernicus Marine Environment Monitoring Service
ECMWF	European Centre for Medium-Range Weather Forecasts
EO	Earth Observation
ESA	European Space Agency
GCOS	Global Observing System for Climate
IOCCG	International Ocean Colour Coordinating Group
MODIS	Moderate Resolution Imaging Spectroradiometer

MERIS	MEdium Resolution Imaging Spectrometer
NASA	National Aeronautics and Space Agency
OC-CCI	Ocean Colour Climate Change Initiative
OLCI	Ocean and Land Colour Instrument
OMAPS	Ocean Colour Multi-Mission Algorithm Prototype System
POLYMER	POLYnomial based algorithm applied to MERIS (though it is now applicable to multiple sensors)
PVP	Product Validation Plan
RBD	Requirements Baseline Document
SeaWiFS	Sea Viewing Wide Field of View Sensor
SeaDAS	SeaWiFS Data Analysis System
SNAP	Sentinel Application Platform
SOW	Statement Of Work
SVC	System Vicarious Calibration
TOA	Top of atmosphere
VIIRS	Visible Infrared Imaging Radiometer Suite

1 Purpose

This requirements baseline document (RBD) covers the requirements that must be met by the prototype processor on the basis of EUMETSAT requirements and those already identified by the wider Ocean Colour community. The document will describe:

- a structured set of high-level requirements for the prototype ocean colour processor system and the generated products,
- the atmospheric correction and ocean colour algorithms to be implemented within the prototype processor,
- all input data (i.e. EO and ancillary data) required to generate the data product(s)

It is also important to outline the methods, test areas, and in-situ observation data sources to be used to validate output products. However, these topics will be covered in the product validation plan and the other RBD (D1.1) written as a counterpart to this document, so will not be covered extensively here.

1.1 Requirement sources

Where relevant the source of a requirement will be given. These requirements result from:

1) The EUMETSET tender general requirements [e.g GR-49, deliverable datasets provided in netCDF CF format]
2) The EUMETSAT statement of work requirements [e.g SOW-11, the review shall take into account the extended spectral resolution of OLCI]
3) User requirements (UR-x) derived from peer review of sources such as GCOS reports, OC-CCI user survey reports or Sentinel-3 Mission Requirements Traceability and validation team reports [SOW-3, GR-3]

2 Intended Processor Structure

The prototype processor will be modular in nature [SOW-16], allowing for modification or comparison of different methods or parameterizations at both the atmospheric correction and in-water product retrieval stages. The processor construction will make use of a 'tagging' scheme such that module tags are used to check the validity of a proposed processor structure. Each module will have a set of 'required', 'forbidden' and 'added' tags. This means that the input to a given module must have all the tags in the required list, none of those in the forbidden list and the output from the module will possess the tags in the added list. The complete list of tags added through a proposed chain can then be used to test if the configuration is valid. It is of note that it is possible for modules to add multiple tags and that not all tags need to be added for a complete processing chain to be valid (for example the tag for smile correction is not required for all sensors).

A schematic of the proposed module format and combination into a processing chain is shown in Figure 1. Given that different approaches to atmospheric correction combine some of the 'modules' shown in the new schematic diagram, it makes more sense to consider variant 'configuration' options rather than all possible module configurations. For example, within the POLYMER atmospheric correction algorithm (as used in OC-CCI) the environmental effects, sun glint and aerosol correction steps are inseparable. In the context of this work, some pre-processing stages are included in the OC-AC (such as instrumental and gaseous corrections).

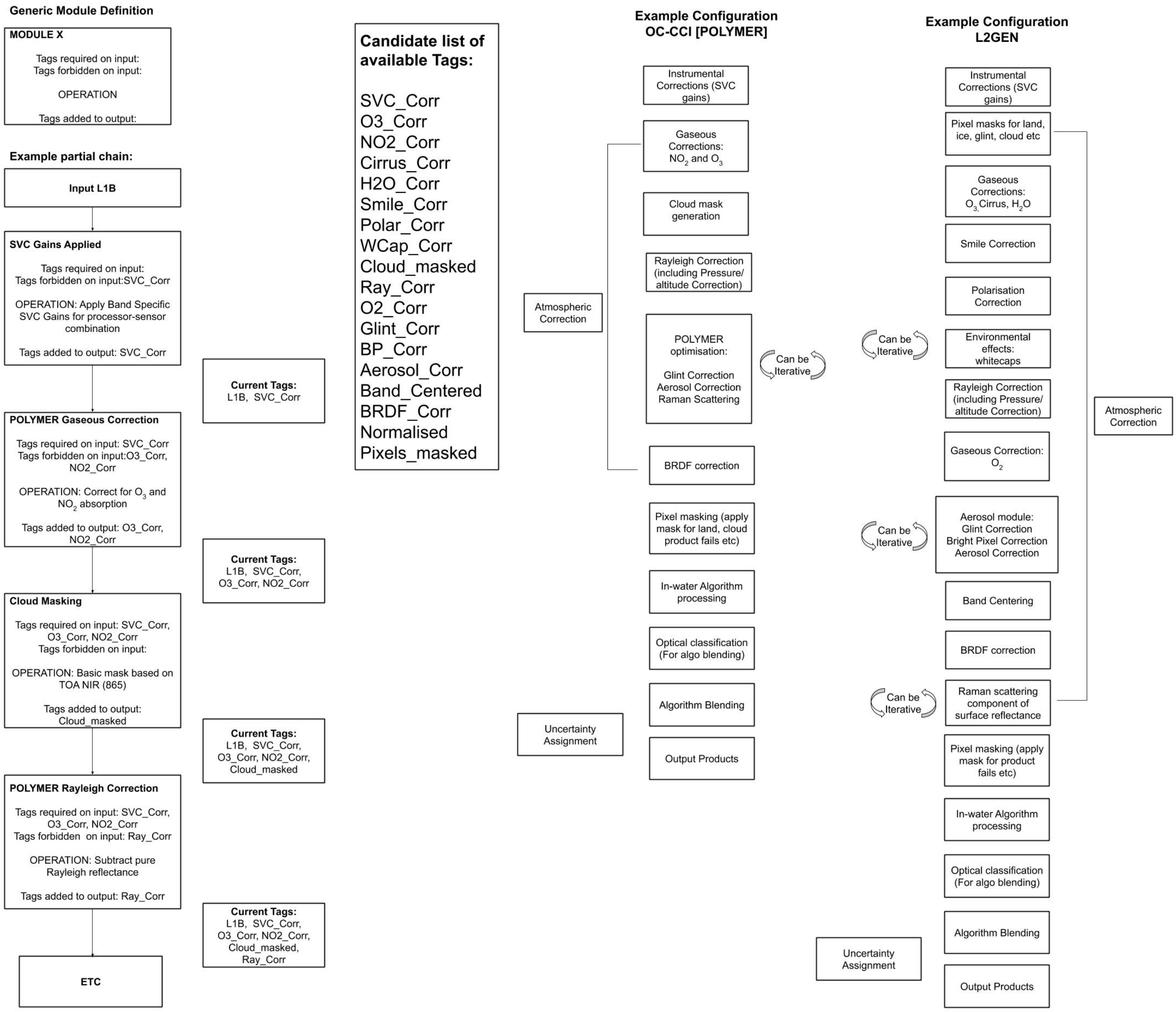

Figure 1 Schematic diagram of module structure and examples of valid constructed processing chains. Not all Tags are required for a chain to be valid as some are sensor or module specific. For example, Smile_Corr is only applicable to MERIS and OLCI sensors.

It was stated by the IOCCG (2012) that it is encouraged that "agencies and users converge on a single ocean-colour data processing software and visualization package, which can be developed and expanded as needed". Currently, NASA is maintaining and developing the SeaWiFS Data Analysis System (SeaDAS) software while ESA is funding development of the Sentinel Application Platform (SNAP). However, convergence is occurring as the latest version of SeaDAS (7.5.3) is the result of a collaboration with the developers of ESA's BEAM software package, which was also the precursor to SNAP. This prototype processor will make use of modules from both these systems for the initial testing configurations in order to continue the harmonisation approach and avoid duplicating effort.

A full description of data formats between modules will be provided in the IODD document but below we provide a table summarising the functional requirements of modules and what is needed as input and output for each stage.

Table 1 OC Processor constituent module requirements

OC processing module	Required Function	Required Input	Required Output	Relevant documentation
Instrumental Correction/SVC gains	Apply system vicarious calibration to improve product quality.	• Input L1B TOA radiance data. • SVC gains LUT for the given atmospheric processor configuration.	Corrected L1B TOA radiances.	SVC ATBD
Gaseous Correction	Correct for the impact of the relevant absorption features due to atmospheric gases within the spectral domain of OLCI (e.g NO_2 Affects bands 1, 2, and 3 of OLCI while O_3 is important for bands 3-16)	• Smile corrected TOA radiances (for example O_2 absorption lines are heterogeneously distributed across band O16) • relevant LUT for gaseous properties • estimate of gaseous concentrations. • viewing and solar geometry • estimate of aerosol thickness	• Pixels flags for algorithm failure. • Gaseous Corrected radiance data in netcdf format.	S3-L2-SD-03-C03-FUB-ATBD_GaseousCorrection https://sentinel.esa.int/documents/247904/349589/OLCI_L2_ATBD_Gaseous_Correction.pdf
Smile Effect	Correct for "curvature of the iso-wavelength line wrt the CCD array rows within a given camera (optical distortion, chromatism) "	• Knowledge of in-FOV variation of wavelength for OLCI cameras. •	Corrected TOA radiance at defined nominal wavelength	S3-L2-SD-03-C04-ACR-ATBD
Rayleigh Correction (including Pressure correction)	Account for the elastic scattering of molecules in the atmosphere, accounting for the impact	• SVC corrected TOA radiances. • Rayleigh scattering LUTs. • Estimates of surface altitude and	Rayleigh corrected TOA radiance.	S3-L2-SD-03-C04-ACR-ATBD

