COPERNICUS SPACE COMPONENT SENTINEL OPTICAL IMAGING

MISSION PERFORMANCE CLUSTER SERVICE

Sen2Water Verification and Validation Report

Ref.: OMPC.ACR.VR.054

Issue: 1.1

Date: 10/12/2024

Contract: 4000136252/21/I-BG

Customer:	ESA	**Document Ref.:**	OMPC.ACR.VR.054
Contract No.:	4000136252/21/I-BG	**Date:**	10/12/2024
		Issue:	1.1

Project:	COPERNICUS SPACE COMPONENT SENTINEL OPTICAL IMAGING MISSION PERFORMANCE CLUSTER SERVICE		
Title:	Sen2Water Verification and Validation Report		
Author(s):	L. Rivoire, M. Böttcher, S. Clerc		
Approved by:		**Authorized by**	J. Bruniquel, OPT-MPC Service Manager
Distribution:	ESA		
Accepted by ESA	S. Dransfeld, ESA TO		V. Boccia, ESA Deputy TO
Filename	OMPC.ACR.VR.054 - - Sen2Water Verification and Validation Report.docx		

ACRI-ST
260 route du Pin Montard
06904 Sophia-Antipolis, France
Tel: +33 (0)4 92 96 75 00 Fax: +33 (0)4 92 96 71 17
www.acri-st.fr

Changes Log

Version	Date	Changes
1.0	13/11/2024	Initial delivery
1.1	10/12/2024	Update scatterplots, add summary graphs and statistics summary tables

List of Changes

Version	Section	Answers to RID	Changes

Table of content

List of Figures

1 Introduction

This document summarises the verification and the validation results of the prototyping version of the Sen2Water processor, developed and delivered by Brockmann Consult to ACRI-ST. This activity is performed in the frame of the "COPERNICUS SPACE COMPONENT SENTINEL OPTICAL IMAGING MISSION PERFORMANCE CLUSTER SERVICE", ESA contract 4000136252/21/I-BG.

1.1 Scope of the document and objectives

The Sen2Water development activity aims at generating Bottom-of-Atmosphere aquatic reflectance layers for Sentinel-2 L2A products. An important constraint is to ensure as far as possible consistent content with respect to reflectance products generated previously by the Copernicus Services (CMEMS and CGLOPS).

Other objectives of the V&V activities are:

- Ensure that the development fulfils the requirements of the SoW MSI L2W RD 2023. In particular, compatibility of the Sen2Water processor with the constraints of Sentinel-2 ground segments shall be demonstrated (see SoW).
- Provide evidence that the Sen2Water has a state-of-the-art performance as assessed, e.g., in the ACIX AQUA benchmark.

1.2 Applicable documents

Document ID	ACR	Description	Version
MSI L2W RD 2023	SoW	Sen2Water Requirements Document, OMPC.BC.RD-MSI-L2, Optical Mission Performance Centre, ESA, October 2023	1.0
OMPC.ACR.PROP.009	Prop	Proposal for the upgrade of the S2 L2A processor to generate Aquatic Reflectances	1.1
OMPC.BC.TN.012	SRD	Sen2Water Requirements Document	1.0
S2-PDGS-TAS-DI-PSD	PSD	Sentinel-2 Product Specification Document	14.9
OMPC.ACR.PLN.13	VVP	Sen2Water Verification and validation plan	i.0

1.3 Reference documents

Document ID	Description	Version
S2-PDGS-MPC-L2A-ATBD 2021	Level-2A Algorithm Theoretical Basis Document, S2-PDGS-MPC-ATBD-L2A, Optical Mission Performance Centre, ESA, November 2021	2.10
MSI L2 IODD 2023	Sen2Cor and Sen2Water Input Output Data Definition, OMPC.TPGZ-BC.IODD-MSI-L2, Optical Mission Performance Centre, ESA, October 2023	1.0
OMPC.TPZG.IOD. 001 2022	Sen2Cor 2.11.00 Input Output Data Definition, Optical Mission Performance Centre, ESA, November 2023	2.11
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
S2-PSD	Sentinel-2 Products Specification Document, *S2-PDGS-TAS-DI-PSD,* ESA	14.9
S2-PDGS-MPC-L2A-PFS	Sentinel-2 MSI – Product Format Specification	14.9
S2-PDD	GMES Space Component – Sentinel-2 Payload Data Ground Segment (PDGS), Product Definition Document	2.3
OMPC-TPZG-SUM-001	Sentinel-2 MSI – Level 2A Prototype Processor Installation and User Manual, Telespazio, OPMC, ESA	2.11
OMPC.TPZG.SRN. 003	Sen2Cor 2.11.00 Software Release Note. Telespazio, OMPC, ESA, 2022	2.11
CMEMS-HR-OC-QUID-009	Quality Information Document for HR OC Products	2022 i2.0
N. Pahlevan et al., 2021	ACIX-Aqua: A global assessment of atmospheric correction methods for Landsat-8 and Sentinel-2 over lakes, rivers, and coastal waters, ttps://doi.org/10.1016/j.rse.2021.112366	
Warren et al., 2019	Assessment of atmospheric correction algorithms for the Sentinel-2A Multi Spectral Imager over coastal and inland waters, https://doi.org/10.1016/j.rse.2019.03.018	
CGLOPS2_QAR_LWQ100_S2	Copernicus Global Land Operations, Lake Water 100 m version, Quality Assessment Report	2020, i1.02

1.4 Acronyms and abbreviations

ACIX: Atmospheric Correction Inter-comparison eXercise

CGLOPS: Copernicus Global Land Operations

CDSE: Copernicus Data Space Environment

CVD: Community Validation Dataset

PSD: Product Specification Document

RD: Requirement Document

SZA: Sun Zenith Angle

TDS: Test Data Set

2 Verification Report

2.1 Objectives and methodology

The objectives of the verification activities are:

- Verification of the correct implementation of the Sen2Water Requirements as specified in document Sen2Water-RD
- Verification that the generated products are compliant with the specifications of the PSD
- Verification of robustness to problematic cases (with no formal requirement associated)

Details on the test plan are provided in the Verification and Validation Plan (VVP).

2.2 Test Results

This section identifies the list of tests for each type of requirements and documents the result of all tests for Sen2Water (scope S).

In the scope column, the letter S and/or L indicates which software is concerned by the test:

- S: Sen2Water stand-alone software
- L: L2A processor

It should be noted that the verification had been performed on v0.4.2 while validation of the next section had been performed with v0.4.1. This explains why the ante-meridian test failed in the validation report while it succeeds here.

2.2.1 Output verification tests

Test ID	Objective	Requirement	Scope	Passed
OUT-1	Sen2Water outputs verification	REQ-05, REQ-07, REQ-14, REQ-23	S	Y
OUT-2	L2A Product verification	REQ-02, REQ-14, REQ-22b, REQ-23	L	-
OUT-3	Inter-comparison of stand-alone and L2A products		S + L	-
OUT-4	Water algorithm selection tests	REQ-04, REQ-05, REQ-06, REQ-21	S	Y

OUT-1 has been performed on the list of inputs specified in the [VVP] and the four additional inputs of the validation report (section 3.2):

```
S2B_MSIL1C_20230808T090559_N0509_R050_T32MRU_20230808T125427.SAFE
S2A_MSIL1C_20230121T111351_N0509_R137_T30UWU_20230121T131033.SAFE
S2B_MSIL1C_20230625T110619_N0509_R137_T30UWU_20230625T114918.SAFE
S2B_MSIL1C_20230823T095559_N0509_R122_T33TVL_20230823T121626.SAFE
S2A_MSIL1C_20231126T100331_N0509_R122_T33TVL_20231126T120138.SAFE
S2A_MSIL1C_20240104T022321_N0510_R103_T51PWN_20240104T032345.SAFE
S2A_MSIL1C_20231121T023011_N0509_R046_T52SBD_20231121T041548.SAFE
S2B_MSIL1C_20240103T221939_N0510_R029_T01KAB_20240103T232410.SAFE
S2A_MSIL1C_20210702T101031_N0500_R022_T32TNM_20230131T141414.SAFE
S2B_MSIL1C_20230806T100559_N0509_R022_T34WFT_20230806T104651.SAFE
S2B_MSIL1C_20231226T105359_N0510_R051_T31SBD_20231226T114540.SAFE
S2B_MSIL1C_20240106T102329_N0510_R065_T31RDH_20240106T122102.SAFE
S2A_MSIL1C_20240617T051231_N0510_R033_T42FXL_20240617T081319.SAFE
S2A_MSIL1C_20240330T140751_N0510_R053_T24VVR_20240330T174815.SAFE
S2A_MSIL1C_20240601T173911_N0510_R098_T12QZJ_20240602T000646.SAFE
S2A_MSIL1C_20240719T102021_N0510_R065_T32TNT_20240719T122006.SAFE
```

The processor software is installed in a directory sen2water-0.4/. The test has been performed in a working directory sen2water-verification that was initially empty.

The inputs have been retrieved from CDSE and unpacked. They have been processed with sen2water by

```
nohup bash -c '
sen2water.sh S2B_MSIL1C_20230808T090559_N0509_R050_T32MRU_20230808T125427.SAFE;
sen2water.sh S2A_MSIL1C_20230121T111351_N0509_R137_T30UWU_20230121T131033.SAFE;
sen2water.sh S2B_MSIL1C_20230625T110619_N0509_R137_T30UWU_20230625T114918.SAFE;
sen2water.sh S2B_MSIL1C_20230823T095559_N0509_R122_T33TVL_20230823T121626.SAFE;
sen2water.sh S2A_MSIL1C_20231126T100331_N0509_R122_T33TVL_20231126T120138.SAFE;
sen2water.sh S2A_MSIL1C_20240104T022321_N0510_R103_T51PWN_20240104T032345.SAFE;
sen2water.sh S2A_MSIL1C_20231121T023011_N0509_R046_T52SBD_20231121T041548.SAFE;
sen2water.sh S2B_MSIL1C_20240103T221939_N0510_R029_T01KAB_20240103T232410.SAFE;
sen2water.sh S2A_MSIL1C_20210702T101031_N0500_R022_T32TNM_20230131T141414.SAFE;
sen2water.sh S2B_MSIL1C_20230806T100559_N0509_R022_T34WFT_20230806T104651.SAFE;
sen2water.sh S2B_MSIL1C_20231226T105359_N0510_R051_T31SBD_20231226T114540.SAFE;
sen2water.sh S2B_MSIL1C_20240106T102329_N0510_R065_T31RDH_20240106T122102.SAFE;
sen2water.sh S2A_MSIL1C_20240617T051231_N0510_R033_T42FXL_20240617T081319.SAFE;
sen2water.sh S2A_MSIL1C_20240330T140751_N0510_R053_T24VVR_20240330T174815.SAFE;
sen2water.sh S2A_MSIL1C_20240601T173911_N0510_R098_T12QZJ_20240602T000646.SAFE;
sen2water.sh S2A_MSIL1C_20240719T102021_N0510_R065_T32TNT_20240719T122006.SAFE"
> s2w.out &
```

