Copernicus Space Component Sentinel Optical Mission

Performance Cluster

Sen2Water Requirements Document

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Changes Log

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1.0	11/10/2023	First version

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1 Introduction

1.1 Purpose and scope

This requirements document defines the software requirements for the Sen2Water processor. It is based on the requirements of the Statement of Work [Sen2Water CR 2022]. And it collects the requirements of the 100m resolution coastal water quality service (HR-OC) within the Copernicus Marine Service and of the 100m resolution lakes water quality service within the Copernicus Global Land Service.

This requirements document is in turn the input to a design of Sen2Water, documented in an Input Output Data Definition [MSI L2 IODD 2023], an Algorithm Theoretical Basis Document [MSI L2 ATBD 2023], and a Software Design Definition [MSI L2 SDD 2023].

1.2 References

The following documents are referenced in this document.

Document ID	Description	Version
Sen2Water CR 2022	OPT-MPC Change Request ESA-EOPG-EOPGMQ-CR-15, ESA, 20.12.2022	1.0
S2-PDGS-TAS-DI-PSD	Sentinel-2 Products Specification Document, S2-PDGS-TAS-DI-PSD, ESA	14.9
CEOS ARD 2021	CEOS Analysis Ready Data Product Family Specification Template, https://ceos.org/ard/files/PFS/CEOS-ARD_PFS_Template.docx, 22.10.2021	1.0
Sentinel-3 Water Mask 2015	Wevers, Jan; Brockmann, Carsten; Kirches, Grit; Stelzer, Kerstin. Sentinel-3 Land Water Mask. Technical Note, https://earth.esa.int/eogateway/documents/ 20142/37627/S3_LandWaterMask_v1_2.pdf/5de313b1-95dd-e9cd-152e-0605ae6a1efd , Brockmann Consult GmbH, 14.08.2015	1.2
MSI L2W IODD 2023	Sen2Cor and Sen2Water Input Output Data Definition Document, OMPC.BC.RD-MSI-L2, Optical Mission Performance Centre, ESA, October 2023	1.0
MSI L2 ATBD 2023	Sen2Cor and Sen2Water Algorithm Theoretical Basis Document, OMPC.TPGZ-BC.ATBD-MSI-L2, Optical Mission Performance Centre, ESA, October 2023	1.0
MSI-L2-SDD 2023	Sen2Cor and Sen2Water Software Design Document, OMPC.TPGZ-BC.SDD-MSI-L2, Optical Mission Performance Centre, ESA, October 2023	1.0

1.3 Acronyms

The following acronyms are used within this document:

Acronym	Description
ATBD	Algorithm Theoretical Basis Document
CAMS	Copernicus Atmosphere Monitoring Service

Acronym	Description
CGLS	Copernicus Global Land Service
CHL	Chlorophyll-a
CR	Change Request
ESA	European Space Agency
HR-OC	High Resolution Ocean Colour
IODD	Input Output Data Definition
L1C	Level 1C
L2	Level 2
L2A	Level 2A
L2W	Level 2 Water
MSI	MultiSpectral Instrument
OMPC	Optical Mission Performance Centre
PDGS	Payload Data Ground Segment
RD	Requirements Document
SAFE	Standard Archive Format for Europe
SDD	Software Design Document
SNAP	Sentinel Application Platform (and Sentinel Toolboxes)
SPM	Suspended particulate matter
TUR	Turbidity

1.4 Document overview

After this formal introduction

Section 2 provides an overview over the coastal water quality service of the Copernicus Marine Service and the lakes water quality service of the Copernicus Global Land Service. It characterizes Sen2Cor that is combined with Sen2Water into a Level 2 processor that creates a Level 2A data product extended by aquatic reflectances.

Section 3 comments the input requirements of the Change Request [Sen2Water CR 2022].

Section 4 refines Change Request requirements for major design decisions how AC algorithms are combined, how ocean and inland water is discriminated, where dynamic identification of water or land pixels is applied, and how the Level 2A output shall look like.

Section 5 collects requirements of the coastal water quality service and of the lakes water quality service that shall take advantage of the extended Level 2A product with the aquatic reflectances.