OC processing module	Required Function	Required Input	Required Output	Relevant documentation
	of surface pressure on Rayleigh scattering.	atmospheric pressure.		
Polarization correction	Correct for polarisation sensitivity of sensor (not required for OLCI)	• TOA radiances • Solar and viewing geometry information.	• Corrected TOA radiance data in netcdf format. •	
Environmental effects	Correct for in the influence of factors such as whitecaps or glint.	• TOA radiances • Solar and viewing geometry information. • Diffuse transmittance estimate. • Estimates of wind speed. • Wind speed thresholds (min and max)	• Corrected TOA radiance data in netcdf format. • Flags for unsuitable conditions (high wind speed or glint).	S3-L2-SD-03-C06-ARG-ATBD S3-L2-SD-03-C09-ARG-ATBD
Bright Pixel Correction	Calculate and apply the correction for NIR reflectance due to 'bright pixels' where the 'dark NIR' assumption fails due to factors like high sediment concentrations.	• Smile, Rayleigh and gaseous absorption corrected TOA radiance data. • LUTs for information such as Bright pixel thresholds. • Optical properties of 'scatterers'.	• Bright NIR corrected TOA radiance data in netcdf format. • Flags if BPC fails.	S3-L2-SD-03-C08-ARG-ATBD_BWAC https://sentinel.esa.int/documents/247904/349589/OLCI_L2_ATBD_Atmospheric_Corrections_Bright_Waters.pdf
Cloud Masking	Identify and provide flags for pixels that are contaminated by cloud pixels or cloud shadows.	• Corrected TOA radiances. • Method for cloud top height estimation • Viewing and solar geometry information	• Cloud and cloud shadow masks.	
Aerosol correction	Correct the TOA total signal to get the marine signal with the best possible accuracy (note	• Viewing and solar geometry information	• water-leaving radiance.	S3-L2-SD-03- C07-LOV-ATBD

OC processing module	Required Function	Required Input	Required Output	Relevant documentation
	this is not to provide aerosol properties, which is the role of aerosol remote sensing, and uses a different approach)	• LUTs of aerosol properties. • TOA radiances after corrections for gaseous absorption, Rayleigh scattering, Bright pixel and environmental effects.		
BRDF correction	Estimate the normalised water leaving reflectance from the non-normalized water reflectance (account for the Bidirectional Reflectance Distribution Function effects associated with the angular distribution of the ratio of upwelling radiance to downwelling irradiance)	• Viewing and solar geometry information • LUTs such as Morel F/Q • water-leaving radiance.	• Normalised water-leaving reflectance.	Morel and Gentili (1996) [RD-14]
Raman scattering correction	Determine the Raman scattering component of Rrs as this can impact optical inversion models.	• Raman excitation response functions per sensor band. • LUTs for Raman scattering properties.	Raman component of water-leaving reflectance.	
Pixel Masking	Remove pixels classified as land or flagged by preceding modules.	• Product Flags • Configuration file of which flags to mask.	• Masked surface reflectance data.	
In water algorithm processing	To derive in-water products (Chlorophyll-a and Kd490) from Rrs data.	• Normalised water-leaving reflectance data. • Configuration file of which flags to mask.	• Chlorophyll-a concentrations for a given set of candidate algorithms. • Kd490 data. • Flags where algorithms fail.	OC in-water Algorithm ATBD (AD-10)

OC processing module	Required Function	Required Input	Required Output	Relevant documentation
Optical classification	To classify the surface reflectance spectra against a defined optical water class set. This will allow optimal algorithm blending and uncertainty estimation.	• LUTs for optical water class set. • Normalised water-leaving reflectance data.	• Flags where optical classification fails. • Optical water class memberships in netcdf format.	Jackson et al (2017) [RD-7]
Algorithm Blending	Provide a seamlessly blended product that makes use of the best candidate algorithm for the optical conditions on a pixel by pixel basis.	• Configuration file of optimal algorithm per optical class • Configuration file of which flags to mask.	• Level-2 data on OC derived products (Chlorophyll-a and Kd490) whose quality remains optimal across different water types.	ATBD for Optimal Algorithm Blending [AD-9]
Product Uncertainty estimates	Provide information on the potential bias and accuracy of the L2 products.	• Optical water class memberships. • LUTs for per water class performance for given products.	• Per-pixel estimates of bias and accuracy.	Jackson et al (2017) [RD-7]
Output Products and standardisation	Last file additions or updates relating to meta-data, versioning, standardisation and product set merging.	• Level-2 product files • Configuration file for meta-data requirements.	• Final level-2 products with standardised meta-data and processing history information.	

3 Product Requirements

The fundamental output of Ocean Colour processing at Level 2 is the spectral water-leaving reflectance for the surface ocean [SOW-7]. From this data, a suite of downstream products can be then be derived. The most commonly requested/utilised derived product is the chlorophyll-a concentration. In addition to spectral reflectance data and chlorophyll-a products the processor will (at a minimum) also be able to produce per-pixel estimates of $K_d(490)$ at Level 2 [SOW-8]. Details of the algorithms to be implemented to produce these products are covered in section 5.2. Full details of the L2 products and formats will be given in the Input Output Data Definition (IODD) document [AD-6] as per [SOW-24]. Here, we will cover the required product specifications in terms of the product set, product accuracy, product flagging and product uncertainty.

3.1 Product Set

The term "water-leaving reflectance" is linguistically odd, as reflectance is a property of a surface and therefore cannot propagate through space. Here, it is used in place of "reflectance based on the water-leaving radiance L_w and the incident irradiance E_d just above the surface" and is defined [SOW-9] as:

$$\rho_w(\theta_v, \phi) = \pi \frac{L_w(\theta_s, \theta_v, \phi)}{E_d(0^+, \theta_s)} \tag{1}$$

In the context of remote sensing, the water leaving radiance is sometimes mentioned as the main product for water colour, however it is more appropriate to use the water reflectance as the main product, which is dimensionless and does not depend on the downwelling irradiance at the surface. Additionally, it is of note that in the context of remote sensing, the surface reflectance estimates are often 'normalised'. Morel and Gentili (1996) defined normalised water-leaving radiance to be "...the radiance that could be measured by a nadir-viewing instrument, if the Sun were at the zenith in the absence of any atmospheric loss, and when the Earth is at its mean distance from the Sun." It is a requirement that the process is capable of producing normalised water leaving reflectance data [SOW-10, SOW-20].
In order to correctly estimate the normalised water leaving reflectance ρ_{wN} from the non-normalized water reflectance $\rho_W(\theta_v, \phi)$, we must account for the Bidirectional Reflectance Distribution Function (BRDF) effects associated with the angular distribution of the ratio of upwelling radiance to downwelling irradiance, just beneath the surface ($\frac{f_0/Q_0}{f/Q}$) , which depends on the water inherent optical properties (IOP) and the observation geometry, and with the angular effects associated with the wavy water-air interface at wind speed W ($\frac{\Re_0(W)}{\Re(W)}$):

$$\rho_{wN} = \frac{\Re_0(W)}{\Re(W)} \frac{f_0(IOP)/Q_0(IOP)}{f(IOP, \theta_s, \theta_v, \phi)/Q(IOP, \theta_s, \theta_v, \phi)} \rho_W(\theta_v, \phi) \tag{2}$$

OLCI provides 21 bands of radiance data (Table 2) at Level 1 [SOW-11] and the processor will be able to handle all as input. The final L2 output products, when full OLCI inputs are provided, shall contain a subset of these 21 bands relevant for ocean colour applications and at a minimum this should include Oa1-12, Oa16 and Oa17.

Table 2 list of OLCI bands and functions

Band	λ centre (nm)	Function
Oa01	400	Aerosol correction, improved water constituent retrieval
Oa02	412.5	Yellow substance and detrital pigments (turbidity)
Oa03	442.5	Chlorophyll absorption maximum, biogeochemistry, vegetation
Oa04	490	High Chlorophyll,
Oa05	510	Chlorophyll, sediment, turbidity, red tide
Oa06	560	Chlorophyll reference (Chlorophyll minimum)
Oa07	620	Sediment loading
Oa08	665	Chlorophyll (2nd Chlorophyll absorption maximum), sediment, yellow substance/vegetation

Band	λ centre (nm)	Function
Oa09	673.75	For improved fluorescence retrieval and to better account for smile together with the bands 665 and 680 nm
Oa10	681.25	Chlorophyll fluorescence peak, red edge
Oa11	708.75	Chlorophyll fluorescence baseline, red edge transition
Oa12	753.75	O2 absorption/clouds, vegetation
Oa13	761.25	O2 absorption band/aerosol correction.
Oa14	764.375	Atmospheric correction
Oa15	767.5	O2A used for cloud top pressure, fluorescence over land
Oa16	778.75	Atmos. corr./aerosol corr.
Oa17	865	Atmospheric correction/aerosol correction, clouds, pixel co-registration
Oa18	885	Water vapour absorption reference band. Common reference band with SLSTR instrument. Vegetation monitoring
Oa19	900	Water vapour absorption/vegetation monitoring (maximum reflectance)
Oa20	940	Water vapour absorption, Atmospheric correction/aerosol correction
Oa21	1 020	Atmospheric correction/aerosol correction

Following the estimation of ocean surface reflectance, the derived ocean colour products (chlorophyll-a and Kd490) are derived. Algorithmic approaches for this are covered in section 5.2 and a summary table of product set requirements [GR-4] is given at the end of this section (
Table 7).

Due to the modular nature of the new processor, there will be a number of possible 'break points' in the processing chain. This means that at some of these intermediate stages, outputs could be created as 'diagnostic variables' [SOW-26] such as calculated Rayleigh reflectances, aerosol reflectances, atmospheric transmittances, estimated glint or whitecap reflectance, or such quantities such as BRDF values and pixel geometries (solar zenith angle etc) [SOW-27]. These diagnostic variables will be provided, as with the primary products, in a netcdf format with associated metadata and for spectral bands where appropriate [GR-49].