The trace of the processor output has been collected in a file s2w.out. It reports successful execution of each of the processor calls. The excerpt shows the trace for one input and output.

```
[…]
resampling to 60m ...
2024-09-24T21:36:56.668 INFO opening inputs
2024-09-24T21:36:58.314 INFO preparing computation
2024-09-24T21:36:58.575 INFO starting computation
2024-09-24T21:39:09.017 INFO output S2A_MSIL1C_20231126T100331_N0509_R122_T33TVL_20231126T120138-
resampled.nc written

S2A_MSIL1C_20231126T100331_N0509_R122_T33TVL_20231126T120138-resampled.nc

Idepix cloud screening ...
Executing processing graph
Initializing Elevation Model

S2A_MSIL1C_20231126T100331_N0509_R122_T33TVL_20231126T120138-idepix.nc

C2RCC atmospheric correction ...
Executing processing graph

S2A_MSIL1C_20231126T100331_N0509_R122_T33TVL_20231126T120138-c2rcc.nc

ACOLITE atmospheric correction ...

S2A_MSI_2023_11_26_10_03_31_S2R_L2R.nc

POLYMER reformatting of cloud mask ...
Executing processing graph
```

```
S2A_MSIL1C_20231126T100331_N0509_R122_T33TVL_20231126T120138-mask.nc

POLYMER atmospheric correction ...
26475 remote DEM tiles existing
69 local DEM tiles available
MSI product, size is 1830x1830
Starting processing at 2024-09-24 21:43:51.477798
Initializing output file "S2A_MSIL1C_20231126T100331_N0509_R122_T33TVL_20231126T120138-polymer.nc"
reading DEM tile /data/yarn/appcache/sen2water-tmp/sen2water-0.4/auxdata/dem/Copernicus 90m Global
DEM/Copernicus_DSM_COG_30_N45_00_E013_00_DEM.tif
[…]
Processing block: size (500, 400), offset (0, 0)
[…]
Done in 0:00:47.218450

S2A_MSIL1C_20231126T100331_N0509_R122_T33TVL_20231126T120138-polymer.nc

Sen2Water switching and output formatting ...
2024-09-24T21:44:39.756 INFO opening inputs
2024-09-24T21:44:40.687 INFO inputs opened
2024-09-24T21:44:40.692 INFO pixel classification prepared
2024-09-24T21:44:44.023 INFO ocean and coastal water switching prepared
2024-09-24T21:44:45.075 INFO inland water switching prepared
2024-09-24T21:44:45.079 INFO output formatting prepared
2024-09-24T21:44:48.248 INFO data written
2024-09-24T21:44:48.248 INFO computing statistics
2024-09-24T21:44:49.514 INFO adding statistics
2024-09-24T21:44:49.522 INFO output S2A_MSIL1C_20231126T100331_N0509_R122_T33TVL_20231126T120138-
s2w.nc written

S2A_MSIL2W_20231126T100331_N0509_R122_T33TVL_20240924T194445.nc
done
```

In contradiction to (REQ-23) log output uses computer local time rather than UTC because this is easier to read for users. If the computer is configured to use UTC then this will be so in the log as well, to make it compliant with (REQ-23).

The outputs of the processor are available in the working directory sen2water-verification:

```
-rw-r--r-- 1 yarn hadoop  9440970 Sep 24 21:36 S2A_MSIL2W_20230121T111351_N0509_R137_T30UWU_20240924T193651.nc
-rw-r--r-- 1 yarn hadoop  6412989 Sep 24 21:44 S2A_MSIL2W_20231126T100331_N0509_R122_T33TVL_20240924T194445.nc
-rw-r--r-- 1 yarn hadoop 62348375 Sep 24 21:55 S2A_MSIL2W_20240104T022321_N0510_R103_T51PWN_20240924T195454.nc
-rw-r--r-- 1 yarn hadoop 41110335 Sep 24 22:05 S2A_MSIL2W_20240330T140751_N0510_R053_T24VVR_20240924T200544.nc
-rw-r--r-- 1 yarn hadoop  1254544 Sep 24 22:11 S2A_MSIL2W_20240601T173911_N0510_R098_T12QZJ_20240924T201139.nc
-rw-r--r-- 1 yarn hadoop 30063402 Sep 24 22:22 S2A_MSIL2W_20240617T051231_N0510_R033_T42FXL_20240924T202156.nc
-rw-r--r-- 1 yarn hadoop  7358347 Sep 24 22:29 S2A_MSIL2W_20240719T102021_N0510_R065_T32TNT_20240924T202941.nc
-rw-r--r-- 1 yarn hadoop  9394752 Sep 24 22:37 S2B_MSIL2W_20230625T110619_N0509_R137_T30UWU_20240924T203737.nc
-rw-r--r-- 1 yarn hadoop 11657399 Sep 24 22:43 S2B_MSIL2W_20230808T090559_N0509_R050_T32MRU_20240924T204341.nc
-rw-r--r-- 1 yarn hadoop  5796438 Sep 24 22:51 S2B_MSIL2W_20230823T095559_N0509_R122_T33TVL_20240924T205125.nc
-rw-r--r-- 1 yarn hadoop 63807726 Sep 24 23:01 S2B_MSIL2W_20231226T105359_N0510_R051_T31SBD_20240924T210102.nc
-rw-r--r-- 1 yarn hadoop 56940881 Sep 24 23:10 S2B_MSIL2W_20240103T221939_N0510_R029_T01KAB_20240924T211017.nc
-rw-r--r-- 1 yarn hadoop   794347 Oct 22 10:10 S2A_MSIL2W_20231121T023011_N0509_R046_T52SBD_20241022T081005.nc
-rw-r--r-- 1 yarn hadoop  4711815 Oct 22 10:17 S2A_MSIL2W_20210702T101031_N0500_R022_T32TNM_20241022T081735.nc
-rw-r--r-- 1 yarn hadoop 68017278 Oct 22 10:26 S2B_MSIL2W_20230806T100559_N0509_R022_T34WFT_20241022T082639.nc
-rw-r--r-- 1 yarn hadoop   492267 Oct 22 10:34 S2B_MSIL2W_20240106T102329_N0510_R065_T31RDH_20241022T083417.nc
```

The structure of the outputs has been verified with ncdump -h :

```
$ ncdump -h S2A_MSIL2W_20230121T111351_N0509_R137_T30UWU_20240924T193651.nc | egrep ') ;|crs ;'
        double y(y) ;
        double x(x) ;
        float Rw443(y, x) ;
        float Rw490(y, x) ;
        float Rw560(y, x) ;
        float Rw665(y, x) ;
        float Rw705(y, x) ;
        float Rw740(y, x) ;
        float Rw783(y, x) ;
        float Rw842(y, x) ;
        float Rw865(y, x) ;
        float Rw945(y, x) ;
        float Rw1375(y, x) ;
        float Rw1610(y, x) ;
        float Rw2190(y, x) ;
        ubyte pixel_class(y, x) ;
        ubyte sen2water_flags(y, x) ;
        int pixel_classif_flags(y, x) ;
        int64 crs ;
```

The Rw variables are the water-leaving reflectances of the MSI bands (REQ-07). sen2water_flags contains quality indicators (REQ-14). The "global attributes" in its stat_* attributes contain further statistics as quality information (REQ-14), and times are provided in UTC (REQ-23):

```
// global attributes:
		:id = "S2A_MSIL2W_20230121T111351_N0509_R137_T30UWU_20240924T193651.nc" ;
		:local_id = "T30UWU_20230121T111351_AQU_60m.nc" ;
		:date_created = "20240924T193651Z" ;
		:tracking_id = "58ad3354-7aac-11ef-9e02-3cfdfea24bbc" ;
		:title = "OPT-MPC Sen2Water water-leaving reflectances in 60m" ;
		:institution = "Brockmann Consult GmbH as part of OPT-MPC for ESA" ;
		:source = "Sentinel-2 MSI L1C" ;
		:auxiliary = "Copernicus 90m DEM,Sen2Water ocean-inland-mask" ;
		:input = "S2A_MSIL1C_20230121T111351_N0509_R137_T30UWU_20230121T131033-resampled.nc" ;
		:processor = "Sen2Water v0.5" ;
		:parameters = "" ;
		:product_version = "05.09" ;
		:history = "Sen2Water switching v{processor_version}; Polymer 4.17beta; Acolite
20210203; C2RCC 9.0cv; Idepix 9.0cv; SNAP-9.0cv S2Resampling" ;
		:references = "https://sentinels.copernicus.eu/web/sentinel/missions/sentinel-2/" ;
		:license = "TBD" ;
		:summary = "The Sen2Water L2W product has been processed from Sentinel-2 MSI L1C by
pixel identification, atmospheric correction with different algorithms, and switching between them for
ocean and inland water pixels. The L2W is provided as part of the Sentinel-2 MSI L2A product parallel
to the outp
ut of Sen2Cor. It can also be generated from L1C with Sen2Water stand-alone." ;
		:keywords = "reflectance, surface water, ocean optics, Copernicus" ;
		:keywords_vocabulary = "NASA Global Change Master Directory (GCMD) Science keywords" ;
		:Conventions = "CF-1.11" ;
		:naming_authority = "www.esa.int" ;
		:standard_name_vocabulary = "NetCDF Climate and Forecast (CF) Metadata Convention" ;
		:creator_name = "Brockmann Consult GmbH as part of OPT-MPC for ESA" ;
		:creator_url = "https://www.brockmann-consult.de/" ;
		:creator_email = "info@brockmann-consult.de" ;
		:contact = "TBD" ;
		:project = "Optical Mission Performance Centre OPT-MPC" ;
		:cmd_data_type = "Grid" ;
		:spatial_resolution = "60m" ;
		:time_coverage_start = "20230121T111351Z" ;
		:platform = "Sentinel-2A" ;
		:sensor = "MSI" ;
		:start_date = "2023-Jan-21 11:13:51.000000" ;
		:stop_date = "2023-Jan-21 11:13:51.000000" ;
		:metadata_profile = "beam" ;
		:stat_clear_ocean_count = 315302LL ;
		:stat_clear_inland_water_count = 2926LL ;
		:stat_clear_land_count = 2735484LL ;
		:stat_snow_ice_ocean_count = 6988LL ;
		:stat_snow_ice_inland_water_count = 13LL ;
		:stat_snow_ice_land_count = 24656LL ;
		:stat_cloud_ocean_count = 53710LL ;
		:stat_cloud_inland_water_count = 2311LL ;
		:stat_cloud_land_count = 207510LL ;
		:stat_valid_ocean_count = 376000LL ;
		:stat_valid_inland_water_count = 5250LL ;
		:stat_valid_land_count = 2967650LL ;
		:stat_valid_count = 3348900LL ;
```

A visual inspection of outputs shows the distribution of water-leaving reflectances (REQ-05).

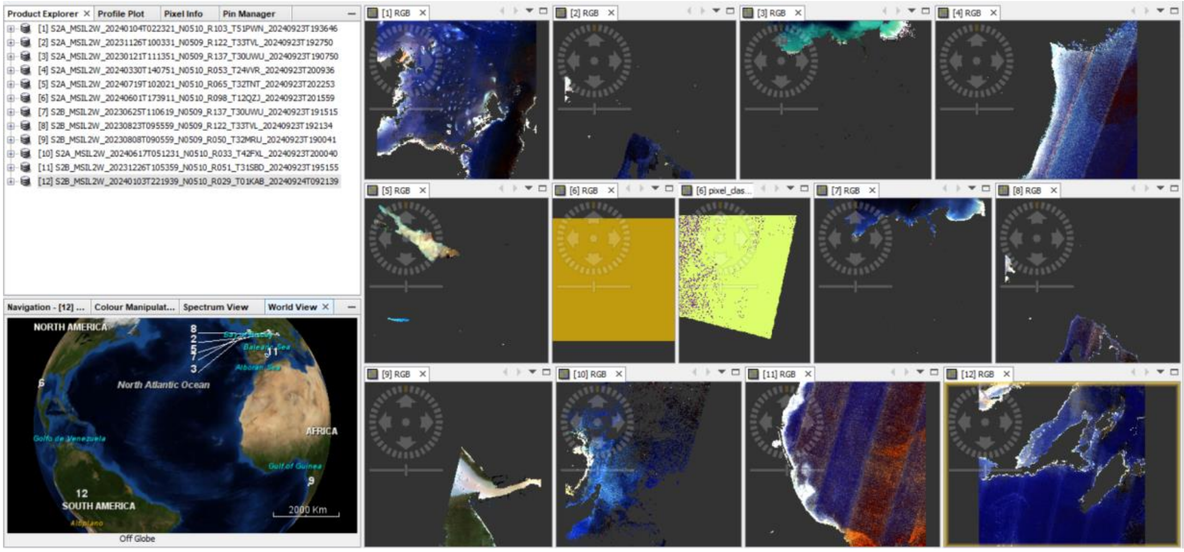

Figure 2-1: Pseudo-RGBs of water-leaving reflectances of 12 verification inputs

Water areas unless flagged because of clouds or other conditions are processed.