Section 6 identifies requirements for the PDGS integration

2 Sen2Water Overview

The Sen2Water processor combines the pre-processing of two complementary services, the coastal water quality service processing for Copernicus Marine Service and the lakes water quality service processing for the Copernicus Global Land Service CGLS. The two services use different chains for pre-processing that are described in two subsections. Sen2Cor operationally generates the former L2 data product and will be part of the target processing chain as well. Sen2Cor and the target chain are described in the next two subsections. The output data product of Sen2Water and the combined chain are introduced in the last subsection.

2.1 Coastal water quality service processing chain heritage

The HR-OC processing chain (Figure 2-1) generates water quality parameters TUR, SPM, CHL, and a few other parameters from Sentinel-2 MSI L1C inputs. It does so for all European coastal ocean waters in a 20 km stripe from the coastline. The pre-processing chain combines C2RCC for clear water and ACOLITE for turbid water with blending in transition zones.

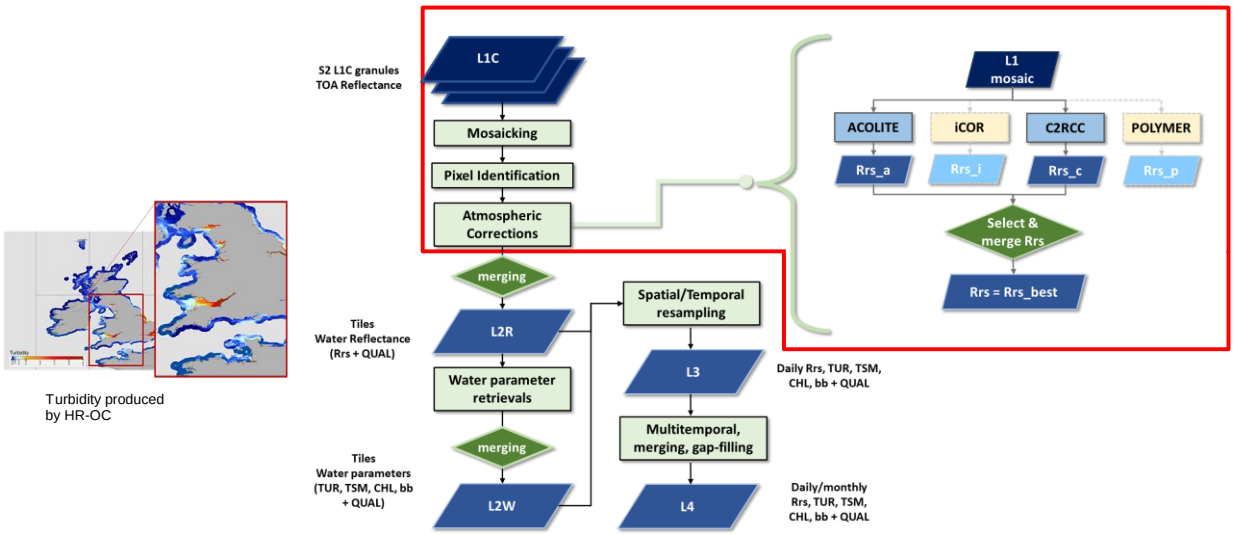

Figure 2-1: Coastal water quality service pre-processing chain with S2Resampling, Idepix, C2RCC, ACOLITE

In addition to C2RCC and ACOLITE, SNAP S2Resampling generates 60 m inputs with carefully determined observation angles. Granules are combined into larger mosaics before processing. A static mask is used to distinguish coastal water, coastal land, and other areas. The SNAP Idepix processor identifies cloud, cloud shadow, ice, and dynamically re-classifies pixels as water or non-water in the coastal zones. Blending generates the AC output and a common set of combined flags.

2.2 Lakes water quality service processing chain heritage

The inland water processing chain shown in Figure 2-2 generates water leaving reflectances, the trophic state index based on chlorophyll concentration and turbidity, from Sentinel-2 MSI L1C inputs. It does so for a set of currently 225 Sentinel-2 granules distributed over Europe and Africa. The pre-processing chain uses POLYMER for atmospheric correction.