3.2 Product Flags

It is essential that pixel flags are provided alongside the products as this allows users to understand and manipulate the data using contextual information. Flags can also be used between/within processing modules to mask pixels that are not suitable for further processing. Where useful we will retain flag information from the input OLCI data and add to this from subsequent modules or processing stages (such as cloud identification) such that final per-pixel flags shall include at minimum [SOW-25]:

- relevant flags carried from the L1B product, e.g. land and water classification, inland water subset of the water classification,

- cloud flags,
- flags indicating intermediate retrieval status, e.g. medium glint, absorbing aerosols, water type classification,
- flags indicating retrieval quality levels, e.g. atmospheric correction warning, chlorophyll failure.

It is common to store product flags in a Bitmask format as this is extremely efficient for combining multiple binary condition flags. This is currently the default procedure used in both NASAs l2gen, and POLYMER atmospheric correction schemes and we will adopt it here also.

Examples of the flags available from the l2gen and POLYMER atmospheric schemes are provided below and more details can be found in the respective processor documentation.

Table 3 l2gen Flags

Bit number	Flag purpose	Flag name
1	atmospheric correction failure from invalid inputs land	ATMFAIL
2	Land	LAND
3	questionable value for one or more parameters severe Sun glint	PRODWARN
4	severe Sun glint	HIGLINT
5	total radiance above knee in any band satellite zenith angle above limit shallow water	HILT
6	satellite zenith angle above limit	HISATZEN
7	shallow water	COASTZ
9	stray light contamination	STRAYLIGHT
10	clouds and/or ice	CLDICE
11	coccolithophore	COCCOLITH
12	turbid, case-2 water	TURBIDW
13	solar zenith angle above limit	HISOLZEN
15	low water leaving radiance at 555nm	LOWLW
16	Chlorophyll-a not calculable	CHLFAIL
17	questionable navigation (e.g tilt change)	NAVWARN
18	absorbing aerosol index above threshold	ABSAER
20	maximium number of iterations of NIR algorithm	MAXAERITER
21	moderate Sun glint	MODGLINT
22	chlorophyll out of range	CHLWARN
23	epsilon out of range	ATMWARN

Bit number	Flag purpose	Flag name
25	sea ice in pixel (based on climatology)	SEAICE
26	navigation failure condition indicated in nav flags	NAVFAIL
27	insufficient valid neighboring pixels for epsilon filtering	FILTER
28	sea surface temperature warning flag (MODIS only)	SSTWARN
29	sea surface temperature failure flag (MODIS only)	SSTFAIL
30	degree of polarization above limit (MODIS only)	HIPOL
31	one or more parameters could not be computed	PRODFAIL

Table 4 POLYMER Flags

Bit number	Flag purpose	Flag name
1	Land mask, either read from level 1 (MERIS) or using a static land/sea mask (MERIS, MODIS, SeaWiFS)	LAND
2	Basic Polymer cloud mask (see section 4.1.1)	CLOUD
3	Invalid level 1 data MERIS: level 1 flags “INVALID”, “SUSPECT” and “COSMETIC” MODIS: input data is set to NaN SeaWiFS: level 1 flags “HILT”, “NAVWARN” and “NAVFAIL”	L1_INVALID
4	Raised when the total backscattering coefficient at 550 nm is a negative value.	NEGATIVE_BB
5	Raised when the optimised parameters (chl or bbs) reach an “out of bounds” value: 0.01 < chl(mg/m3) < 100 -0.005 < bbNC(m-1) < 0.1	OUT_OF_BOUNDS
6	Error in the LUT interpolation (raised for example on MODIS night pixels)	EXCEPTION
7	Raised when detecting anomalous results in presence of thick aerosol plume, detected by the following expression: “Rnir/Rw_max > 10 – 1.5*logchl” Where Rnir is the TOA reflectance in the NIR (865 or equivalent) band, corrected for Raileigh scattering, Rw_max is the maximum water reflectance over all bands, and logchl is the 10-based logarithm of the chlorophyll concentration.	THICK_AEROSOL
8	Raised when the air mass (1/cos(thv)+1/cos(ths)) is greater than 5. Pixels are considered of reduced quality and should not be used.	HIGH_AIR_MASS
9	Raised when the optimization is performed in case 2 mode (see section 3.4). This does not invalidate the pixel.	CASE2
10	Raised when, at any band, t*Rw or the atmospheric signal Ratm exceed the TOA reflectance corrected for Rayleigh scattering. This flag is used for triggering re-initialization of the	INCONSISTENCY

Bit number	Flag purpose	Flag name
	optimization process for next pixel, but should not be used for pixel filtering (leads to over-flagging in some cases, in particular for MERIS)	

Each module can add flags to the data structure but should not remove flags that have been put in place from other modules. The act of actually masking products through flag criteria can therefore potentially be applied at multiple intermediate stages through the atmospheric correction and ocean colour processing chain. For example, one may wish to mask all pixels that are potentially contaminated by sun glint before processing spectral reflectance values to produce chlorophyll-a estimates, or one might wish to mask pixels where the chlorophyll-a estimate is beyond the range considered reliable for a given in-water algorithm. The example shown below is a masking operation used at the stage of binning data after atmospheric correction which combines masks from the POLYMER atmospheric correction algorithm and from IDEPIX pixel classification (used to identify cloud and ice pixels in addition to the checks performed within polymer):

```
not(pixel_classif_flags.F_INVALID or pixel_classif_flags.F_CLOUD or
pixel_classif_flags.F_LAND or pixel_classif_flags.F_SNOW_ICE or
pixel_classif_flags.F_MIXED_PIXEL or pixel_classif_flags.F_CLOUD_BUFFER or
pixel_classif_flags.F_CLOUD_SHADOW) and ((polymer.bitmask && 1023) == 0)
```

The OC processor will preserve flags raised by differing modules or processing stages such that they can be applied or used for analysis at a later stage. This means that there could be multiple flags available for a single pixel and condition (such as L2gen.CLDICE, polymer.CLOUD and IDEPIX.F_CLOUD for identifying cloud). The processor will allow for these name variations through the use of a masking expressions options that can be set within a configuration file.

3.3 Product Accuracy

In addition to being having key spectral bands available, it is essential that satellite derived ocean colour products are of a high enough quality to meet the needs of both water quality measurement requirements (AD-8) and climate change scientists (AD-7). The exact needs and desires of the community continue to evolve as new technologies and products are tested by agencies such as NASA and ESA. However, we can consider the performance requirement set by the Global Observing System for Climate (GCOS) [UR-1] in support of the United Nations Framework Convention on Climate Change (UNFCCC), and the results of the OC-CCI user survey [UR-2], as the minimum current requirements of the ocean colour community [SOW-5].
Obviously the users of near-real-time (NRT) products should expect that NRT products will come with a lower accuracy than those produced during reprocessing activities, during which factors such as higher quality ancillary data sources and the latest available SVC corrections will enhance data quality. This means that although the processing time requirements for NRT are quite demanding, the quality criteria are less well constrained. For example, the CMEMS [UR-3] project current estimates a Quality index for NRT ocean colour data as:

$$QI = \frac{CurrentDataPixel - ClimatologyDataPixel}{STDDataPixel}, \qquad 3$$

where CurrentDataPixel is the daily observation and ClimatologyDataPixel and STDDataPixel are the climatology mean and standard deviation, respectively. The QI daily distribution is then analysed to show the spread in QI values relative to the STD.

The OC-CCI user survey showed threshold (minimum) accuracy and precision requirements for chl-a of 10–25% (modellers) and 25–50% (EO scientists) with a goal of < 10%. This goal was considered to be equivalent to the uncertainty in *in situ* observation (CCI URD, 2014). The GCOS and Ocean Colour Community requirements relevant to level 2 product generation (i.e not including factors such as temporal coverage) are summarised in **Table 5** and **Table 6**.

Table 5 GCOS Ocean Colour Product requirements (GCOS 2011,2016)

Variable/Parameter	Horizontal Resolution	Accuracy
Water Leaving Radiance	4km	5% (for blue/green wavelengths)
Chlorophyll-a concentration	30km (later reduce to 4km)	30%

Table 6 OC-CCI User requirements

Variable/Parameter		Horizontal Resolution	Accuracy
Water Leaving Radiance	EO scientists	0.1 - 1 km	~ 10 %
	Modellers	10 - 100 km	10 - 25 %
Chlorophyll-a concentration	EO scientists	0.1 -1 km	10-25%
	Modellers	1 - 10 km	10-25%
K_d(490)	EO scientists	0.1 - 1 km	~ 10 %
	Modellers	1 - 10 km	10 - 25 %

Given that the signal of interest for ocean colour (water-leaving radiance) is a fraction of the signal received by the instrument in orbit, it has long been clear that good calibration and a high radiometric sensitivity are extremely important for ocean colour (Gordon 1987, IOCCG 2012). For reference, IOCCG (2013) evaluates the uncertainty associated with a radiance-based calibration of MERIS (Medium Resolution Imaging Spectrometer) through a solar diffuser at 3%, though this includes a 2% uncertainty of solar irradiance (Thuillier et al. 2003) which can be factored out when working with reflectance spectra. Differences between on-orbit lunar observations conducted by SeaWiFS, MODIS Aqua and Terra have been observed at 1-8% (Eplee et al. 2011). Ultimately, uncertainties of 2% for TOA radiance has been proposed as a realistic target, although still lower uncertainties would be certainly welcome (IOCCG 2012, IOCCG *2019*).

Despite the best efforts of satellite sensor constructors and operators to characterise all the sensor radiometric and spectral properties pre-launch (e.g sensor spectral response function, dark current, radiometric angular, detector-to-detector differences, linearity (or variations around it), sensitivity for polarised light and straylight, etc) these properties may not be perfectly known and may drift over the sensor lifetime. Periodic assessment by the sensor operators can identify deviations and will usually result in a gain correction to the sensor.

In addition to updates to the sensor calibration parameters, there will remain the requirement for a System Vicarious Calibration (SVC). The SVC is a relative radiometric calibration to sensors that minimizes uncertainties in the water-leaving radiance derived from the TOA radiance. This are produced for a given sensor and processor configuration and it is therefore essential that the prototype processor is able to utilise SVC gains for application to the level 1 data [SOW-19]. A number of approaches have been developed to derive SVC gain coefficients, but all rely on match-ups between in-situ measurements and remotely sensed reflectance estimates. The details of the SVC approach to be used as part of the offline processor will be covered in the relevant ATBD, but it is important to note here that the development of multi-band-optimisation based atmospheric correction algorithms such as POLYMER has made the process of SVC gain estimation much more complicated as a single band gain correction provokes a multi-band response.