OUT-4 has been performed by inspecting single outputs and the respective static mask that has been used as auxiliary data.

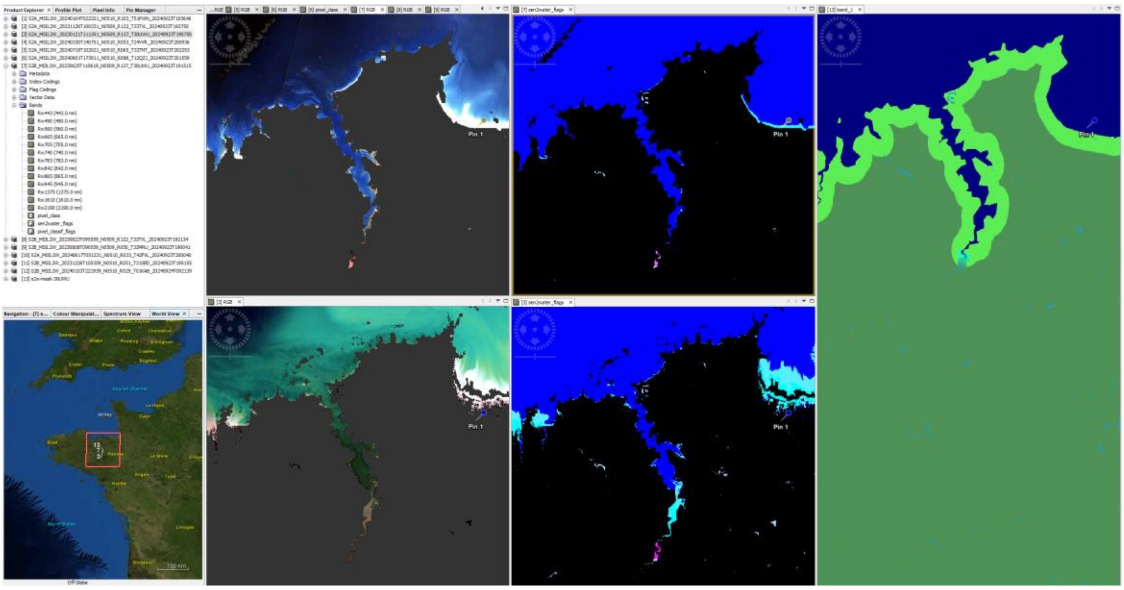

Figure 2-2: L2W of granule 30UWU at 2023-06-25 and 2023-01-21: left Pseudo-RGBs, middle selected algorithms, right static mask for ocean-inland water discrimination

- The images on the left show aquatic reflectances over water (REQ-05).
- The images in the middle demonstrate the switch from one algorithm to another in turbid waters in river mouths and close to the coast. (REQ-04). The mask shows blue for C2RCC, turquoise for ACOLITE, darker turquoise in the switching zone between them, and light blue for POLYMER in lakes and rivers. The small lakes get their separate class (even lighter blue, difficult to distinguish here because of the small area of the lakes.) Pink is used for out-of-range data reported by the respective algorithm used.

- The static mask on the right distinguishes ocean and inland water. The coastal zone is a buffer that changes into ocean where the static mask is not accurate or is temporarily flooded (REQ-06). The other direction is detected as well, as shown in this example at the pin.

2.2.2 Operational verification tests

Test ID	Objective	Requirement	Scope	Passed
OPE-1	Sen2Water run and configuration tests	REQ-08, REQ-13	S	Y
OPE-2	L2A processor run and configuration tests, including aquatic layer selection	REQ-03, REQ-11, REQ-12, REQ-17	L	-
OPE-3	Parallel processing	REQ-09, REQ-10	S, L	Y / -

OPE-1 extends OUT-1 and what has been reported there for the trace output with a few more aspects. The calling convention of sen2water (REQ-08) is

```
$ sen2water.sh --help
sen2water.sh <options> <l1cpath>
e.g.
sen2water.sh S2A_MSIL1C_20240104T103431_N0510_R108_T32UME_20240104T123149.SAFE
options
--c2rccanc embedded | constant
--acoliteanc embedded | constant
--polymeranc embedded | nasa | constant
--dem 'Copernicus 90m Global DEM' | 'Copernicus 30m Global DEM'
--withdetfoofilter
--withcleanup
--chunksize 610 | 1830 | 915 | 366 | 305 | 183 | 122 | 61
```

e.g.

```
sen2water.sh S2A_MSIL1C_20240104T103431_N0510_R108_T32UME_20240104T123149.SAFE
```

Dynamic auxiliary data is embedded in the L1C input. In addition, the Copernicus DEM is used by the processors. Its location is specified within the runtime structure during installation by a symbolic link to a directory where it is hosted (REQ-13).

```
$ ls -l sen2water-0.4
total 24
drwxr-xr-x 11 yarn hadoop 4096 Jul 19 16:56 auxdata -> /data/sen2water-auxdata
drwxr-xr-x  2 yarn hadoop 4096 Sep 24 22:23 bin
drwxr-xr-x  2 yarn hadoop 4096 Jul 19 09:46 etc
drwxr-xr-x 10 yarn hadoop 4096 Jul 19 19:13 lib
drwxr-xr-x  2 yarn hadoop 4096 Jul  4 13:11 licenses
-rw-r--r--  1 yarn hadoop 3327 Sep 24 21:24 README

$ ls -l sen2water-0.4/auxdata/dem/Copernicus\ 90m\ Global\ DEM/
total 214672
-rw-r--r-- 1 yarn hadoop 4712464 Sep 17 11:54 Copernicus_DSM_COG_30_N02_00_E035_00_DEM.tif
-rw-r--r-- 1 yarn hadoop 4348992 Sep 17 11:54 Copernicus_DSM_COG_30_N02_00_E036_00_DEM.tif
-rw-r--r-- 1 yarn hadoop 4385974 Sep 17 11:54 Copernicus_DSM_COG_30_N03_00_E035_00_DEM.tif
[...]
```

For OPE-3 the internal parallelisation is demonstrated by the output of the different steps of the processors in s2w.out:

```
resampling to 60m ...

real    2m44.390s
user    11m1.019s
sys     0m45.852s

Idepix cloud screening ...

real    1m44.104s
user    4m28.083s
sys     0m4.940s

C2RCC atmospheric correction ...

real    1m9.468s
user    3m24.682s
sys     0m1.769s

ACOLITE atmospheric correction ...

real    1m29.535s
user    0m42.443s
sys     0m28.093s

POLYMER reformatting of cloud mask ...

real    0m20.660s
user    0m11.720s
sys     0m0.536s

POLYMER atmospheric correction ...

real    0m56.776s
user    2m42.118s
sys     0m11.231s

Sen2Water switching and output formatting ...

real    0m9.891s
user    0m19.843s
sys     0m1.614s
```

'real' is the wall clock time of the step, 'user' and 'sys' are core computing times in user and kernel mode respectively. The ratio of (user+sys) / real is the concurrency. The different steps show concurrencies (REQ-10) between 4.25 and 2, in one step a concurrency of 1.

2.2.3 Installation, environment, and performance test

Test ID	Objective	Requirement	Scope	Passed
ENV-1	Open-source repository check	REQ-18	S	N
ENV-2	Sen2Water installation tests	REQ-24	S	Y
ENV-6	Sen2Water performance test	REQ-20	S	Y
ENV-3	L2A processor installation tests	REQ-24	L	-

Test ID	Objective	Requirement	Scope	Passed
ENV-4	Run on PDGS environment, RAM and CPU profile	REQ-15. REQ-19, REQ-20	L	-
ENV-5	Cloud platform test	REQ-19, REQ-22a	S, L	Y / -

ENV-1 is verified by inspection of the respective repositories (REQ-18):

SNAP	https://github.com:senbox-org/snap-engine.git h https://github.com:senbox-org/s3tbx.git https://github.com:senbox-org/s2tbx.git https://github.com/bcdev/calvalus2.git	
C2RCC	https://github.com:senbox-org/s3tbx.git	
Idepix	https://github.com/bcdev/snap-idepix.git	
ACOLITE	https://github.com/acolite/acolite.git	
POLYMER	https://github.com/hygeos/polymer.git	
Sen2Water	https://github.com/bcdev/snap-idepix.git	not yet public

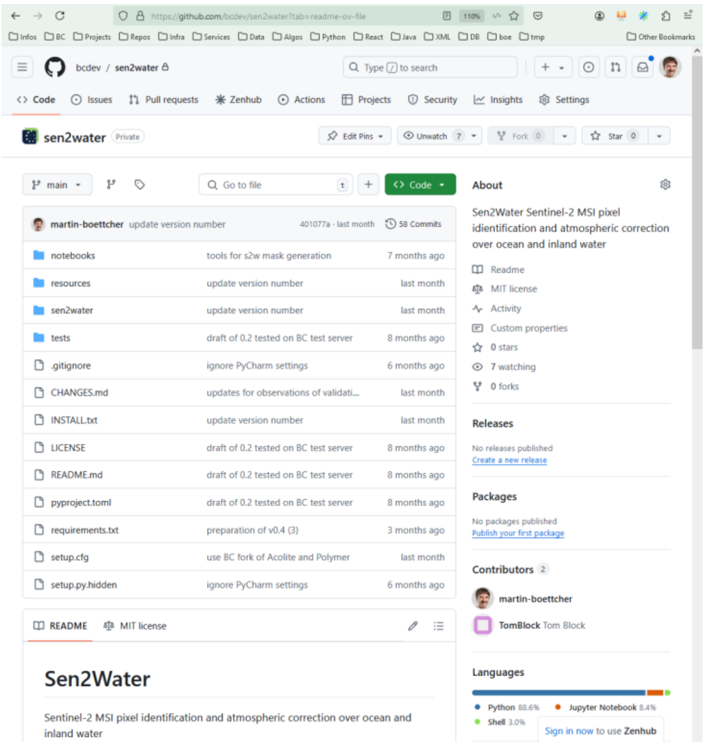

Figure 2-3: Sen2Water GitHub repository

ENV-2 is verified by inspection of an installation. The software has been installed by unpacking a .tar.gz in the installation directory, in this case sen2water-tmp. It could have been any other directory (REQ-24).

```
sen2water-tmp (s2w)$ tree -L 2 sen2water-0.4
sen2water-0.4
├── auxdata -> /data/sen2water-auxdata
```

```
├── bin
│   ├── hrocresampling.sh
│   ├── msiresampling.sh
│   ├── mys2w
│   └── sen2water.sh
├── etc
│   ├── acolite.parameters
│   ├── c2rcc-graph.xml
│   ├── idepix-graph.xml
│   ├── polymer-mask-graph.xml
│   ├── polymer.parameters
│   ├── s2resampling-graph.xml
│   ├── s2w-merge-graph.xml
│   └── snap.properties
├── lib
│   ├── acolite
│   ├── c2rcc
│   ├── conda
│   ├── idepix
│   ├── jre
│   ├── msiresampling
│   ├── polymer
│   └── snap
├── licenses
│   ├── ACOLITE-LICENCE.txt -> ../lib/acolite/LICENCE.txt
│   ├── CONDA-LICENSE.txt -> ../lib/conda/LICENSE.txt
│   ├── Idepix-LICENSE.txt -> ../lib/idepix/LICENSE.txt
│   ├── JRE-LICENSE -> ../lib/jre/LICENSE
│   ├── LICENSE-sen2water
│   ├── POLYMER-LICENCE.txt -> ../lib/polymer/LICENCE.TXT
│   └── SNAP-LICENSE.txt -> ../lib/snap/LICENSE.txt
└── README
sen2water-tmp (s2w)$ tree -L 1 /data/sen2water-auxdata
sen2water-auxdata
├── acolite
├── color_palettes
├── dem
├── polymer
├── proj-data
├── s2w-global-mask
├── s2w-lists
├── s2w-mask
└── watermask
```

The auxiliary data can be separated from the software package by symbolic links. Within the auxiliary data symbolic links can point to an existing directory with the Copernicus DEM. The runtime directory is independent of the software location. In the tests the working directory was

```
sen2water-tmp/validation2/
```

This is the directory the processor writes intermediates and the output to.