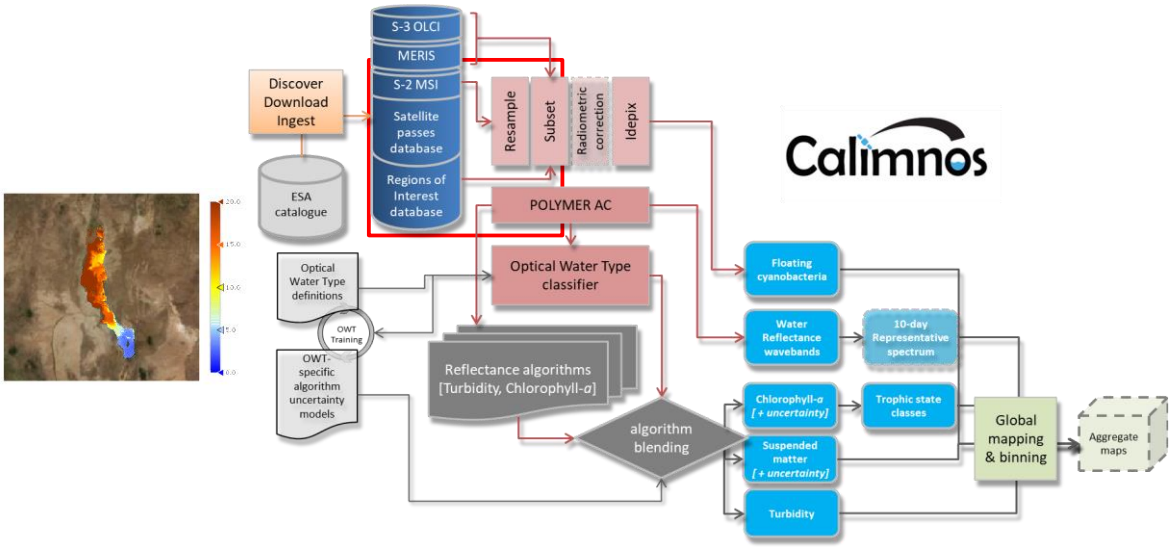

Figure 2-2: CGLS inland water pre-processing chain with S2Resampling, Idepix, POLYMER

Prior to POLYMER, SNAP S2Resampling generates 60m inputs with corrected observation angles. The SNAP Idepix processor distinguishes clear water dynamically from cloud, and other pixel classes.

2.3 Sen2Cor heritage

Sen2Cor is a processor for Sentinel-2 Level 2A product generation and formatting; it performs the atmospheric correction and terrain correction of Top-Of-Atmosphere Level 1C input data. The sequence of processing steps is shown in Figure 2-3. Sen2Cor creates Bottom-Of-Atmosphere, i.e. surface reflectance images; and additionally, Aerosol Optical Thickness-, Water Vapor-, Scene Classification Map and Quality Indicators for cloud and snow probabilities. Its output product format is equivalent to the Level 1C User Product: JPEG 2000 images, with three different resolutions, 60, 20 and 10 m.