As the state of the art for ocean colour sensors has moved forward at a rapid pace since the GCOS requirements were first compiled and modern sensors are more than capable of meeting the horizontal resolutions deemed suitable by GCOS. Whether the newest suite of sensors can meet the accuracy requirements, at these high resolutions, across the diversity of optical conditions seen in the global domain remains to be proven. The construction of the new prototype processor is not guaranteed to produce ocean colour products that meet these accuracy requirements, but the modular approach and capability to blend ocean colour algorithms (discussed in section 5.2.3) will allow multiple in-water algorithms to be combined in order to optimise final product accuracy across a range of optical conditions. This will also allow relatively simple ‘upgrades’ of modules/processing algorithms following future developments. For example, if a new chlorophyll-a algorithm is developed it could be included in the processor blending scheme without modifying other aspects of the processor.

3.4 Product Uncertainties

According the Guide to the Expression of Uncertainty in Measurement (GUM, 2008): “The uncertainty of the result of a measurement reflects the lack of exact knowledge of the value of the measurand.”

Noting that “the result of a measurement (even following correction for known systematic errors) can unknowably be very close to the value of the measurand (and hence have a negligible error) even though it may have a large uncertainty. Thus the uncertainty of the result of a measurement should not be confused with the remaining unknown error.”
When discussing providing estimates of uncertainty then those would be given as a standard deviation (an expression of the standard error).

Given that the performance of both atmospheric correction and in-water ocean colour algorithms is not uniform across the range of sampled environments it is important that users are provided with information on the quality of the Level 2 products on a pixel by pixel basis [GR-7, GR-9]. This will be done through the provision of corresponding uncertainty products for each of the provided Level 2 products.

The provision of uncertainty metrics alongside the primary data is becoming more common in the ocean colour community and has been a central tenet of the Ocean Colour Climate Change Initiative (OC-CCI). Having uncertainties is now considered indispensable or desirable by 75% of the survey Ocean Colour community, while only 15% classed them as not being required. According to the community, uncertainty estimates should be estimated from a combination of in situ data, atmospheric and in-water processing algorithms and a longer time-series of observations. Currently the OC-CCI uncertainty metrics provided are root-mean-square difference and bias, from which the standard deviation (an expression of standard uncertainty) can also be computed.

In an ideal system the uncertainty estimates provided for a product would result from a formal error propagation of known initial measurement uncertainties at the sensor level [GR-8]. Unfortunately, the inclusion of techniques such as neural networks and spectral matching in the atmospheric correction or in-water algorithm processing can hamper the creation of a complete error budget. Work to provide formal uncertainty estimates for ocean colour is ongoing so it cannot be guaranteed that this will be integrated into the prototype processor. As a minimum the prototype processor will instead make use of the methods developed by the OC-CCI project. This approach involves using optical water type classification techniques and an in-situ database of ocean colour measurements from a range of water conditions in order to map the product performance (as assessed using matchups against in-situ measurements) onto global products on a pixel by pixel basis.

Table 7 Summary table of Product Set requirements

Product Set requirement	Sources
Provide native resolution normalised water leaving reflectances at OLCI OC wavebands, including BRDF correction.	SOW-7, SOW-10, SOW-11, SOW-20
Provide native resolution Chlorophyll-a product	SOW 7, SOW-8
Provide native resolution Kd490 product	SOW 7, SOW-8
Provide Uncertainties (per pixel) for the above products, following the QA4EO approach (if possible)	GR-7, GR-8, GR-9
Provide per-pixel flag information, formed from a combination of input L1B flags and those generated within the processor configuration	SOW-25
Allow the output of 'diagnostic variables' from intermediate stages in the OC-processing chain.	SOW-26, SOW-27

Table 8 Summary table of per product requirements

Product requirement	Normalised water leaving reflectance	Chlorophyll-a	Kd490	Source
Scope	Global Provided for all OLCI OC wavebands	Global	Global	SOW-7,SOW-8,SOW-11, UR-1, UR2
Physical units	Sr^{-1}	$mg\ m^{-3}$	m^{-1}	
Accuracy	5% (less stringent for NRT)	30% (less stringent for NRT)	20% (less stringent for NRT)	UR-1, UR-2, UR-3
Precision	Stated to at least 0.001	Stated to at least 0.01	Stated to at least 0.01	UR-1, UR-2, UR-3
Spatial resolution	300m	300m	300m	SOW-8
Timeliness	<0.5 day (For NRT processing)	<0.5 day (For NRT processing)	<0.5 day (For NRT processing)	SOW-35, UR-2, UR-3

Product requirement	Normalised water leaving reflectance	Chlorophyll-a	Kd490	Source
Source EO missions	Sentinel 3A and 3B	Sentinel 3A and 3B	Sentinel 3A and 3B	SOW-13
Reference measurements	QC'd in-situ database from sources such as AERONET OC sites.	QC'd in-situ database	QC'd in-situ database	UR-2

4 Additional Processor functionality requirements

4.1 Timeliness of production

Given that there are now two OLCI sensors on orbit, providing hundreds of Gigabytes (GB) of level 1 data per day, it is essential that the processor is sufficiently efficient that it can process from level 1 to level 2 in a timely manner. A typical day of OLCI data might contain ≅ 211 granules for 1 sensor (or >400 for 3A and 3B).

Considering a project such as CMEMS, NRT requirements on processing speed can be a significant challenge. CMEMS NRT data is currently produced with a target delivery time of +1d 18:00 for daily data and +10d 18:00 monthly composites. The spatial requirements are 1km for regional seas, and 4km for global products but those are less than the native sensor resolution that we are required to process here.

It is intended that the ocean colour processor can be deployed in a grid (parallel) processing environment, such that if processing a single granule can be performed in 2-5 hours then running across approximately 50 nodes should be more than sufficient to allow processing to keep pace with input data generation [SOW-35].

4.2 Input and output Data formats

Within this project, the term 'ocean colour processor' refers to a system to process input data at level 1B to output ocean surface products at level 2. A complete description of the data inputs, data structures and product outputs is provided in the Input Output Definition Document (IODD) but we will include some information below for context alongside the processor requirements.

The Level 1B data set, QC'd [GR-14] and provided by EUMETSAT [GR-51], will contain (per pixel) calibrated and geolocated at-aperture (top-of-atmosphere) radiances generated from Level-0 sensor counts, pixel surface classification, instrument radiometric and spectral information (wavelength, full width at half maximum (FWHM), solar flux, datetime information, and bright pixel flagging [SOW-33]. Additionally, the file must contain meteorological values (typically at tie points) including total ozone, total columnar water vapour, humidity, atmospheric temperature profiles at tie pressure levels, horizontal wind at 10m altitude, sea level pressure [SOW-34]. Given the numerous re-processing operations that have been undertaken for the OLCI S3A data, it should be noted that the L1B data provided by EUMETSAT should have a consistent baseline reprocessing version, which is clearly documented and stated in the L1B meta-data.

The initial focus will be on the Ocean and Land Colour Imager (OLCI) aboard Sentinel 3A and 3B, but the structure of processor configuration files will be such that the they are extensible to historical ocean colour (MODIS, MERIS, VIIRS and SeaWiFS) or future instruments for which ocean colour may be a secondary objective (e.g SEVIRI, FCI, 3MI) instruments [SOW-16].

Given the size of Level 1B full resolution OLCI granules it is common for users to only want to process or work with a subsection of a granule. Therefore, provided the structure and metadata of the file remain consistent, the processor should be able to handle 'minifile' or partial granule spatial subsets [SOW-32]. In principle this is often how granules are processed 'behind the scenes' as much of the code is designed to operate with chunking (processing and writing sections of data to prevent loading everything into memory).

It is essential that common data formats are used throughout the operational processor chain from Level 1 input to output level 2 (and level 3) ocean colour products. File formats should also be extremely memory efficient as the total volumes of data to process and store for routine ocean colour applications can be on the order of Terabytes (TB) and may soon reach Petabytes (PB), with individual files reaching GB in size. It is also important that standardised community-agreed nomenclature is used for dimension and product names, units and descriptions. Bearing all of these points in mind, all product files will be stored as NetCDF4 files and where possible will follow the Climate and Forecast (CF) Metadata convention. Ancillary data files such as look-up-tables (LUTs), configuration files [SOW-31], or manifest files may be stored in other formats but should contain sufficient metadata that they can be clearly interpreted.

Table 9 Summary of processor functionality requirements

Processor requirements	**Source**
Ability to process OLCI data fast enough for NRT (eg <12 hours)	SOW-35, UR-2, UR-3
All outputs and intermediate products in netCDF format.	GR-17, GR-49, UR-2,
able to process subsets of full files	SOW-32
Processor must be modular and extensible, making use of config files and LUTs where required	GR-12, SOW-16, SOW-31
allow input of radiometric gains from SVC updates	SOW-19
Offer Choice of atmospheric correction including POLYMER, baseline and Alternative scheme from SACSO	SOW-38, SOW-18

Table 10 Summary of input data requirements

Input Data Requirements	**Source**
EUMETSAT to provide files with necessary auxillary data including meteorological values such as total ozone, total columnar water vapour, humidity, atmospheric temperature profiles at tie pressure levels, horizontal wind at 10m altitude, sea level pressure	GR-51, SOW-34
EUMETSAT to provide consistent baseline processing files at L1B (TOA) with geolocation information.	GR-52, SOW-33
Supplied L1B files will have pixel surface classification and bright pixel flags available	GR-14, SOW-34

5 Algorithmic Approaches

Full details of algorithms used for both atmospheric correction and in-water products will be provided in Algorithm Theoretical Baseline documents (ATBDs). Here we will cover the requirements of the processor in terms of its flexibility to incorporate multiple algorithms as options to switch in and out for different processing configurations.