ENV-6 is verified by the times in s2w.out. The sum of the steps for the different inputs are:

Input	Elapsed	Core
S2B_MSIL1C_20230808T090559_N0509_R050_T32MRU_20230808T125427.SAFE	498	1169
S2A_MSIL1C_20230121T111351_N0509_R137_T30UWU_20230121T131033.SAFE	469	1383
S2B_MSIL1C_20230625T110619_N0509_R137_T30UWU_20230625T114918.SAFE	384	1305
S2B_MSIL1C_20230823T095559_N0509_R122_T33TVL_20230823T121626.SAFE	497	1299
S2A_MSIL1C_20231126T100331_N0509_R122_T33TVL_20231126T120138.SAFE	464	1365
S2A_MSIL1C_20240104T022321_N0510_R103_T51PWN_20240104T032345.SAFE	584	1894
S2A_MSIL1C_20231121T023011_N0509_R046_T52SBD_20231121T041548.SAFE	277	816
S2B_MSIL1C_20240103T221939_N0510_R029_T01KAB_20240103T232410.SAFE	577	1760
S2A_MSIL1C_20210702T101031_N0500_R022_T32TNM_20230131T141414.SAFE	450	1241
S2B_MSIL1C_20230806T100559_N0509_R022_T34WFT_20230806T104651.SAFE	546	1884
S2B_MSIL1C_20231226T105359_N0510_R051_T31SBD_20231226T114540.SAFE	590	1297
S2B_MSIL1C_20240106T102329_N0510_R065_T31RDH_20240106T122102.SAFE	458	1135
S2A_MSIL1C_20240617T051231_N0510_R033_T42FXL_20240617T081319.SAFE	515	1777
S2A_MSIL1C_20240330T140751_N0510_R053_T24VVR_20240330T174815.SAFE	508	1640
S2A_MSIL1C_20240601T173911_N0510_R098_T12QZJ_20240602T000646.SAFE	413	1066
S2A_MSIL1C_20240719T102021_N0510_R065_T32TNT_20240719T122006.SAFE	546	1316

The times are in seconds and have been determined by a single run on a quad-core machine with hyperthreading with 32 GB RAM. By experience, different runs deviate by about 10% from each other. None of the runtimes is beyond the required 40 minutes (REQ-20), even if considering core seconds.

ENV-5 has been verified by test. Sen2Water has been installed and run on a freshly created VM on Creodias (REQ-22a) using a smaller dual-core virtual machine running CentOS 9 (REQ-19). The trace of this test is:

```
$ cat /etc/os-release
NAME="CentOS Stream"
VERSION="9"
...
REDHAT_SUPPORT_PRODUCT="Red Hat Enterprise Linux 9"
REDHAT_SUPPORT_PRODUCT_VERSION="CentOS Stream"
$ # install Sen2Water
$ ls -l
total 1643356
-rw-r--r--. 1 eouser eouser   69926912 Oct 22 11:03 sen2water-0.4.2-202410122.tar.gz
-rw-r--r--. 1 eouser eouser 1612863465 Oct 22 11:03 sen2water-auxdata-0.4.tar.gz
$ tar xf sen2water-auxdata-0.4.tar.gz
$ tar xf sen2water-0.4.2-202410122.tar.gz
$ # set up working dir with input
$ mkdir validation
$ cd validation
$ . ../sen2water-0.4/bin/mys2w
using Sen2Water in /home/eouser/sen2water-0.4
$ cp -r /eodata/Sentinel-
2/MSI/L1C/2024/01/06/S2B_MSIL1C_20240106T102329_N0510_R065_T31RDH_20240106T122102.SAFE
.
$ # run processor
$ time sen2water.sh S2B_MSIL1C_20240106T102329_N0510_R065_T31RDH_20240106T122102.SAFE
resampling to 60m ...
2024-10-22T11:09:51.460 INFO opening inputs
...
S2B_MSIL2W_20240106T102329_N0510_R065_T31RDH_20241022T151836.nc
done

real    8m49.905s
user    11m46.227s
sys     0m35.692s
```

```
$ ls -l *L2W*
-rw-r--r--. 1 eouser eouser 492206 Oct 22 11:18
S2B_MSIL2W_20240106T102329_N0510_R065_T31RDH_20241022T151836.nc
```

Sen2Water runs on a CentOS 9 VM on Creodias without problems.

2.2.4 Robustness tests

Test ID	Objective	Requirement	Scope	Passed
ROB-1	Small number of water pixels	Shall provide an output	S	Y
ROB-2	Antimeridian tile	Shall provide an output	S	Y
ROB-3	Product with missing packets	Shall provide an output on valid pixels	S	Y
ROB-4	Product with high SZA	Shall provide an output with flags	S	Y
ROB-5	Product with missing AUX data	Shall provide an output based on default values, with “degraded” quality warning	S	N
ROB-6	Incomplete parameters or missing input	Shall result in error	L	Y (for S)
ROB-7	Prime meridian tile	Shall provide an output	S	Y

The respective outputs of the tests are:

Test ID	Input	
ROB-1	S2A_MSIL2W_20231121T023011_N0509_R046_T52SBD_20241022T081005.nc	
ROB-2	S2B_MSIL2W_20240103T221939_N0510_R029_T01KAB_20240924T092139.nc	
ROB-3	S2A_MSIL2W_20210702T101031_N0500_R022_T32TNM_20241022T081735.nc	
ROB-4	S2B_MSIL2W_20230806T100559_N0509_R022_T34WFT_20241022T082639.nc	
ROB-5	-	patched
ROB-6	-	missing
ROB-7	S2B_MSIL2W_20231226T105359_N0510_R051_T31SBD_20240923T195155.nc	

ROB-1 shows the small part of available observation that has been successfully processed.

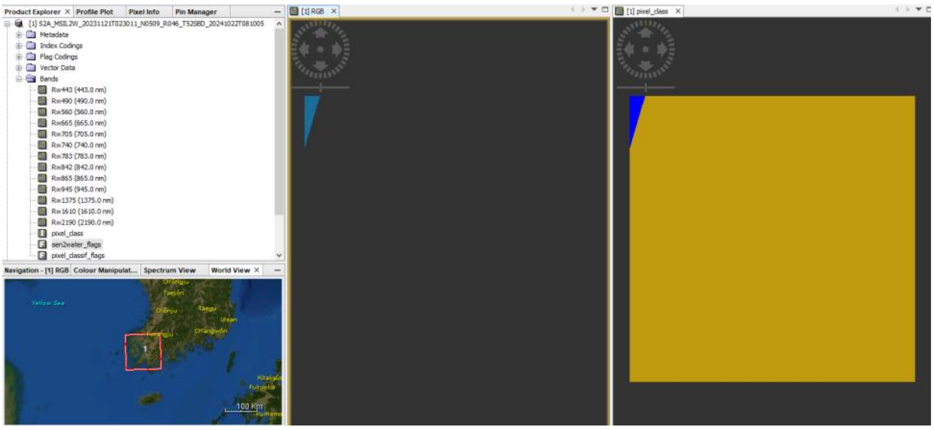

Figure 2-4: ROB-1 L2W of ganule 52SBD with a small water area: pseudo-RGB left, pixel_class right

ROB-2 had failed initially but succeeds after a fix in v0.4.2. There are no artefacts at the ante-meridian.

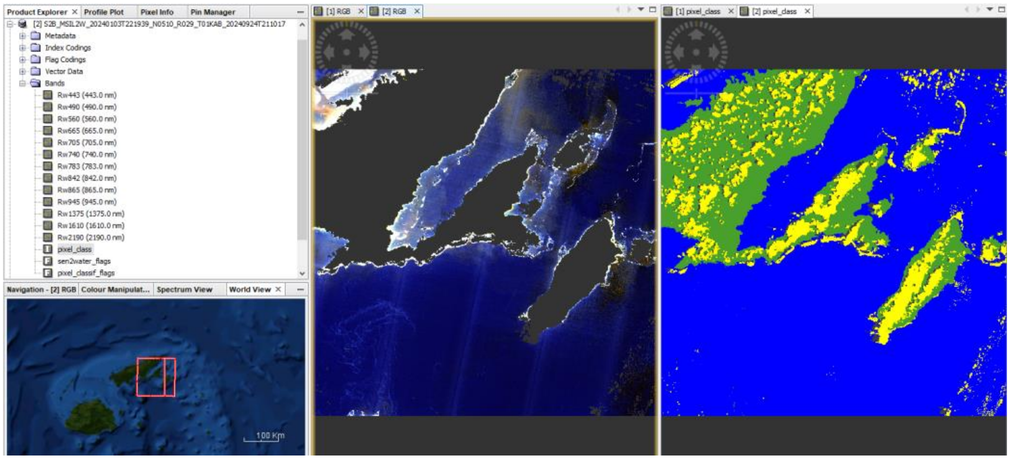

Figure 2-5: ROB-2 granule of 01KAB: no artefacts at ante-meridian (fixed in version 0.4.2)

ROB-3 has processed valid areas of the input with missing packets.

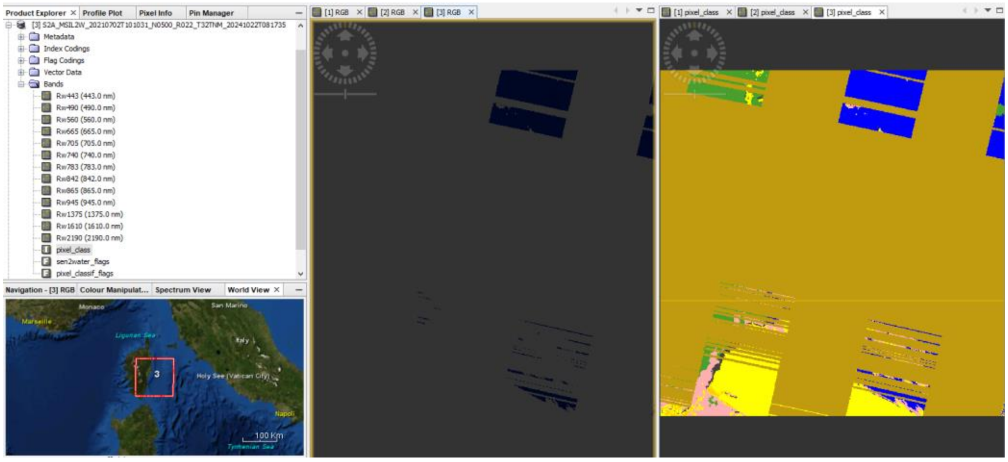

Figure 2-6: ROB-3 granule of 32TNM: missing packets, but valid areas are processed

ROB-4 has processed large parts of the image despite of high SZA.