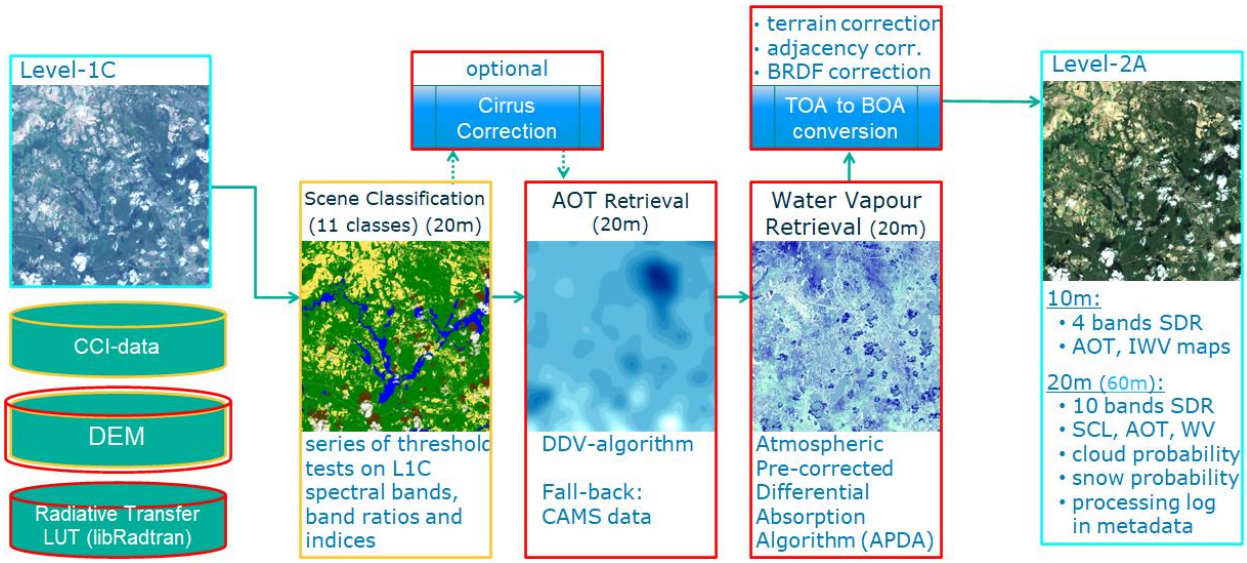

Figure 2-3: Overview of Sen2cor processing chain

Sen2Cor is designed to perform atmospheric correction of land surfaces. It is used operationally since December 2018 to generate official L2A products. Since January 2022, Sen2Cor can use aerosol information from auxiliary CAMS (Copernicus Atmosphere Monitoring Service) when it is not possible to retrieve aerosol content from the scene itself. It is applied to both, land pixels and water pixels.

2.4 Target processing chain configuration

There are two target configurations: Sen2Water stand-alone and the new Level 2A processor. Sen2Cor exists as stand-alone module as well. the combined Level 2A processor configuration is shown in Figure 2-4. The combined processor processes L1C in PDI format.

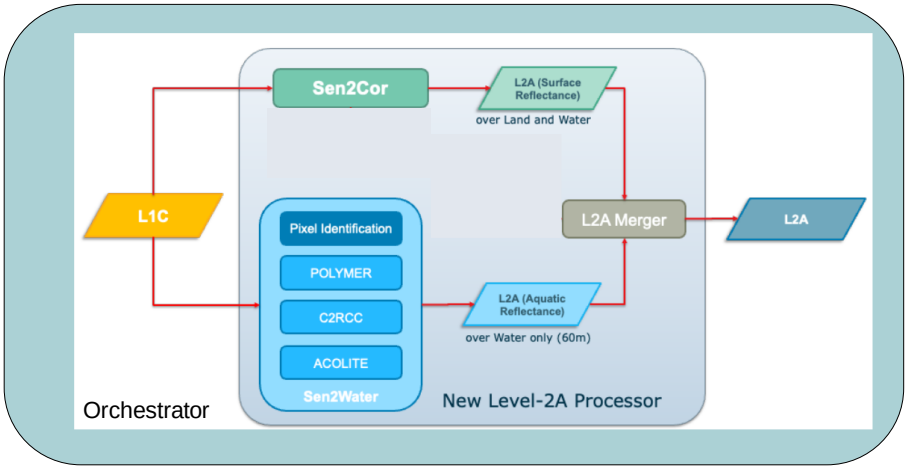

Figure 2-4: New Level 2A processor with Sen2Cor and Sen2Water

Sen2Water in stand-alone configuration processes L1C data in end user product format (EUP). The Sen2Water processor comprises S2Resampling, Idepix and three different AC processors that are applied to water areas. Selection and blending combine their outputs into the L2W aquatic reflectance data product.

The new Level-2A processor combines Sen2Cor and Sen2Water. They can be run concurrently. A merger creates the final output that includes both the generic and aquatic reflectances and respective flags.

2.5 Target output data product

Sen2Water as stand-alone data processor generates an output data product L2W in 60 m with atmospherically corrected aquatic reflectances for water pixels. Bands required for in-water retrieval are B1, B2, B3, B4, B5, B6, B7, and B8A. The other MSI bands will be corrected as well for verification purposes. It will cover ocean and inland water bodies. L2W is provided in Sentinel-2 granules of 1830 x 1830 pixels. Additional flags further characterize the quality of the retrieval. L2W will be provided as NetCDF4 data file with CF-compliant metadata.