5.1 Atmospheric correction algorithms

As mentioned above it will be of use to think of processor configurations rather than stage by stage. The prototype processor will initially have three configuration options by default. Those will be the 'NASA' configuration (based on NASA's L2gen processor), the POLYMER atmospheric correction configuration [SOW-18] and the Alternative Aerosol Processor configuration [SOW-38]. These are discussed in more detail below. If the source code is made openly available for the current OLCI baseline processor then that will also be included into the configuration options if possible.

5.1.1 NASA L2gen configuration

The following was derived from L2gen code within SeaDAS 7.5. See section 6.1 for the comments from the source code justifying this configuration.

Processing stage	**Calculations performed**
Pressure/altitude correction	• Pressure correct the Rayleigh optical thickness
Environmental effects + Rayleigh Correction + Gasesous Corrections	• Correct for ozone absorption. (inbound and outbound and put inbound back when computing Lw) • Cirrus correction - subtract off cirrus reflectance • Correct for transmittance of water vapor above cirrus clouds • Apply smile correction • Apply polarization correction • Remove whitecap radiance • Subtract the Rayleigh contribution • Correct for O2 absorption (replace O2 losses)
Iteration for aerosol with corrections for non-zero nLw(NIR)	• Initialise tLw as surface + aerosol radiance • Compute and subtract glint radiance • Adjust for non-zero NIR water-leaving radiances using input Rrs (or mumm or IOP model) • Compute the aerosol contribution • Subtract aerosols and normalise • estimate chlorophyll (test for warning flag)
Band centering	• Convert water-leaving radiances from band-averaged to band-centered.

Processing stage	Calculations performed
	• Switch mean solar irradiance from band-averaged to band centered also.
BRDF correction	• Compute f/Q correction and apply to nLw (according to FOQMOREL).
Compute derived products	• Compute final Rrs • Compute final chl from final nLw (needed for flagging)
Raman Scattering Correction	• Determine Raman scattering contribution to Rrs
Pixel Masking	• Apply L2gen Masks

5.1.2 Polymer configuration

For full details of the POLYMER algorithm we would refer readers to Steinmetz et al (2011, 2018).

Processing stage	Calculations performed
Vicarious calibration	• Apply vicarious calibration coefficients
Gaseous correction	• Correct for ozone absorption based on ancillary data • Correct for NO2 absorption based on climatology data
Cloud masking (optional: external cloud mask can be provided to Polymer)	• Calculate a basic cloud mask based on a threshold on the absolute value and standard deviation of the TOA reflectance in the NIR (865nm)
Rayleigh correction	• Subtract the pure Rayleigh reflectance
Polymer iterative optimization	• Iterative optimization scheme: determine the atmospheric model parameters (3 parameters) and water reflectance model parameters (2 parameters) that best fit the input signal
Water reflectance calculation	• Subtract the model atmospheric reflectance from the observation, and divide by the total pure-Rayleigh

Processing stage	Calculations performed
	atmospheric transmission, to obtain the directional water reflectance
Normalization	• Water reflectance bidirectional normalization: use the water reflectance model to normalise the water reflectance to a nadir-nadir observation • Spectral normalization: use the water reflectance spectrum to normalise from the per-detector measured wavelength (MERIS and OLCI only) to a common central wavelength

5.1.3 Alternative Aerosol processor configuration

The alternative aerosol processor developed in the EUMETSAT SACSO project is being developed on the basis of the Polymer processor: its structure is not yet consolidated but should be very similar to the structure of Polymer (see previous section).

5.2 In water algorithms

5.2.1 Empirical Algorithms

A variety of empirical chlorophyll algorithms have been developed in order to estimate chlorophyll-a concentration from remote sensing reflectance data. These include band ratio algorithms such as NASAs OC2, OC3, and OC4 algorithms and colour-index (CI) algorithms such as that of Hu et al. (2012). The requirement for reparameterization of the empirical relationship for each sensor and algorithm combination can lead to a great number of 'empirical chlorophyll-a algorithms', for example O'Reilly and Werdell (2019) provide 65 different parameterisations for versions of the OC4, OC5 and OC6 relationships. The diversity of the data used to determine the empirical relationship is also of key importance when we consider if algorithms can be applied globally or are more suitable for regional applications. For example, within the Copernicus Marine Environment Monitoring Service (CMEMS) a number of regionally tuned algorithms are used to provide chlorophyll-a products for the Atlantic, Baltic and Mediterranean waters.

It is to be expected that empirical relationships derived for one biogeochemical environment might not hold across the large diversity of conditions seen in the global oceans. This means that either the relationship must be generic enough to cover the majority of observed global data or we must blend different optimal algorithms depending on their suitability for use in the optical conditions at the pixel in question.

The use of empirical relationships does not just apply to chlorophyll-a products. A number of algorithms for estimating *$K_d(490)$* rely on empirically derived parameterisations such as that of Werdell et al. (2005):

$$K_d(490) = 10^{\left(a0+\sum_{i=1}^{4} a_i \log_{10}\left(\frac{R_{rs}(\lambda_{blue})}{R_{rs}(\lambda_{green})}\right)^i\right)} + 0.0166 \quad (4)$$

where a^0, a^1, a^2, a^3, and a^4 are derived empirically for each sensor.

The prototype processor will include a separate module to allow for the selection of Kd(490) from a list of candidate algorithms (which will grow with future developments for the latest generation of ocean colour sensors). The initial list of candidate $K_d(490)$ algorithms will include:

- The MERIS parameterised version of the above equation (where 490nm is used as the blue band, 560nm as the green band and a^0 to a^4 are -0.8641,-1.6549, 2.0112, -2.5174, -1.1035).
- The "OK2-560" algorithm proposed by Morel et al. (2007) which is based on the 490-560 reflectance ratio, and has the same form as that given above with $R_{rs}(\lambda_{blue})$ replaced by $\rho_N(490)$ and $R_{rs}(\lambda_{green})$ replaced by $\rho_N(560)$, and a^0, a^1, a^2, a^3, and a^4 are -0.82789, -1.64219, 0.90261, -1.62685 and 0.088504 respectively.

An additional candidate algorithm for initial comparison could be that of Lee et al. (2005) but this would also require the use of an algorithm for the generation of Inherent Optical Properties (IOPs).

5.2.2 Analytical and Semi-analytical algorithms

A fully analytical approach to ocean colour products uses radiative transfer theory to provide a relationship between upwelling irradiance or radiance and the in-water constituents. Inversion of the radiative transfer model then allows the derivation of in water properties from radiance/reflectance measurements at multiple wavelengths. Semi-analytical approaches involve the use of empirical relationships for some components of the bio-optical modelling (Carder et al. 1999). Examples of semi-analytical models are the HOPE (Lee et al. 1998, 1999), QAA (Lee et al. 2002, 2009), GSM (Maritorena et al., 2002) and GIOP (Franz and Werdell, 2010; Werdell et al., 2013) models.

As the semi-analytical approaches also depend upon empirical relationships these algorithms can end up having multiple variants for different sensors or regions. For example, Xue et al (2019) tuned a version of the QAA algorithm for use with OLCI Rrs data over turbid inland waters. The prototype processor will contain the functionality to implement a number of existing semi-analytical models where they have been parameterised for the wavebands available from the input sensor and any underlying empirical relationships remain valid.

5.2.3 Algorithm Blending schemes

In order to try and break the dependence of product quality on water types [sow-15], from open ocean to coastal waters, the OC-CCI project implemented a blending approach based on the fuzzy classification of optical water types (Jackson et al 2017). This allows the utilization of multiple algorithms, each providing optimal results in differing optical environments, in a seamless manner. This approach can be used to combine any set of 'optimal' chlorophyll-a algorithms provided 1) a representative optical water class set that represents the global diversity of R_{rs} data for a given sensor and 2) sufficient in-situ data is available to discern the optimal approach for each optical water class in a given set. This process does not provide a uniform 'quality' across all waters (see Figure 2 for example of bias and RMSD for differing optical water types in the OC-CCI blended product). Instead this approach aims to maximise quality irrespective of water type rather than favouring performance under a prescribed set of conditions or adopting a single 'best overall' algorithm.

The prototype processor will include fuzzy classification and algorithm blending options which will read in information on the number of classes, spectral bands to use, class definitions and per class optimal algorithms from a configuration file.