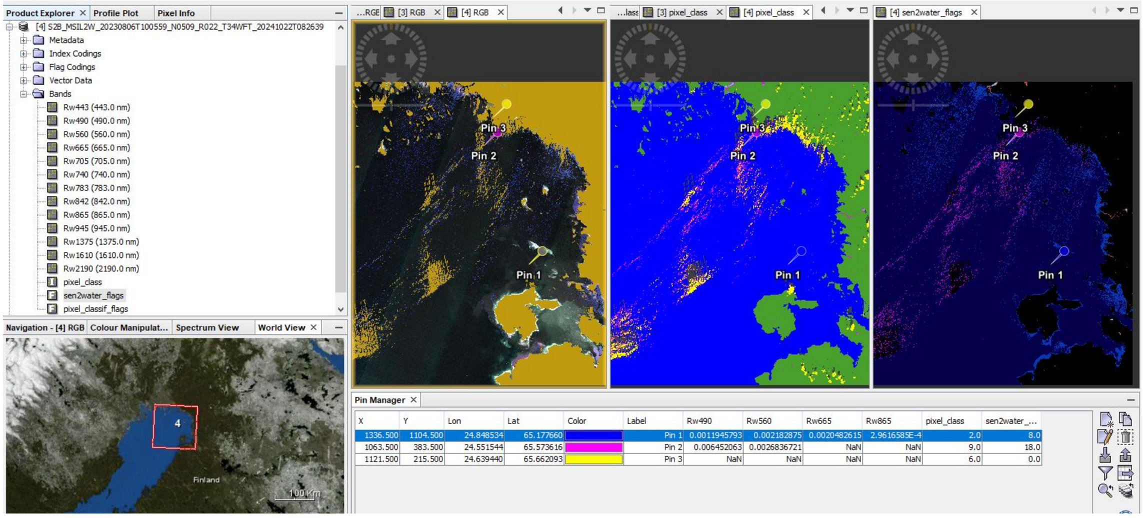

Figure 2-7: ROB-4 granule of 34WFT: Pin 1 in clear ocean successfully processed by C2RCC, Pin 2 flagged AC out-of-range, Pin-3 in cloud shadow

ROB-5 returns with an exception that aux variables are missing. The AUX_DATA directory had been removed from the input before starting the processor:

```
$ rm -r S2B_MSIL1C_20230808T090559_N0509_R050_T32MRU_20230808T125427.SAFE/GRANULE/L1C_T32
MRU_A033538_20230808T092730/AUX_DATA

$ sen2water.sh S2B_MSIL1C_20230808T090559_N0509_R050_T32MRU_20230808T125427.SAFE

KeyError: "No variable named 'aux_latitude'. Variables on the dataset include ['x60',
'y60', 'spatial_ref_60', 'B10', 'x10', ..., 'vaa_B
10', 'vza_B11', 'vaa_B11', 'vza_B12', 'vaa_B12']"
```

This is not what is expected by the validation team. If there are products without AUX_DATA then this is an open issue.

ROB-6 returns with the usage information if no input is specified with the command.

```
$ sen2water.sh
sen2water.sh <options> <l1cpath>
e.g.
sen2water.sh S2A_MSIL1C_20240104T103431_N0510_R108_T32UME_20240104T123149.SAFE
options
--c2rccanc embedded | constant
--acoliteanc embedded | constant
--polymeranc embedded | nasa | constant
--dem 'Copernicus 90m Global DEM' | 'Copernicus 30m Global DEM'
--withdetfoofilter
--withcleanup
--chunksize 610 | 1830 | 915 | 366 | 305 | 183 | 122 | 61
```

This is as expected.

ROB-7 shows no artefacts at main meridian.

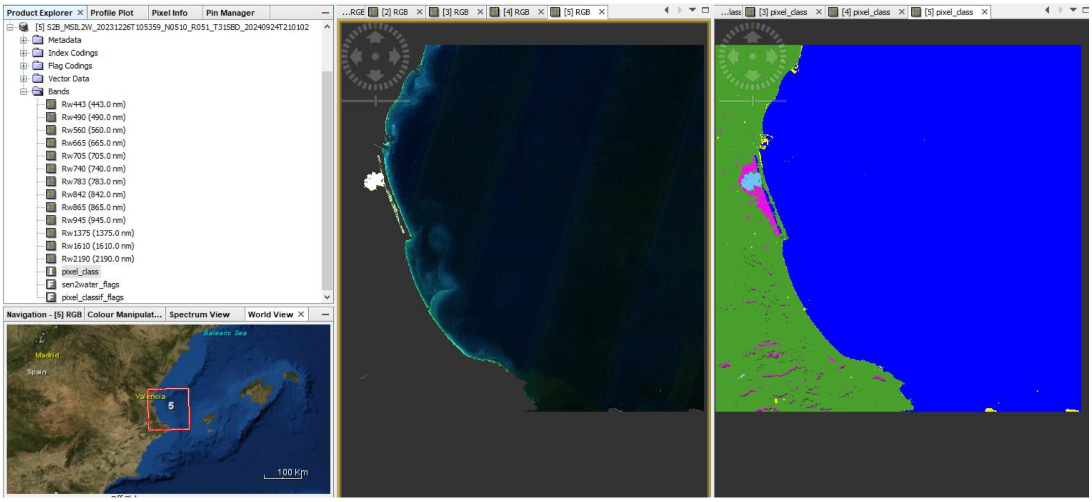

Figure 2-8: ROB-7 of granule 32SBD: no artefacts at main meridian

2.3 Conclusions and way forward

2.3.1 Tests not performed

All tests for Sen2Water without the embedding Sentinel-2A processor have been performed.

2.3.2 Tests not successful and open issues at the end of the verification

ROB-5 raises an error because the expected embedded auxiliary data cannot be found. If there are operational products without auxiliary data that shall be processed, then this becomes an open issue.

ENV-1 is not yet fully fulfilled because the Sen2Water software repository is not yet open. We recommend opening it with the public release of Sen2Water.

2.3.3 Conclusions

There are no specific conclusions from verification.

3 Validation Report

3.1 Objectives and methodology

The objectives of the validation activity are:

- Detect any anomaly impacting data quality
- Ensure that Sen2Water provides fit-for-purpose products replacing the current processing of Copernicus services. Therefore, the validation plan draws from the existing plans for the land and marine services.
- Compare with published results from the published ACIX AQUA benchmark to ensure that results are state-of-the-art. This objective will be more relevant for other users and is in line with requirement [REQ-27].

Note that the objective at this stage is not to fully characterize the uncertainty of the Sen2Water products in an operational perspective. Additional routine validation activities should be performed once the processing enters in operation. In particular, a systematic validation of the pixel classification will not be performed in the frame of the Sen2Water development. Similarly, sensibility studies are out of scope.

The validation plan will include three types of approaches:

- Visual inspection and quality assessment
- Comparison with in-situ data over coastal waters and lakes
- Comparison with Sentinel-3 OLCI products of equivalent multi-sensor LR composites

Level 2 Sen2Water products will be often compared to level 2 Sen2Cor products, which is the current reference for reflectance over all surfaces.

To fulfil the validation activities, a dataset of S2 L1C products has been collected (from CDSE). Only L1C products with processing baseline 05.XX have been used (Collection 1 products for archive products).

Sen2Water version v0.4.1 is used to perform the validation.

3.2 Test data set and methodology

3.2.1 Visual inspection

A detailed visual inspection was performed on the TDS products and on additional products of interest. The inspected products are listed hereafter :

- S2B_MSIL1C_20230808T090559_N0509_R050_T32MRU_20230808T125427.SAFE
- S2A_MSIL1C_20230121T111351_N0509_R137_T30UWU_20230121T131033.SAFE
- S2B_MSIL1C_20230625T110619_N0509_R137_T30UWU_20230625T114918.SAFE
- S2B_MSIL1C_20230823T095559_N0509_R122_T33TVL_20230823T121626.SAFE
- S2A_MSIL1C_20231126T100331_N0509_R122_T33TVL_20231126T120138.SAFE

- S2A_MSIL1C_20240104T022321_N0510_R103_T51PWN_20240104T032345.SAFE
- S2A_MSIL1C_20231121T023011_N0509_R046_T52SBD_20231121T041548.SAFE
- S2B_MSIL1C_20240103T221939_N0510_R029_T01KAB_20240103T232410.SAFE
- S2A_MSIL1C_20210702T101031_N0500_R022_T32TNM_20230131T141414.SAFE
- S2B_MSIL1C_20230806T100559_N0509_R022_T34WFT_20230806T104651.SAFE
- S2B_MSIL1C_20231226T105359_N0510_R051_T31SBD_20231226T114540.SAFE
- S2A_MSIL1C_20240617T051231_N0510_R033_T42FXL_20240617T081319.SAFE (additional product with white caps)
- S2A_MSIL1C_20240330T140751_N0510_R053_T24VVR_20240330T174815.SAFE (additional product with sea ice – ice floe)
- S2A_MSIL1C_20240601T173911_N0510_R098_T12QZJ_20240602T000646.SAFE (additional product with sun glint)
- S2A_MSIL1C_20240719T102021_N0510_R065_T32TNT_20240719T122006.SAFE (additional product with inland water)

For each product, reflectances and pixel classification are inspected. Possible image discontinuities, noise, stripes or “flat” areas are searched for. Comparison of images over the same site at different times is conducted to look for possible permanent features.

3.2.2 In-situ data: AERONET-OC

In-situ data from the Aerosol Robotic Network (AERONET-OC, Zibordi et al., 2009) is used.

The AERONET-OC database contains water-leaving radiances measured in various places around the globe. We decided to use measurements made after the 01/01/2022, to validate only the most recent Sentinel-2 observations. We use in-situ measurements at level 2.0 (quality-assured data) when available and at level 1.5 (cloud cleared and quality-controlled data) otherwise. The wavelengths at which measurements are made are not standardized, thus we retain only measurements for which radiances have been measured at wavelengths 412 nm, 442 nm, 490 nm, 530 nm, 551 nm and 668 nm, with a tolerance of plus or minus 2 nm. These six wavelengths are required for the spectral resampling presented later. After having applied these selection criteria, we obtain 4332 valid in-situ-measurements in 9 different sites, as of March 2024.

Water-leaving radiances are then converted into water-leaving reflectances using equation [A] below:

$$\rho_w = \frac{\pi \cdot L_w}{E \cdot \cos(\theta_s)}$$

with ρ_w the water-leaving reflectance, L_w the water-leaving radiance, E the solar irradiance at the wavelength of the measurement and θ_s the sun zenith angle. The TSIS solar spectrum at 1 nm sampling resolution is used (see Coddington et al., 2023) to compute the solar irradiance at the wavelength of the measurement.

Finally, the water-leaving reflectances are spectrally resampled to match Sentinel-2 spectral response functions using the deep neural approach presented in Pahlevan et al., 2021, and available on github (see

Brandon, 2017). A dataset of in-situ measurements is produced using Sentinel-2A spectral response and another one for Sentinel-2B, by changing the parameters of the deep neural approach.

3.2.3 In-situ data: GLORIA

Most of the in-situ measurements from the AERONET-OC database are made in coastal waters. To compare satellite measurements to in-situ measurements made in inland waters, the GLObal Reflectance community dataset for Imaging and optical sensing of Aquatic environments (GLORIA, see Lehmann et al., 2023) database is also used.

The GLORIA database is smaller than the AERONET-OC database. Thus, there are only 33 valid in-situ measurements made after the 01/01/2022. For this reason, we decided to extend the temporal window for the GLORIA dataset, back to 01/01/2020: we obtain 627 valid measurements. A measurement is valid when no flag (provided in the database) is raised. The GLORIA dataset is a hyperspectral dataset containing water-leaving reflectances. Thus, there is no need for a conversion using a solar spectrum, as we already have reflectances, except a multiplication by pi to convert remote sensing reflectances in water leaving reflectances. The hyperspectral reflectances are converted to Sentinel-2A and Sentinel-2B like reflectances by convoluting them with the spectral response functions of each sensor. The 627 valid in-situ measurements are spread over 55 different sites.

Products from AERONET-OC database and GLORIA database are located in 64 different sites, as presented in figure below.