The combined processor generates the Sen2Cor output enriched by the L2W, i.e. with aquatic reflectances and flags for water areas in 60 m in addition to the outputs of Sen2Cor. The L2W content is part of the SAFE product format.

3 Understanding of the Change Request requirements

This chapter comments the input requirements of the Change Request [Sen2Water CR 2022]. These requirements convey expectations of ESA on the Sen2Water processor. They are commented here in four tables with a first level of assessments how they will be fulfilled. For important algorithmic decisions the next section characterize with more detailed derived requirements how the Change Request requirement can be fulfilled. There are references to respective subsections in the comment column of the respective SoW requirement.

3.1 The output generated

Table 3-1: Software requirements addressing the output generated

No	Requirement summary	Comment
[REQ-01]	processor shall integrate Sen2Cor, Sen2Water, and an L2A_merger.	software design
[REQ-02]	single comprehensive Level-2A product with surface reflectance and aquatic reflectance layers, as simple addition to current L2A	product definition
[REQ-04]	algorithm selection depending on kind of water (clear, turbid)	Sen2Water algorithm definition (may be partially in conflict with continuity requirement of the services)
[REQ-05]	aquatic reflectance only over water	Sen2Water algorithm definition
[REQ-06]	static mask for inland and open waters, buffer for dynamic change	Sen2Water algorithm definition, see dynamic water identification in section 4.1 and 4.2
[REQ-07]	aquatic reflectance for all MSI bands except B10	Product definition, Sen2Water algorithm definition, see restriction of existing water processors in section 4.3
[REQ-13]	Level-2A processor can use dynamic aux in L1C. Additional aux shall be communicated.	Sen2Water algorithm definition, external dynamic auxiliary data used in current services see section 4.5
[REQ-14]	Sen2Water quality indicators in QI_DATA and in summary metadata	Sen2Water product definition
[REQ-16]	Sen2Water shall meet CEOS ARD PFS threshold requirements	product definition
[REQ-23]	UTC in metadata and logs	software implementation

In this first set of requirements REQ-04 is fulfilled for ocean products with a selection of processors depending on a proxy band ratio expression for turbidity. There currently is no such selection of processors for lakes in the lake water quality service. For lakes only what is available in POLYMER to

process turbid and clear waters serves this requirement. If service continuity is considered more important as this new requirement, then this approach is initially kept for Sen2Water. A later evolution as investigated in the CERTO project may lead to a different approach, similar to the one applied for ocean waters. Sen2Water shall be prepared for that.

There are separate subsections below that refine requirements on land water masks, bands to be included, and auxiliary data used.

The CEOS ARD PFS template [CEOS ARD 2021] defines threshold requirements for metadata to be included in the product. Some of the requirements, if applied to the L2W stand-alone product require that metadata is transferred from the L1C input into the L2W.

3.2 The way of processing

Table 3-2: Software requirements addressing the way of processing

No	Requirement summary	Comment
[REQ-03]	selection of surface reflectance and/or aquatic reflectance by configuration	L2 processor parameters and workflow definition
[REQ-08]	Sen2Water stand-alone	Sen2Water stand-alone configuration, calling convention, runtime structure
[REQ-09]	parallel (independent) execution of Sen2Cor and Sen2Water	L2 processor workflow definition
[REQ-10]	use internal parallelisation	Sen2Cor elements, workflow definition, Sen2Water elements, workflow definition
[REQ-11]	Level-2A processor PDGS mode	L2 processor PDGS integration
[REQ-12]	GIP_PROBA2 to define processing baseline	L2 processor parameters
[REQ-15]	Integration into PDGS	L2 processor PDGS integration
[REQ-17]	Level-2A processor shall manage GIPP and their applicability dates	L2 processor PDGS integration
[REQ-18]	Open-source algorithms, GitHub repositories	Sen2Cor elements, Sen2Water elements, L2 processor repository

Most of the second set of requirements are on the level of the combined processor, its control and its workflow. Parallelisation is also relevant for Sen2Water's internal workflow.