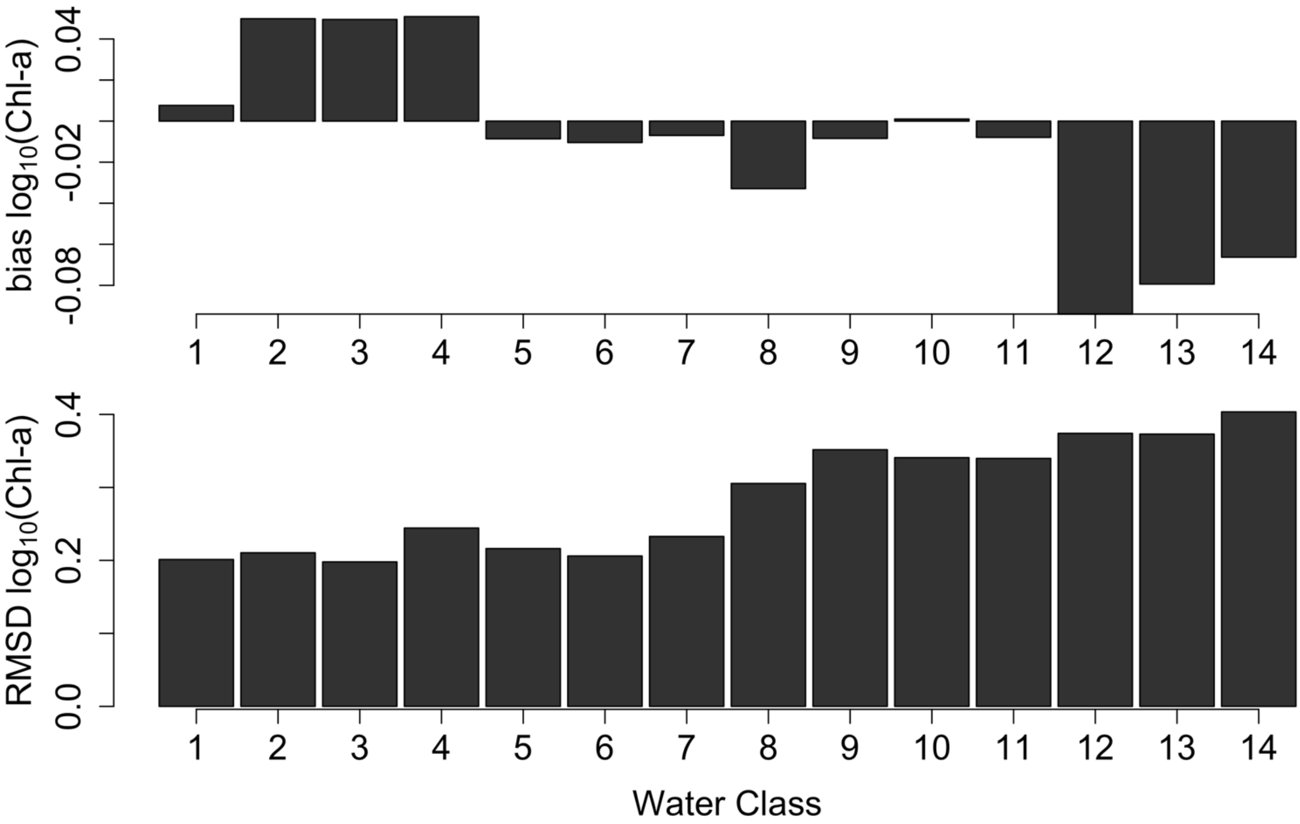

Figure 2 Metrics of product performance (bias and RMSD) across water types.

Table 11 Summary of algorithmic requirements

Algorithmic requirements	Source
Ability to implement POLYMER and alternative aerosol atmospheric processing configurations	SOW-38, SOW-18
minimise the dependency of L2 product quality on water type i.e. open ocean, seas, coastal and inland water	SOW-15

6 Appendices

6.1 Appendix 1: L2gen atmocor2 order of operations

Below is a formatted subset of the atmocor2 code that is used within the NASA l2gen atmospheric correction scheme. To aid clarity, this subset shows only the comments describing what operations and corrections are being calculated in the order that they appear (and maintaining indentation for loops/iteration) in the processor.

```
/* atmocor2() - atmospheric correction, converts Lt -> nLw                        */
/* C-version, September 2004, B. Franz                                            */
/* ---------------------------------------------------------------------------- */
  /* Initialize output values. If any input radiances are negative, just return. */
  /* If any expected channels are negative */

  /* Calculate airmass*/
  /* Remove pre-computed atmospheric effects */
  /* -------------------------------------- */
     /* Pressure correct the Rayleigh optical thickness */
     /* Copy TOA radiance to temp var, eliminate missing bands */
     /* Correct for ozone absorption.  We correct for inbound and outbound here, */
     /* then we put the inbound back when computing Lw.                        */
     /* Do Cirrus correction - subtract off cirrus reflectance from Ltemp */
     /* Add cirrus_opt to input */
     /* Apply smile correction delta */
     /* Apply polarization correction */
     /* Remove whitecap radiance */
     /* Subtract the Rayleigh contribution for this geometry. */
     /* Correct for O2 absorption (replace O2 losses) */
  /* Compute BRDF correction, if not dependent on radiance */
  /* Initialize iteration loop */
  /* new glint_opt usage - a 2 will use the simple TLg from atmocor1 */
  /* Begin interations for aerosol with corrections for non-zero nLw(NIR) */
     /* Initialize tLw as surface + aerosol radiance */
     /*  Compute and subtract glint radiance */
     /* Adjust for non-zero NIR water-leaving radiances using input Rrs
  (or MUMM or IOP model if options chosen)*/
             /* Convert NIR reflectance to TOA W-L radiance */
             /* Avoid over-subtraction */
             /* Remove estimated NIR water-leaving radiance */
     /*  Compute the aerosol contribution */
     /* Subtract aerosols and normalize */
         /* Compute new estimated chlorophyll */
            /* Aerosol determination failure */
     /* If NIR/SWIR switching, do secondary test for turbidity & reset if needed */
  /* If the atmospheric correction failed, we don't need to do more.        */
  /* If we used a NIR Lw correction, we record the tLw as it was predicted. */
  /* Convert water-leaving radiances from band-averaged to band-centered.   */
  /* Switch mean solar irradiance from band-averaged to band centered also. */
  /* Compute f/Q correction and apply to nLw */
  /* Compute final Rrs */
  /* Compute final chl from final nLw (needed for flagging) */
  /*Determine Raman scattering contribution to Rrs*/
```

6.2 Appendix 2: SOW requirements traceability matrix

Tasks	Requirement Reference	Requirement summary	Relevant document and section
Task 1: Scientific review and requirements consolidation	SOW req 1	The study shall establish a Requirements Baseline for Ocean Colour Level 2 algorithm and products, as specified in [AD-1].	• Baseline Requirement Document (Ocean Colour Level 2 Algorithm and Products): Whole Document
	GR R-1	The Contractor shall start with an analysis of EUMETSAT requirements, and derive a consolidated and elaborated requirement set in a Requirements Baseline Document (RB).	• Baseline Requirement Document (Ocean Colour Level 2 Algorithm and Products) • Requirement Baseline Document for Offline Processor: Whole Document
	SOW req 2	The study shall establish a Requirements Baseline for the OC validation methodology, its implementation, and diagnostic datasets, based on this SoW and on the relevant OC-CCI documentation ([RD-21]).	• Requirement Baseline Document for Offline Processor: section 3.5 • Product Validation Plan: sections 2-4.
	SOW req 3	The requirements consolidation shall include the L2 product specifications and scientific requirements of CMEMS and a broader user community. The requirements shall be collected by liaison with CMEMS's OC-TAC and by review of CMEMS, OC-CCI and community documentation.	• Baseline Requirement Document (Ocean Colour Level 2 Algorithm and Products) • Requirement Baseline Document for Offline Processor: Whole Document
	SOW req 4	The OC L2 products Requirements Baseline shall be the reference for the OC validation activity.	• Requirement Baseline Document for Offline Processor: section 3.5 • Product Validation Plan: sections 2-4.

Tasks	Requirement Reference	Requirement summary	Relevant document and section
	SOW req 5	The study shall apply OC-CCI experience in L2 algorithm user requirements and algorithm performance with relevance to S3/OLCI and possible extensions to other EUMETSAT missions.	• Baseline Requirement Document (Ocean Colour Level 2 Algorithm and Products): section 3. • Requirement Baseline Document for Offline Processor: section 3.5 • Product Validation Plan: sections 2-4.
	SOW req 6	The scientific review shall cover state-of-the-art and innovation in OC L2 algorithm developments beyond the current OC-CCI baseline.	• Baseline Requirement Document (Ocean Colour Level 2 Algorithm and Products): section 3.
	GR R-2	A critical review of the state-of-the-art in the scientific field related to the retrievals of the applicable product(s) shall be prepared and presented in the Requirements Baseline Document.	• Baseline Requirement Document (Ocean Colour Level 2 Algorithm and Products): section 2 + 3
	GR R-3	The critical review shall be based on peer-reviewed scientific and technical publications.	• Baseline Requirement Document (Ocean Colour Level 2 Algorithm and Products): section 2 + 3
	SOW req 7	The key products required from the OC-AC shall be: a) water-leaving reflectances at the instrument spatial and temporal sampling (i.e. per pixel) and at all nominal spectral bands relevant to Ocean Colour ([RD-25]), b) corresponding uncertainties at the same sampling and spectral bands.	• Baseline Requirement Document (Ocean Colour Level 2 Algorithm and Products): section 3
	SOW req 8	The key products required from the OC-WR shall be: a) chlorophyll-a concentration and Kd490 at the instrument spatial and temporal sampling (i.e. per pixel) ([RD-25]); b) corresponding uncertainties for both products at the same sampling.	• Baseline Requirement Document (Ocean Colour Level 2 Algorithm and Products): section 3

Tasks	Requirement Reference	Requirement summary	Relevant document and section
	GR R-7	Uncertainty issues shall be specifically addressed for each product.	• Baseline Requirement Document (Ocean Colour Level 2 Algorithm and Products): section 3.4
	GR R-8	Uncertainty characterisation for each product shall follow the approach outlined by QA4EO.	• Baseline Requirement Document (Ocean Colour Level 2 Algorithm and Products): section 3.4
	GR R-9	New products shall be accompanied with per-pixel uncertainties.	• Baseline Requirement Document (Ocean Colour Level 2 Algorithm and Products): section 3.4
	GR R-4	The RB shall include a consolidation and refinement of product requirements on the basis of EUMETSAT requirements and those already identified in the proposal, establishing - a structured set of individual high-level requirements for the applicable product(s) to be generated, - the algorithms to be implemented either in the form of refinements to existing algorithms or as newly developed alternative algorithms, - all input data (i.e. EO and ancillary data) required to generate the data product(s), - as well as methods, test areas, and in-situ observation data sources to be used to validate them. Note: product requirements include scope, physical unit(s), accuracy, precision, spatial and temporal resolution, spatial and temporal coverage, spatial sampling, timeliness, source EO mission(s), reference measurements /observations.	• Baseline Requirement Document (Ocean Colour Level 2 Algorithm and Products): Tables 7-10 • Product Validation Plan: section 2.