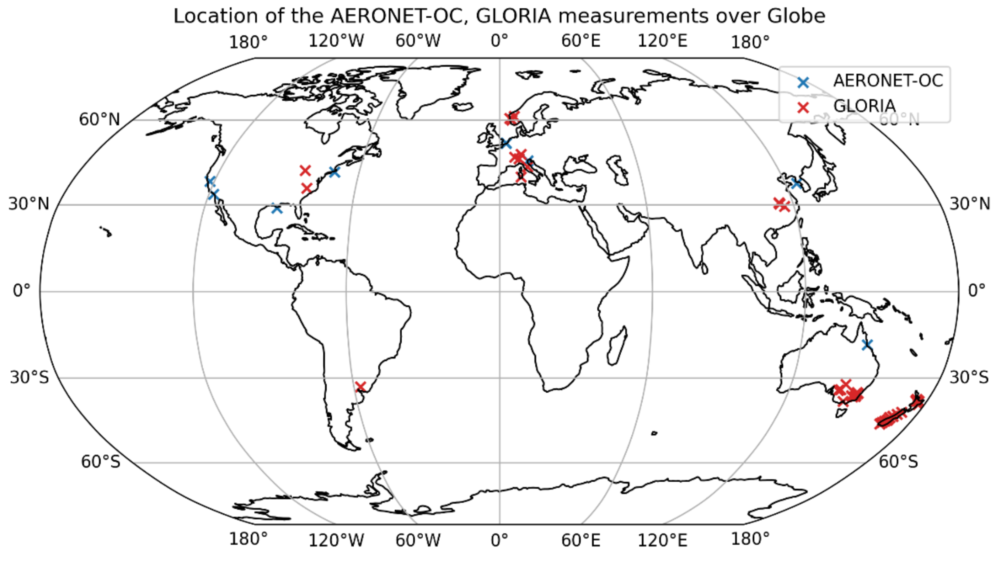

Figure 3-1: location of the 9 AERONET-OC and 55 GLORIA in-situ measurement sites over the globe

3.2.4 In-situ and satellite data match-ups

For each valid in-situ measurement obtained after the pre-processing, a request is made to the Copernicus Data Space Ecosystem to find Sentinel-2 products at the location of the in-situ measurement. A temporal difference of less than 3 hours between the in-situ measurement and the satellite measurement is accepted for coastal measurements, and a temporal difference of 24 hours is accepted for inland measurements. Before any filtering, 294 matchups are obtained for AERONET-OC data and 115 for GLORIA data.

Level 1C and level 2A products are downloaded, and level 2W products are computed using Sen2Water processor version 0.4.1 and level 1C products. Level 2A and level 2W products are compared.

Level 2A products are resampled at a 60 m resolution by averaging pixels into macro-pixels. Level 2W products are already at a 60m resolution. Nine 60 m pixels are extracted around the in-situ measurement for both levels 2A and 2W. Satellite reflectances are extracted, as well as classification flags stating whether the macro-pixels are clear water pixels or not, for both levels 2A and 2W.

Two different validation pipelines are created.

i. First validation pipeline ("products" pipeline)

In the first one, only flags from level 2W are used. The median of the macro-pixels that are flagged as clear water is computed and is directly compared to the in-situ measurement. If all macro-pixels are flagged as non-clear water, then the matchup is not used. This pipeline aims at validating the processor from a user perspective, who will only use flags from the product and will not perform any additional filtering.

ii. Second validation pipeline ("algorithms" pipeline)

In the second one, flags from level 2W are used. Moreover, for each macro-pixel, a masking criteria is used, computed using level 2A reflectances (we do not use level 2W reflectances as they are not computed in the SWIR) and taken from Pahlevan et al., 2021:

$$\rho_w(1610\,nm) > 0.025 \; or \; std\big(\rho_w(1610\,nm)\big) > \; 0.01 \qquad \text{[B]}$$

With $\rho_w(1610\,nm)$ the water-leaving reflectance at 1610 nm, std the standard deviation applied to all non-nan macro-pixels.

A second criteria is presented and used in Pahlevan et al., 2021, based on standard deviation of pixels at 1610 nm and fluorescence line height. However, this criteria is very restrictive and removes too many products (only 69 products of all water types are retained, whereas 165 are retained if this criteria is not applied), thus it has been decided not to use this criteria in order to improve statistical significance of the results.

Moreover, a threshold of 5 valid macro-pixels is used in this second pipeline, meaning that at least 5 macro-pixels must be valid to compute the median, otherwise the matchup is discarded.

Once the median is computed, outliers are removed. For each band and each level, the mean absolute difference (MAD) between the satellite and in-situ measurements is computed, and each absolute difference (AD) higher than three times the MAD is discarded. Similarly, the mean absolute percentage difference (MAPD) between the satellite and in-situ measurements is computed, and each absolute percentage difference (APD) higher than three times the MAPD is discarded.

Finally, for each matchup, all reflectances - for the four bands at 442 nm, 490 nm, 551 nm and 668 nm for both levels 2A and 2W – must be positive. If at least one reflectance is negative, then the matchup is discarded.

This pipeline aims at validating the processor from a scientific, robust perspective, where only meaningful matchups are used after a strict filter.

iii. Common validation pipeline

For the two validation pipelines, the satellite and in-situ reflectances must be valid for the four bands at 442 nm, 490 nm, 551 nm and 668 nm for both levels 2A and 2W in order for the matchup to be accepted.

Otherwise, the matchup is discarded. This ensures that metrics are computed similarly for all bands and for both levels.

The advantage of using the median of the set of valid pixels is that it automatically discards the few pixels that can be contaminated by a structure and that are not flagged. For example, if one pixel over the nine pixels is contaminated by a structure and has not been flagged, the median will use the value of another pixel, which is more representative of the area of interest, and the contaminated pixel will not have any impact on the final value.

iv. Number of matchups obtained

At the end of the first validation pipeline (the "products" pipeline), 268 matchups are left, with 201 over coastal oceans, 62 over lakes, 3 over rivers and 2 not classified. After the second validation pipeline (the "algorithms" pipeline), the pipeline with the most drastic filtering, 165 matchups are left, with 106 over coastal oceans, 56 over lakes and 2 not classified. As very few matchups are available over rivers and in the "not classified" class, no specific analysis is performed for these matchups. They are considered in the "all water types" analysis.

3.2.5 Matchups performance indicators

In order to evaluate the difference between satellite level 2A and 2W data when compared to in-situ measurements, different metrics are set up. Each time, the four Sentinel-2 bands at 440 nm, 490 nm, 560 nm and 665 nm are displayed, with results for both Sen2Water and Sen2Cor processors and for the two validation pipelines.

To measure the bias between satellite and in-situ measurements, mean difference and β metric are used.

To measure the spread of satellite measurements around in-situ measurements, root mean square differences (RMSD) and ε metric are used.

The β and ε metrics are presented in equations [C] and [D] below :

$\beta = 100 \times sign(Z) \times (10^{|Z|} - 1)$ [C]

where $Z = median(log_{10}(satellite\,reflectance \div insitu\,reflectance))$

$\varepsilon = 100 \times (10^{Y} - 1)$ [D]

where $Y = median|log_{10}(satellite\,reflectance \div insitu\,reflectance)|$

Coefficients of determination are also compared for the different processors, bands and validation pipelines.

3.2.6 Product inter-comparison

Sen2Water products are compared to OLCI Level 2 Ocean Colour Full Resolution. Time difference between the acquisitions by OLCI and MSI is as short as possible. Products are collocated and spectra are compared at various locations over the water pixels. Histograms of relative differences for different bands are also computed.

The following products are compared:

- Products S2A_MSIL1C_20240719T102021_N0510_R065_T32TNT_20240719T122006 and S3B_OL_2_WFR____20240719T100805_20240719T101105_20240720T165702_0179_095_236_2160_MAR_O_NT_003

- Products S2A_MSIL1C_20240104T022321_N0510_R103_T51PWN_20240104T032345 and S3B_OL_2_WFR____20240104T015920_20240104T020220_20240105T093953_0179_088_117_2700_MAR_O_NT_003
- Products S2B_MSIL1C_20230806T100559_N0509_R022_T34WFT_20230806T104651 and S3A_OL_2_WFR____20230806T092211_20230806T092511_20230807T221544_0179_102_036_1800_MAR_O_NT_003

3.3 Test results

3.3.1 Visual inspection and quality assessment

For all inspected products, only bands 1, 2, 3, 4, 5, 6 and 8A have valid reflectances on open oceans. Bands 7, 8, 9, 10, 11 and 12 are set to NaN on open oceans. This is coherent with requirement [REQ-07] which mentions the restrictions of C2RCC water processor.

a) Product S2B_MSIL1C_20230808T090559_N0509_R050_T32MRU_20230808T125427.SAFE

Almost all water pixels are flagged as cloudy, yet no cloud is visible to the naked eye on all flagged parts of this product. L1C band 10 image has a mean reflectance of about 0.001, thus we can assume that no thin cirrus is present in the scene. Some water pixels near the shore are flagged as clear ocean water, when no to little difference with pixels flagged as cloudy is noticeable.

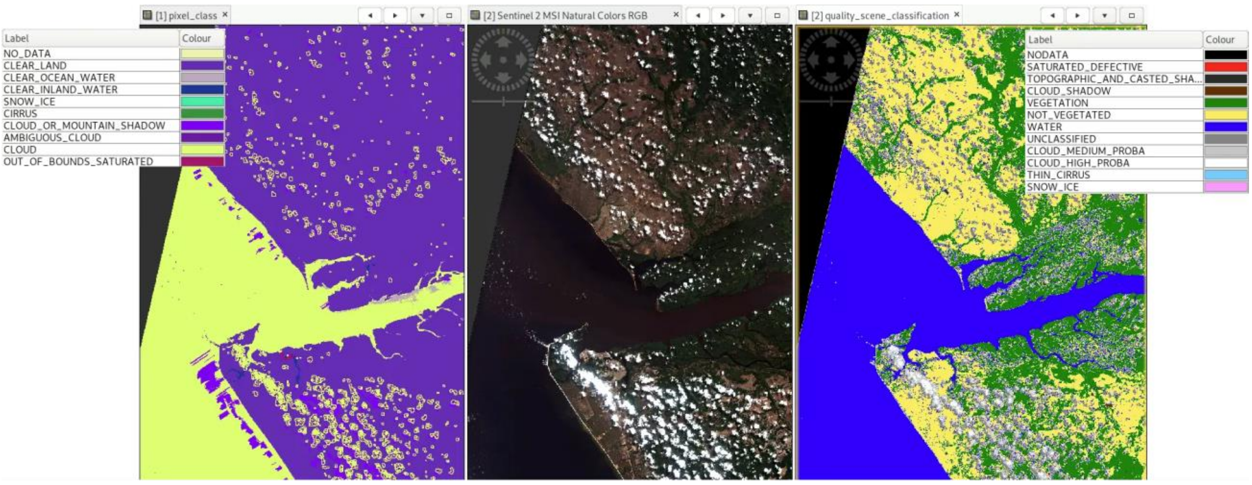

Figure 3-2: Sen2Water pixel classification (left), Sen2Cor RGB reflectance (middle) and Sen2Cor pixel classification (right) show that while ocean is classified as “water” and not “cloud” with Sen2Cor, it is classified as “cloud” with Sen2Water, although it seems that no cloud is present.

A repetition of the test with Sen2Water version v0.4.2 resolves the issue.