3.3 Environment and performance

Table 3-3: Requirements addressing performance and verification

No	Requirement summary	Comment
[REQ-19]	Intel-based platform, CentOS	operating system dependent elements
[REQ-20]	40 minutes per tile for Sen2Water	internal parallelisation

No	Requirement summary	Comment
[REQ-21]	Input variability land, inland, coastal, ocean	test
[REQ-22]	Cloud platform, compatible with Sentinel-2 Product Unit Definition and Metadata ICD	test
[REQ-24]	installation target folder	Sen2Water stand-alone

The third set of requirements address the platform performance. Overall runtime is related to parallelisation.

3.4 Scientific validation

Table 3-4: Requirements addressing scientific validation

No	Requirement summary	Comment
[REQ-25]	Sen2Water scientific validation	validation
[REQ-26]	Variability of products for validation (latitudes, inland, open waters)	validation data
[REQ-27]	Time series of one year for validation, e.g. ACIX-Aqua dataset	validation data

The fourth set of requirements characterize the validation that is expected.

4 Sen2Water design decisions

This chapter refines Change Request requirements for major design decisions. Major design decisions are the combination of AC algorithms and the discrimination of ocean and inland water, dynamic identification of coastal land or water pixels, the bands and quality masks to be included into the Sen2Water output, and the format of the output, also when included in the Level 2A product.

4.1 Global (ocean) water mask

There are different processors applied to coastal ocean water in the coastal water quality service and to inland water in the lakes water quality service. One of the requirements of services is continuity (see section 5). To meet these two service requirements Sen2Water needs a way to distinguish ocean water from inland water. This must be a geographic distinction because other features, in particular turbidity, may vary. (If the criterion to switch the algorithm were on turbidity the algorithm applied to turbid lakes would change compared to the current lakes water quality service.)

The approach characterised by the following requirements uses a global land-ocean-inland water mask as input. The coastal water quality service has derived its mask from a coastal lines mask in a 1:1 million scale from the Geoportal of the European Commission (EUROSTAT) (https://ec.europa.eu/eurostat/web/gisco/geodata/reference-data/administrative-units-statistical-units). While HR-OC has processed a 20 km stripe of coastal water the restriction to 20 km shall be dropped for Sen2Water.

From such a static mask a derived mask can be computed that contains buffer areas in addition. This derived mask will be combined with dynamic pixel identification to detect changes in both directions to account for inaccuracies in the land-water mask and to dynamic coastlines.

Table 4-1: Requirements for ocean-inland water discrimination

[RD-100]	A global water mask used as input for a derived mask shall distinguish ocean from land and from inland water. The mask will be used to derive a mask with 60m resolution. The resolution and accuracy shall be adequate for this purpose (see paragraph below). It is considered an advantage if the mask selected is consistent with masks used for other missions, in particular for Sentinel-3 OLCI.
[RD-105]	The mask will be buffered in both directions to define a zone for dynamic (ocean) water identification. It shall be ensured that buffering does not lead to leakage of the ocean mask into lakes close to the coast.
[RD-110]	The derived mask shall be projected to all Sentinel-2 granules Tnnxxx in UTM projection at 60m.
[RD-115]	The derived mask shall be compared to and if necessary corrected with the HR-OC mask over Europe.
[RD-120]	The Sentinel-3 Land Water Mask [Sentinel-3 Water Mask 2015] shall be considered as candidate for the input mask.

The mask will be buffered in both directions to define a zone for dynamic (ocean) water identification. Therefore, the global input mask does not need to be accurate at 60m resolution. A coarser mask can still be used. The size of the buffer shall be selected such that it is sufficient for the mask accuracy.

Note that the inland water mask is not necessarily used to distinguish land and water for processing. This can be completely done by dynamic pixel identification, as it is done in the lakes water quality processing chain.

4.2 Dynamic water identification

Table 4-2: Requirements for dynamic water identification

[RD-125]	Dynamic pixel identification shall distinguish at least clear water, clear land, snow/ice, and pixels affected by cloud and cloud shadow.
[RD-130]	Dynamic pixel identification shall be used for all inland water bodies to identify water pixels. This includes pixels in the transition zone between ocean and inland water.
[RD-135]	Dynamic pixel identification shall be used for coastal pixels to re-classify pixels inside the static land mask as water, and to re-classify pixels inside the static ocean mask as land.

4.3 Aquatic reflectance bands

REQ-07 requires that the output contains reflectances of all MSI bands except B10. Only bands up to B8A are relevant for water retrieval. C2RCC atmospheric correction does not correct all bands. The other two algorithms correct all input bands, and they write a B10 that has passed the correction algorithm as well.