Tasks	Requirement Reference	Requirement summary	Relevant document and section
	SOW req 9	The exact physical definition of the water-leaving reflectance product shall be part of the user requirements consolidation. This whole document refers to 'water-leaving reflectances', however it is understood that this parameter can change depending on the requirements.	• Baseline Requirement Document (Ocean Colour Level 2 Algorithm and Products): section 3.1
	SOW req 10	Water-leaving reflectances shall be normalized to the reflectance that would be measured exiting the flat water surface with the Sun at zenith and with the atmosphere absent. They should also be corrected for the directional viewing effects with a BRDF suitable for the specific waters. If the Requirements Baseline requests not to normalize the water-leaving reflectance products, the BRDF shall still be provided per pixel in the L2 product.	• Baseline Requirement Document (Ocean Colour Level 2 Algorithm and Products): section 3.1 and table 7.
	SOW req 11	The scientific review shall take into account the capabilities of S3/OLCI extended spectral resolution, 400 – 1020nm, including the O2 absorption bands ([RD-11]).	• Baseline Requirement Document (Ocean Colour Level 2 Algorithm and Products): section 3.1 and table 7.
	SOW req 12	OC System Vicarious Calibration needs shall be included in the review ([RD-26]).	• Baseline Requirement Document (Ocean Colour Level 2 Algorithm and Products): table 1 and table 9.
Task 2: Algorithm development	SOW req 13	The Requirements Baseline for the prototype processor and associated validation methodology shall be implemented, specifically for S3/OLCI (both Sentinel 3A and 3B).	• Baseline Requirement Document (Ocean Colour Level 2 Algorithm and Products): table 8.
	GR R-5	The extended global retrieval algorithms for the applicable product(s) shall specifically address designated area(s) as per the Requirements Baseline, as well as be applicable for use with the applicable satellite/instrument(s).	• Baseline Requirement Document (Ocean Colour Level 2 Algorithm and Products): Section 3.3 and table 8.

Tasks	Requirement Reference	Requirement summary	Relevant document and section
	SOW req 14	The ATBD shall provide the detailed description of the algorithms applied in the implementation of the prototype.	• ATBDs (SVC, Blending, in-water algorithms, atmospheric correction).
	GR R-43	The contents of ATBD documents shall be as follows: -Product Overview -Product Description -Product Requirements -Scientific state-of-the-art -Satellite Instrument Description -Assessment of Instrument Benefits and Capabilities wrt the Product -Algorithm Description -Processing Outline -Algorithm Input -Theoretical Descrition (Physical and Mathematical) -Algorithm Output -Performance Estimates (Test Data Description, Sensor Effects, Retrieval Errors) -Practical Considerations (High-Level Description of Prototyped Software, Numerical Computation Considerations, Programming and Procedural Considerations, Quality Assessment and Diagnostics, Exception Handling) -Validation -Assumptions and Limitations -Performance Assumptions -Potential Improvements	• ATBDs (SVC, Blending, in-water algorithms, atmospheric correction).
	GR R-6	The format of the output products shall be defined in the Product Specification Document (PSD).	• PSD has been incorporated into the IODD.
	SOW req 15	The OC algorithm shall minimize the dependency of L2 product quality on water type i.e. open ocean, seas, coastal and inland waters, atmospheric conditions (e.g. maritime and non-maritime/absorbing aerosols), and on solar and viewing geometries.	• Baseline Requirement Document (Ocean Colour Level 2 Algorithm and Products): Section 3.3

Tasks	Requirement Reference	Requirement summary	Relevant document and section
	SOW req 16	The OC algorithm shall be scientifically and technically designed to be modular and extensible. Future extensions (beyond this study) shall be considered in the algorithm and prototype design and architecture. Individual algorithm components shall be in distinct algorithm modules and shall allow for inclusion of updated and new modules and extensions to geostationary, e.g. MTG/FCI and MSG/SEVIRI, and polar missions, e.g. EPS-SG/3MI.	• Baseline Requirement Document (Ocean Colour Level 2 Algorithm and Products): Section 3.3, 4.2 and table 9.
	GR R-11	The coding of the algorithms shall be suitable for integration into EUMETSAT's Offline environment.	• Baseline Requirement Document (Ocean Colour Level 2 Algorithm and Products): Section 4.
	GR R-12	The coding shall be modular, clearly readable, commented, portable, as much generic as possible; any use of libraries with background IPRs and/or under commercial licence shall be submitted to prior EUMETSAT written approval.	• Baseline Requirement Document (Ocean Colour Level 2 Algorithm and Products): Section 4.
	GR R-13	An installation and user manual shall be provided with the software delivery, see [R- 46] for the specification of the contents.	NA
	GR R-46	The contents of the installation and software user manual shall be as follows: -Purpose of the software -Contents of the software delivery -Operational environment (Hardware configuration, software configuration, Operational constraints, External dependencies) -Installation (setup and initialisation, verification) -Operational manual (General operational principles and getting started, Normal operations, Error conditions, Recovery operations)	NA
	SOW req 17	The algorithm development process shall be planned such that it includes iterations on the product generation and algorithm/product validation in order to narrow down on the most accurate algorithm for S3/OLCI.	• We are not proposing to develop new algorithms within this project. We will test existing candidates developed by others. See

Tasks	Requirement Reference	Requirement summary	Relevant document and section
			Requirement Baseline Document for Offline Processor.
	SOW req 18	The OLCI version of the POLYMER algorithm ([RD-17]) should be considered to be incorporated into the processing chain. Note 1: if POLYMER is implemented, an adequate license shall be procured by the Study Team, and this shall include allowance for EUMETSAT to make full use of it for prototyping, modification and testing. Note 2: EUMETSAT does not mandate the use of POLYMER in this study, but the performance of the prototype must be at least as good as OC-CCI or make best use of OC-CCI experience.	• Baseline Requirement Document (Ocean Colour Level 2 Algorithm and Products): Table 9 and section 5.1.2
	SOW req 19	The algorithm prototype shall accept on input radiometric gains coming from System Vicarious Calibration (SVC) [RD-26] or a similar procedure.	• Baseline Requirement Document (Ocean Colour Level 2 Algorithm and Products): Figure 1, table 1 and table 9.
	SOW req 20	The OC prototype shall include post-processing of the outputs of the OC-AC module, i.e. normalisation of the water-leaving reflectance.	• Baseline Requirement Document (Ocean Colour Level 2 Algorithm and Products): Figure 1, table 1 and table 9.
	SOW req 21	The algorithm development shall include an interface workshop with EUMETSAT, supported by the OC-AC Aerosol Study.	NA
	SOW req 22	The Interface workshop shall aim at the consistency between the Alternative OC-AC Aerosol module IODD, delivered by EUMETSAT and the prototype IODD.	NA

Tasks	Requirement Reference	Requirement summary	Relevant document and section
	SOW req 23	The IODD shall cover the formats applied within this Study to: a) L2 Products b) Inputs and outputs of the intermediate modules (including the OC-AC Module, and others to be agreed with EUMETSAT) c) Diagnostic data	• IODD: Whole document
	GR R-10	Each product's algorithms shall be described in detail in an Input Output Data Definition Document (IODD) and an Algorithm Theoretical Basis Document (ATBD) and a Detailed Processing Model (DPM) document. Note: ATBD contents shall be as per [R- 43]. Note: IODD contents shall be as per [R- 44]. Note: DPM contents shall be as per [R- 45].	• IODD • ATBDs (SVC, Blending, in-water algorithms, atmospheric correction)
	SOW req 24	The L2 product definition in the IODD shall include the file format, per-pixel flags, ancillary information and standard and additional diagnostic outputs.	• IODD: Whole document
	GR R-44	The contents of IODD documents shall be as follows: -List of input file types, auxiliary inputs data file types, output file types: -For each file type: -naming convention -data format description	• IODD: Whole document
	SOW req 25	Per-pixel flags shall include at minimum: a) relevant flags carried from the L1B product, e.g. land and water classification, inland water subset of the water classification, b) cloud flag, c) flags indicating intermediate retrieval status, e.g. medium glint, absorbing aerosols, water type classification, d) flags indicating retrieval quality levels, e.g. atmospheric correction warning, chlorophyll failure.	• Baseline Requirement Document (Ocean Colour Level 2 Algorithm and Products): Section 3.2. • IODD: Whole document
	SOW req 26	The prototype shall be able to output diagnostic variables included in the Product Validation Plan, in addition to the key products.	• Baseline Requirement Document (Ocean Colour Level 2 Algorithm and

Tasks	Requirement Reference	Requirement summary	Relevant document and section
			Products: Section 3.1, Table 7.
	SOW req 27	The set of diagnostic variables to be produced in one run of the prototype shall be user configurable. Examples of variables include: (TOA radiances, Rayleigh reflectances, aerosol reflectances or simliar, including the Rayleigh-aerosol contribution if relevant, all transmittances, reflectances related to surface and environement [sun glint, white caps], aerosol [e.g aerosol reflectances, Rayleigh aerosol multi-scattering, aerosol module type], quantitites related to the decoupling between the water and the atmosphere or BPC, BRDF values, all pixel geometries) The radiances and reflectances shall be provided at all instrument spectral bands except at those not suitable for Ocean Colour retrievals.	• Requirement Baseline Document for Offline Processor: Section 3.5.2
	SOW req 28	The round-robin intercomparison and validation shall be able to take into account the diagnostic variables as well as the key products.	• Requirement Baseline Document for Offline Processor: Section 3.2.2
	SOW req 29	The prototype shall be able to run in test modes accepting geophysical parameters which are predefined on input. As a minimum the following three options shall be available: a) predefined on input water-leaving reflectances, and provision on output of corresponding TOA radiance (VIS SVC mode), b) predefined on input aerosol (e.g. AOT, Ångström exponent or model type) and provision on output of corresponding TOA radiances (NIR SVC mode), c) predefined on input aerosol properties (e.g. AOT, Ångström exponent or model type) and provision on output of corresponding water-leaving reflectances.	• Requirement Baseline Document for Offline Processor: Section 3.4.2
	SOW req 30	The SVC mode (Req-29) shall apply the same algorithm modules as in the standard (i.e. forward) processing and inverted modules where required.	The SVC module cannot be run in inverse mode.