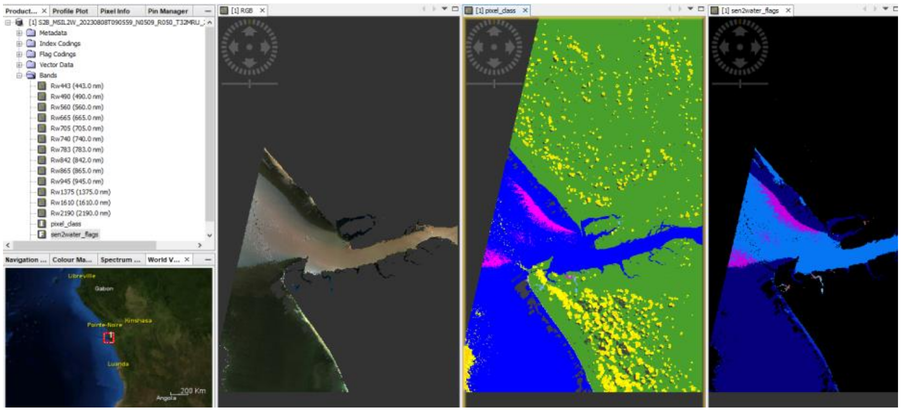

Figure 3-3: Same scene re-processed with Sen2Water v0.4.2, left pseudo-RGB of water-leaving reflectances, middle pixel_class which is mainly clear water in the ocean, right algorithm selection with ACOLITE (light blue) in turbid water, and AC out-of-range flags (pink)

b) Product S2A_MSIL1C_20230121T111351_N0509_R137_T30UWU_20230121T131033.SAFE

Beaches, foreshores and riverbanks are often labelled as "cloud" in low-tide situation, which is the case in this product (high tide situation corresponds to the following product, namely S2B_MSIL1C_20230625T110619_N0509_R137_T30UWU_20230625T114918.SAFE).

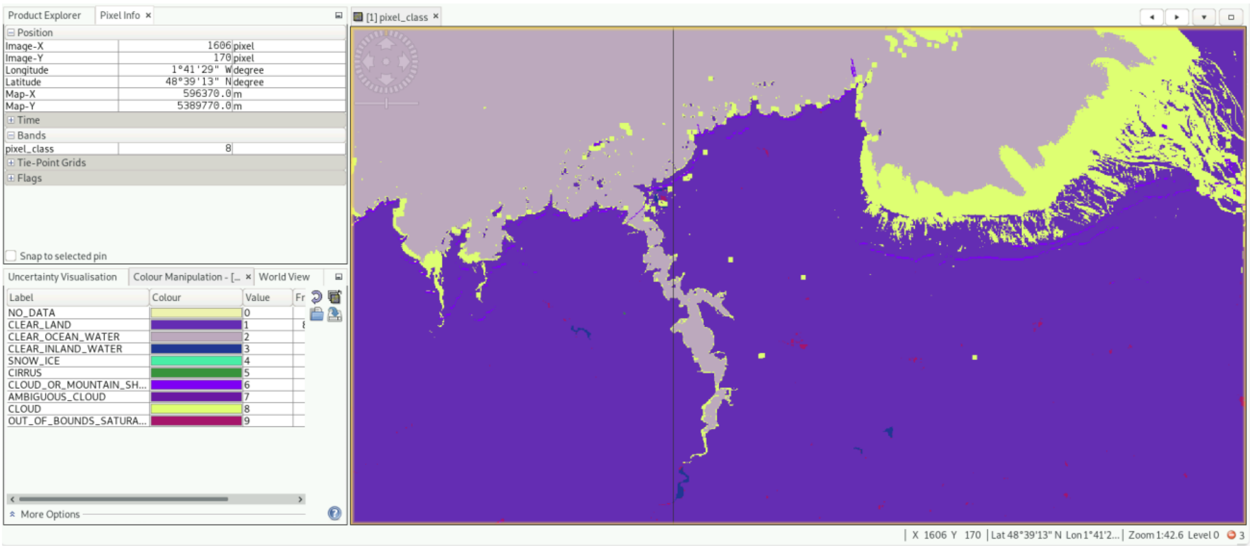

Figure 3-4: pixels are labelled as "clouds" on tidal land according to the pixel classification, while they should be labelled as "clear land"

Water spectra for five different points are displayed in the figure below. The five points are located in areas where only processor C2RCC is used. All spectra look reasonable for clear coastal waters. No negative reflectance is measured.

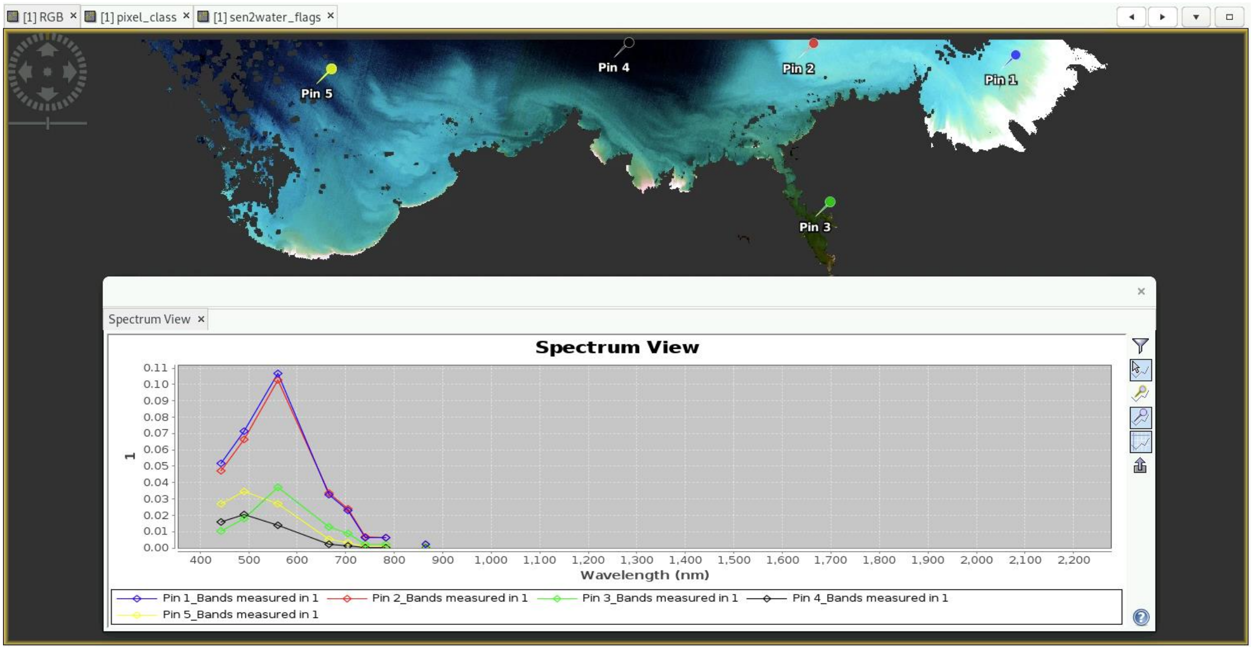

Figure 3-5: Sen2Water RGB reflectance and water spectra for five different points over coastal ocean

c) Product S2B_MSIL1C_20230625T110619_N0509_R137_T30UWU_20230625T114918.SAFE

This product corresponds to the same tile as the previous product, but for a high tide situation, whereas the previous one was low tide.

Sea mask is clearly taking into account the tide: it evolves with low and high tide.

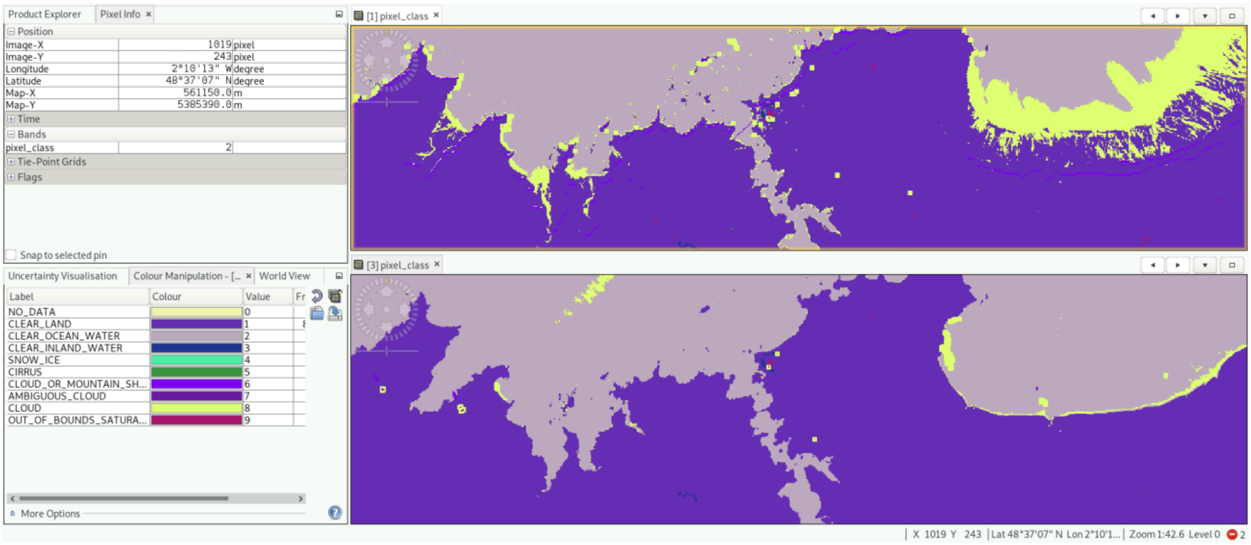

Figure 3-6: low and high tide pixel classification comparison: land-sea limit moves with tide in the top product (low tide, S2A_MSIL1C_20230121T111351_N0509_R137_T30UWU_20230121T131033) compared to the lower product (high tide, S2B_MSIL1C_20230625T110619_N0509_R137_T30UWU_20230625T114918)

Some beaches, foreshores and riverbanks are sometimes labelled as "cloud", on the right hand part of the image.

Limit between two detectors is clearly visible on ocean. Indeed, reflectance at the limit of two detectors is very different from surrounding reflectances: it can be two to three times lower, or two to three times higher, or even nan.

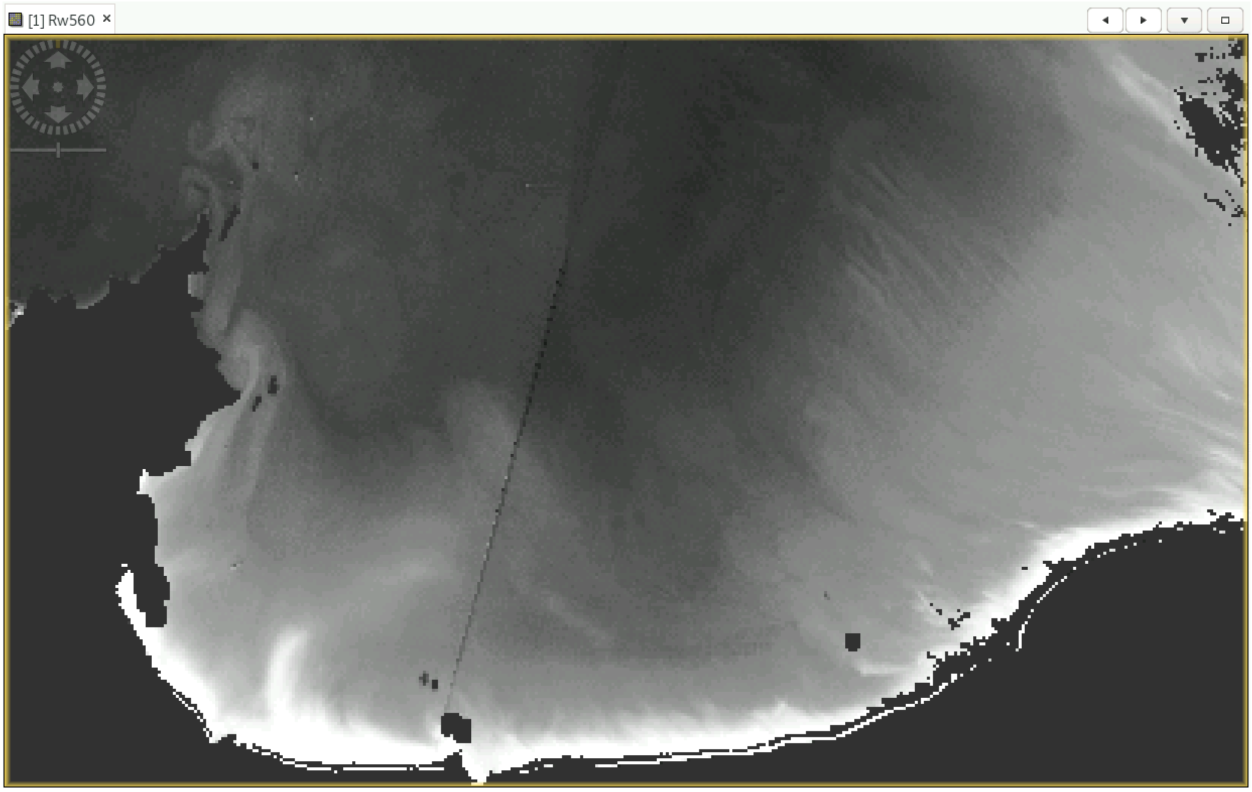

Figure 3-7: limit between two detectors is clearly visible at 560 nm, with some pixels NaN on the limit (reflectance range is $1 \cdot 10^{-3}$ to $1 \cdot 10^{-1}$)

d) Product S2B_MSIL1C_20230823T095559_N0509_R122_T33TVL_20230823T121626.SAFE

Stripes and detectors limit are clearly visible in this product. It is interesting to mention that both across and along-track stripes are visible.