[RD-140]	For continuity reasons the superset of all bands provided by the algorithms shall be output of Sen2Water. These are all 13 bands.
[RD-145]	Algorithms that correct only a subset of the bands shall set the values of the other bands to NaN. C2RCC corrects B1, B2, B3, B4, B5, B6, B7, B8A.

The reason to keep all bands in the L2W is that they can be used for quality checks of the atmospheric correction. A reason to drop them is space. A L2W with 8 bands is smaller than a L2W with 13 bands.

4.4 Digital Elevation Model

Different DEMs are in use by the processors of the two services:

- Idepix uses SRTM 1Sec HGT and GETASSE30 for the lakes water quality service, GETASSE30 for the coastal water quality service.
- POLYMER does not use a DEM in the lakes water quality service chain because it uses surface pressure from the dynamic auxiliary data.
- C2RCC uses GETASSE30
- ACOLITE does not use a DEM in the CMEMS HR-OC chain

[RD-150]	The processing steps that use a DEM in Sen2Water shall use the Copernicus 90m DEM by default. Idepix shall be parameterised to use the Copernicus DEM. The DEM to be used shall be a parameter of Sen2Water.
[RD-155]	C2RCC shall be changed to support the use of the Copernicus DEM.
[RD-160]	POLYMER shall be changed to support the use of the Copernicus DEM. (L1C contains mean sea level pressure, not surface pressure.)
[RD-165]	Missing DEM tiles shall be downloaded automatically in the stand-alone version of Sen2Water. The cache directory for DEM download shall be a parameter. It is expected that the DEM is provided for the combined processor used in PDGS.

4.5 Dynamic auxiliary data

Dynamic auxiliary data of atmospheric conditions are used for the atmospheric correction:

- POLYMER uses ozone, surface pressure, and wind speed dynamic auxiliary data. The auxiliary data is from NASA/Goddard's Global Modelling and Assimilation Office GMAO. It is downloaded from OBPG. Alternatively, POLYMER can use ERA5 data.
- C2RCC did not use dynamic auxiliary data in the HR-OC chain. It is able to use TOMSOMI ozone and NCEP pressure downloaded from OBPG. By parameterisation it can also use the ECMWF data contained in the L1C.
- ACOLITE can use dynamic auxiliary data for ozone, water vapour, pressure, and wind speed. It can download them from OBPG. It did not use dynamic auxiliary data in the HR-OC chain.

[RD-170]	The AC algorithms shall use the dynamic auxiliary data for atmospheric conditions contained in the L1C product (since baseline 04.00).
[RD-175]	POLYMER shall be changed to use the dynamic auxiliary data contained in the L1C.
[RD-180]	ACOLITE shall be changed to use the dynamic auxiliary data contained in the L1C.

4.6 Blending at the ocean-inland water interface

Based on a distinction of ocean and inland water areas introduced in subsection Global (ocean) water mask there is a spatial interface between ocean and inland waters at river mouths and estuaries. Because different algorithms are used for ocean and inland waters, a decision is required how to switch between the two algorithms at that interface. If the switch is simply from one to the other algorithm then the result will contain a visible artefact of changed water leaving reflectances at the interface line.

[RD-185]	The ocean waters shall be processed with the HR-OC CMEMS algorithm, i.e. a combination of ACOLITE and C2RCC.
[RD-190]	The rivers further upstream belong to the inland waters and shall in principle be processed with the inland water algorithms, i.e. POLYMER.

[RD-195]	A transition zone of n km from the ocean-inland interface into the river shall be used to transition smoothly from one algorithm to the other. The line of the ocean-inland water interface shall be taken from the static mask. The combination of ACOLITE/C2RCC and POLYMER results shall be based on the distance from the ocean-inland water interface in inland direction.

As stated in RD-105 the method of buffering shall ensure that the ocean algorithm does not leak into lakes close to the coast if they are separated from ocean by land. The transition shall only be applied at water-to-water interfaces.

To define the transition zone in the direction of inland only ensures that ocean pixels are continued to be processed with the HR-OC CMEMS algorithms.