Tasks	Requirement Reference	Requirement summary	Relevant document and section
	SOW req 31	The OC algorithm prototype shall be as generic as possible wrt algorithms and missions. For example, it shall make use of external look-up-tables and parametrization files allowing for configuration without code modifications, where possible.	• Baseline Requirement Document (Ocean Colour Level 2 Algorithm and Products): Figure 1, table 1.
	SOW req 32	The prototype shall be able to process S3/OLCI L1B files which do not cover the full instrument processing dissemination units, i.e. minifile extractions, and shall be able to process and output a user selected region of interest of a L1B input product.	• Baseline Requirement Document (Ocean Colour Level 2 Algorithm and Products: Section 4.2, Table 9.
	SOW req 33	The input for the OC algorithm prototype shall be L1B calibrated and geolocated TOA radiances per pixel / detector ([RD-25]).	• Baseline Requirement Document (Ocean Colour Level 2 Algorithm and Products: Section 4.2, Table 10. • IODD
	SOW req 34	The following additional information shall be assumed to be included in the L1B products or provided with L1B products: a) pixel surface classification: land, water and fresh inland water. b) instrument radiometric and spectral information, such as wavelength, full width at half maximum (FWHM) and solar flux per detector. Spectral response functions per detector are typically provided separately ([RD-11]). c) latitude, longitude, altitude per pixel / detector and time stamp of data rows. d) meteorological values, typically at tie points, including total ozone, total columnar water vapour, humidity, atmospheric temperature profiles at tie pressure levels, horizontal wind at 10m altitude, sea level pressure. e) bright pixel flag in OLCI L1B products.	• Baseline Requirement Document (Ocean Colour Level 2 Algorithm and Products: Section 4.2, Table 10. • IODD

Tasks	Requirement Reference	Requirement summary	Relevant document and section
	SOW req 35	The prototype processor shall be designed so that it could be suitable for near-real time processing with regards to the speed.	• Baseline Requirement Document (Ocean Colour Level 2 Algorithm and Products: Section 4.1, Table 9.
	SOW req 36	The study shall perform the integration of the Alternative OC-AC Aerosol module in its reference OC processing chain.	• Baseline Requirement Document (Ocean Colour Level 2 Algorithm and Products: Section 4.1, Table 9.
	SOW req 37	Integration testing of the Alternative OC-AC Aerosol module shall be performed according to the PVP.	• PVP: section 2.2
	SOW req 38	The prototype shall offer a choice of processing with the reference OC-AC module or the Alternative OC-AC Aerosol module (e.g. by a simple configuration parameter).	• Baseline Requirement Document (Ocean Colour Level 2 Algorithm and Products: Section 4.2, Table 9.
Task 3: Product generation	SOW req 39	The study shall assemble a set of test input and reference data fulfilling all of the needs of the Product Validation Plan.	• PVP: Section 2
	GR R-16	The specification of the diagnostic datasets shall be agreed with EUMETSAT in advance.	• PVP: Section 2
	SOW req 40	The definition of diagnostic datasets shall be provided in the Product Validation Plan (PVP).	• PVP: Section 2
	GR R-14	The input dataset from the applicable satellite/instrument(s)/product(s), and the necessary auxiliary data, shall be quality checked prior to use.	• Baseline Requirement Document (Ocean Colour Level 2 Algorithm and Products: Section 4.2
	SOW req 41	The study shall process test input data and generate product and additional diagnostic variables as per the Product Validation Plan, using the reference prototype.	• PVP: Section 2

Tasks	Requirement Reference	Requirement summary	Relevant document and section
	GR R-17	A complete reprocessing of selected data products (=data record generation) for a defined area and time shall be agreed with EUMETSAT and performed, validated and provided in the netCDF CF format [RD-1].	• PVP: Section 3
	SOW req 42	The study shall process test input data and generate product and additional diagnostic variables as per the Product Validation Plan, using the Alternative OC-AC Aerosol module.	• PVP: Section 3
	GR R-15	Processing of diagnostic datasets for the applicable satellite/instrument(s) shall be performed, validated and provided in the netCDF CF format.	• PVP: Section 2
Task 4: Validation and round-robin inter-comparisons for S3/OLCI	SOW req 43	The study shall implement the verification and validation framework as per the requirements baseline for the OC validation methodology.	• Requirement Baseline Document for Offline Processor: Section 3.5
	SOW req 44	The verification and validation framework shall be provided for both the algorithm (including algorithm modules and parametrizations) and the products.	• Requirement Baseline Document for Offline Processor: Section 3.5 • PVP: Section 4
	SOW req 45	The study shall establish the verification and validation approach applicable for any OC-AC Aerosol module to be included in a round robin intercomparison.	• Requirement Baseline Document for Offline Processor: Section 3.2
	GR R-24	The study shall build on the validation experiences made during past projects.	• Requirement Baseline Document for Offline Processor: Section 3.2, 3.3.
	SOW req 46	The verification and validation approaches shall be documented in the Product Validation Plan (PVP).	• PVP: Whole document
	GR R-21	A Product Validation Plan (PVP) shall be provided describing the validation objectives, validation criteria, validation data and test approaches. Note: PVP contents shall be as per [R- 47]	• PVP: Whole document

Tasks	Requirement Reference	Requirement summary	Relevant document and section
	GR R-47	The Product Validation Plan shall contain the following information as a minimum: -Validation objectives -Validation criteria -Validation data -Validation team and responsibilities -Validation methodology -Schedule -Expected outputs	• PVP: Whole document
	SOW req 47	The PVP shall define key algorithm and product performance indicators subject of the consolidated requirements from the RB, including the uncertainties of S3/OLCI water-leaving reflectance, chlorophyll and Kd490 retrievals across different water and atmospheric conditions.	• PVP: Sections 4 and 5.
	SOW req 48	The PVP should consider the evaluation of additional diagnostic variables as per Req-27.	• PVP: Section 2.3.
	GR R-18	The algorithm shall be validated with respect to accuracy, as well as with respect to possible systematic and structural random errors following QA4EO guidelines.	• Baseline Requirement Document (Ocean Colour Level 2 Algorithm and Products): section 3.4, table 7.
	GR R-19	Product validation shall be performed using documented community recognised approaches/methodologies as outlined by the QA4EO guidelines.	• Baseline Requirement Document (Ocean Colour Level 2 Algorithm and Products): section 3.4, table 7.
	GR R-22	Product validation shall be performed using the latest versions of the selected datasets in order to assess benefits of new approach in terms of accuracy.	• PVP: Section 2.
	SOW req 49	The PVP shall identify all the required diagnostic datasets.	• PVP: Section 2.

Tasks	Requirement Reference	Requirement summary	Relevant document and section
	SOW req 50	The study shall review the EUMETSAT provided Product Validation Plan for the Alternative OC-AC Aerosol module, in particular identifying the tests (and corresponding diagnostic data sets) to be applied after the integration and in the round robin intercomparison.	• PVP: Section 2.
	SOW req 51	The PVP shall incorporate a relevant subset of the Alternative OC-AC Aerosol module validation tests.	• PVP: Section 2.
	SOW req 52	The diagnostic data sets shall include global and seasonal S3/OLCI time series, statistically representative of atmospheric and water conditions in open ocean, coastal and inland waters.	• PVP: Section 2.
	SOW req 53	The diagnostic datasets should include S3/OLCI test cases covering : a) various aerosols, i.e. coarse scattering sea salt aerosols, ultra-violet/deep-blue absorbing dust, and fine weakly and strongly deep-blue/VIS absorbing aerosols; b) various types of phytoplankton, and c) various contributions of absorbing and scattering water constituents (i.e. coloured dissolved matter and particulates); according to the scope of the algorithm as defined in the Requirements Baseline.	• PVP: Section 2.
	SOW req 54	The diagnostic datasets should include reference validation data, i.e. high-quality *in situ* measurements for open ocean, seas, coastal and inland waters, and the various types of aerosols, phytoplankton, and absorbing and scattering water constituents, according to the scope of the algorithm.	• PVP: Section 2.
	GR R-20	Validation data sets shall be identified in advance and agreed with EUMETSAT. They may include in situ observations and/or comparable products from other missions.	• PVP: Section 2 and 4.
	GR R-23	Comparisons shall also be performed side-by-side with existing EUMETSAT and non-EUMETSAT satellite products, when applicable, in order to assess benefits of the new approach in terms of accuracy.	• PVP: Section 2 and 4.

Tasks	Requirement Reference	Requirement summary	Relevant document and section
	SOW req 55	The study shall include diagnostic dataset workshop with EUMETSAT, supported by the OC-AC Aerosol Study.	NA
	SOW req 56	The diagnostic dataset workshop shall aim at identifying a relevant subset of the Alternative OC-AC Aerosol module diagnostic dataset, for incorporation in this study's diagnostic datasets.	NA
	SOW req 57	The round-robin intercomparison shall be applied to the reference chain (see Req- 15) and to the Alternative OC-AC Aerosol module.	• Requirement Baseline Document for Offline Processor: Section 3.2
	SOW req 58	The round robin intercomparison shall be able to reprocess test cases from the Alternative OC-AC Aerosol module validation and compare them with EUMETSAT provided data.	• Requirement Baseline Document for Offline Processor: Section 3.2
	SOW req 59	Verification and validation results in the Product Validation and evolution Report (PVR) shall report the performance of the OC algorithms against the product requirements in the RB document.	• PVR
	GR R-25	A Product Validation and evolution Report (PVR) shall be prepared describing the findings. Note: PVR contents shall be as per [R- 48]	• PVR
	GR R-26	The Product Validation and evolution Report (PVR) shall contain full details of tests, evaluation and their results, stating the compliance against the agreed product requirements.	• PVR
	GR R-48	The Product Validation and Evolution Report shall contain the following information as a minimum: -Results of the validation activities -Analysis and evaluation of the results -Open points and recommendations for additional validation activities -Recommendations for evolution of the product -Conclusions	• PVR
Generated Datasets	GR R-49	All deliverable datasets and data files shall be provided in netCDF CF format.	• IODD

Tasks	Requirement Reference	Requirement summary	Relevant document and section
	GR R-50	The diagnostic datasets shall be made available on a FTP server by the contractor for extended validation by selected researchers to be agreed with EUMETSAT.	NA (data delivery not document)
	GR R-51	EUMETSAT shall provide the input data (including such non-specific auxiliary files as Digital Elevation Model, forecast or analysis fields…) required for the project.	• Baseline Requirement Document (Ocean Colour Level 2 Algorithm and Products): section 4.2, table 10. • IODD
	GR R-52	Product format definition for the provided input data shall be provided by EUMETSAT.	• IODD