REQ-04 requires that the algorithm is selected depending on the kind of water. If the distinction between ocean and inland water serves at kind of water then the requirements are in line with that. This is also in line with the requirement of the services for continuity of the time series.

In case of reprocessing there is a different choice possible: To combine different algorithms also for inland water, depending on turbidity or some other data-dependent property. If the choice is identical to the one in ocean between C2RCC and ACOLITE then the smooth transition could be ensured by using the same algorithm combination for ocean and inland water, instead of the blending by geographic criteria.

5 Requirements of the coastal water quality service and the lakes water quality service

This chapter collects requirements of the services for the way of processing and the L2W data product. The purpose of Sen2Water is that the services can replace their own pre-processing by the L2W data product. To achieve that the following high-level requirements are defined.

5.1 Continuity and consistency of the time series

[RD-300]	Continuity and consistency with the coastal water quality service time series The L2W product provided by the PDGS shall contain water-leaving reflectances that continue the time series of intermediates produced in the operational chain of the coastal water quality service (HR-OC) of the Copernicus Marine Service for coastal ocean water. This can be achieved by using the same combination of C2RCC and ACOLITE and the same parameterisation as in the operational coastal water quality service chain.
[RD-305]	Continuity and consistency with the lakes water quality service time series The L2W product provided by the PDGS shall contain water-leaving reflectances that continue the time series of intermediates produced for lake water in the operational chain of the lakes water quality service of CGLS. This can be achieved by using the same POLYMER processor and the same parameterisation as in the operational lakes water quality service processing chain.

The restriction of this requirement to the water bodies which have been processed so far in the services opens options for the interface between ocean and inland (section 4.6)

The requirements further allow improvements and harmonisations if they do not have a large or negative impact on the result that breaks the time series consistency. The exchange of the DEM used will not change something for ocean water as all DEMs can be expected to provide “sea level” here. The exchange of dynamic auxiliary data source from OBPG to ECMWF should also have a minor impact only. But this needs to be investigated.

5.2 Way forward for ongoing and future development

The services so far had been free to improve their pre-processing. This has happened within both services that have upgraded Idepix or Polymer.

HR-OC currently prepares an update that will plug-in a de-striping step before (!) atmospheric correction to compensate for visible stripes of the different detectors, in particular in case of glint. Such improvements shall still be possible with L2W being processed in the ground segment.

[RD-310]	PDGS shall incorporate upgrades of the Sen2Water processor if there are major improvements of the algorithms required by one of the services.
[RD-315]	The upgrades shall be aligned with upgrades of Sen2Cor if possible.
[RD-320]	If upgrades have an impact on both service chains (like de-striping) it shall be analysed for both services whether the impact is positive and accepted.

5.3 Operational requirements

The two services are operational and have corresponding requirements for the L2W data product that will be their input.

[RD-325]	The aquatic reflectance product shall be available in NRT (within 6 hours after acquisition normally, 24 hours after acquisition at maximum) to the coastal water quality service and the lakes water quality service.
[RD-330]	The services shall be able to safe processing time by using the L2W. (rephrased: The L2W must be the product that the services need, not something different.)
[RD-335]	The L2W shall be available as an item that can be accessed without downloading the complete L2 data product. This is easily achieved by making the L2W a NetCDF4 file within the complete L2A data product and by providing access to components of a product, e.g. in S3 cloud storage.

6 Requirements for PDGS integration

This chapter collects requirements of the PDGS relevant for the integration of the combination of Sen2Cor and Sen2Water into the PDGS operational service.

[RD-400]	The combined processor shall read PDI format inputs.
[RD-405]	The combined processor shall write PDI format outputs that are converted into EUP format by a later step.
[RD-410]	The combined processor shall call both Sen2Cor and Sen2Water. It shall merge the results of both into a common L2A.
[RD-415]	The call of Sen2Water and the merger shall be avoided for granules that do not contain water pixels.
[RD-420]	Whether Sen2Water and the merger are called shall be controlled by a processor configuration parameter.
[RD-425]	The local path of the DEM shall be provided as processing parameter.

Note that Sen2Water stand-alone shall read the L1C End User Product (EUP) format. Sen2Water in any case generates the L2W product component. It is the merger that integrates it into the L2A, and a later step that generates the EUR.