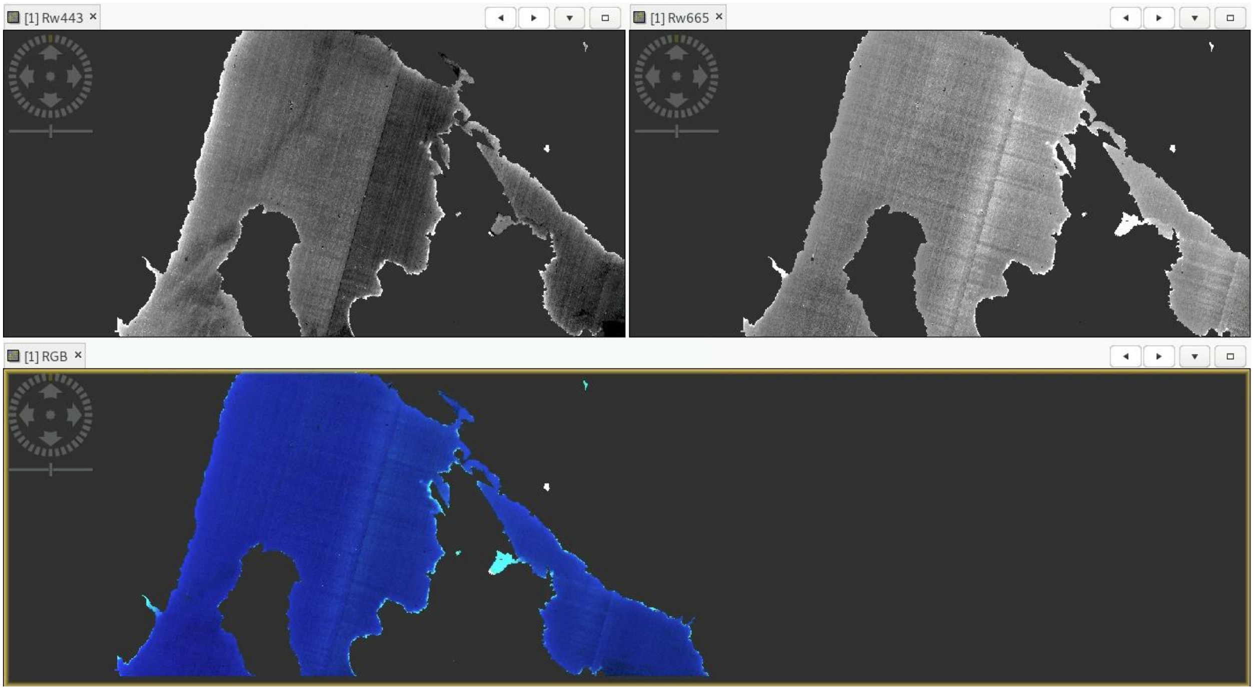

Figure 3-8: stripes and detectors limit on clear ocean waters are visible for reflectances at 440 nm (top left figure, reflectance range is $1 \cdot 10^{-2}$ to $2 \cdot 10^{-2}$) and 665 nm (top right figure, reflectance range is $1 \cdot 10^{-4}$ to $1 \cdot 10^{-3}$), but barely on Sen2Water RGB image (bottom)

e) Seasonal lakes

Product S2A_MSIL1C_20231126T100331_N0509_R122_T33TVL_20231126T120138.SAFE

Two seasonal lakes are in this product and are absent in the previous product. They are detected and not flagged as “clear land”, but they are falsely flagged as “out of bounds saturated”.

Product S2B_MSIL1C_20230823T095559_N0509_R122_T33TVL_20230823T121626

In this acquisition over the same area, the seasonal lakes are not present. In the L2W product, the area is flagged as “with polymer” and “polymer invalid”. No reflectance is available over the area.

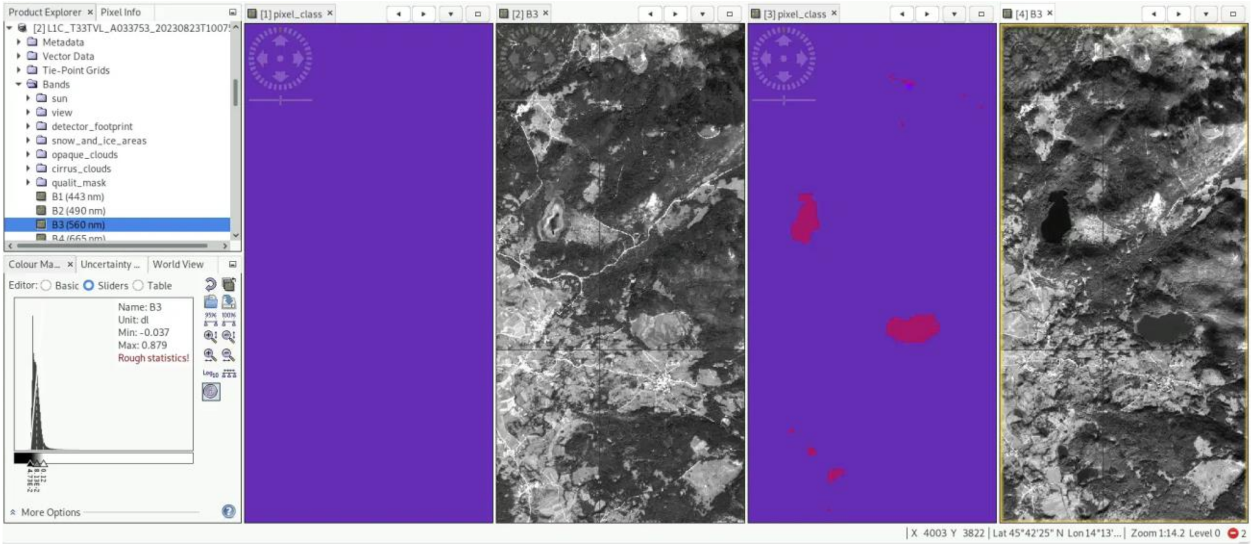

Figure 3-9: comparison of tile T33TVL over Lake Palčje, Slovenia, on the 23/08/2023 (left) and on the 26/11/2023 (right), with Sen2Water pixel classification and L1C band 3 : seasonal lakes are detected but not flagged as clear inland water

f) Product S2A_MSIL1C_20240104T022321_N0510_R103_T51PWN_20240104T032345.SAFE

This product looks good. Areas flagged as cloud shadow seem overestimated for some clouds, on the right hand side of the image for example.

Figure 3-10: cloud shadows in the pixel classification mask (top) seem overestimated when compared to L1C RGB reflectances (bottom)

g) Product S2A_MSIL1C_20231121T023011_N0509_R046_T52SBD_20231121T041548.SAFE

This product is very small, with only about 60 kilometres square, located west of South Korea. All pixels are flagged as clear water. Reflectances are very noisy and stripes can be seen, although the disturbance levels are very small in absolute terms. On bands 1 to 4, stripes seem to occur in two orthogonal directions, along-track but also across-track.

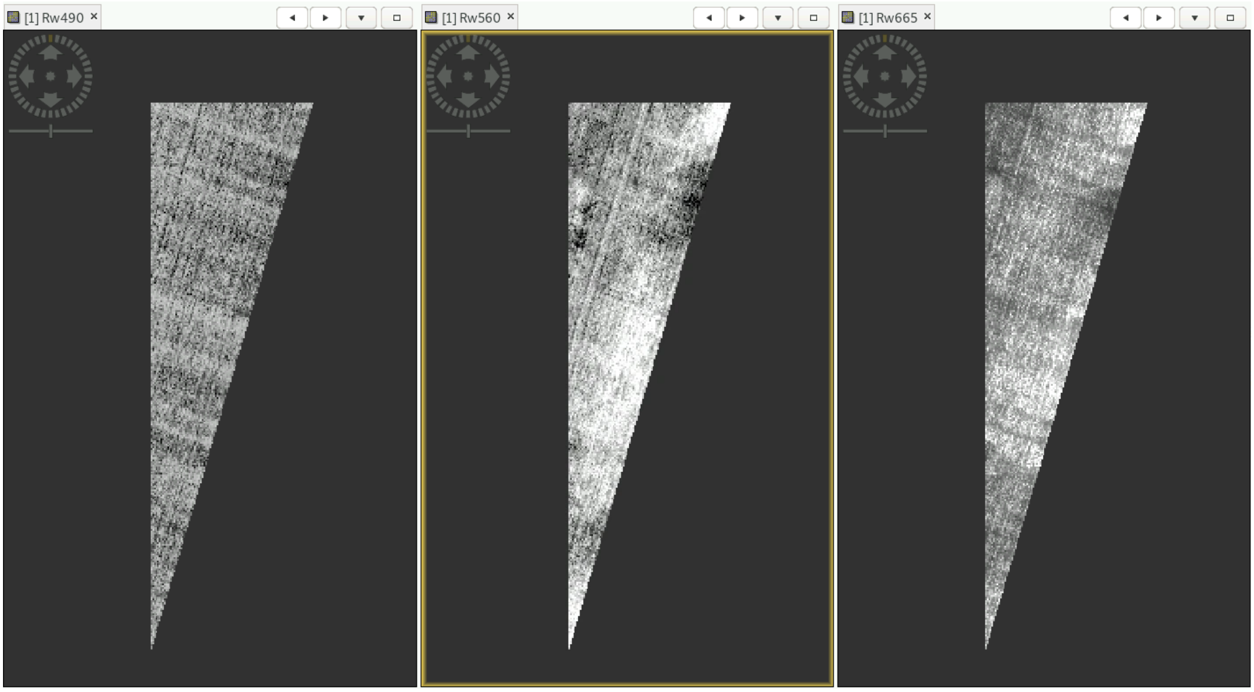

Figure 3-11: Sen2Water bands 2 (left), 3 (middle) and 4 (right) are noisy and some stripes can be seen (band 2 reflectance range is $5 \cdot 10^{-2}$ to $7 \cdot 10^{-2}$, band 3 reflectance range is $8.2 \cdot 10^{-2}$ to $8.8 \cdot 10^{-2}$ and band 4 reflectance range is $1.5 \cdot 10^{-2}$ to $2.5 \cdot 10^{-2}$)

Water spectra are displayed in figure below for two different points.

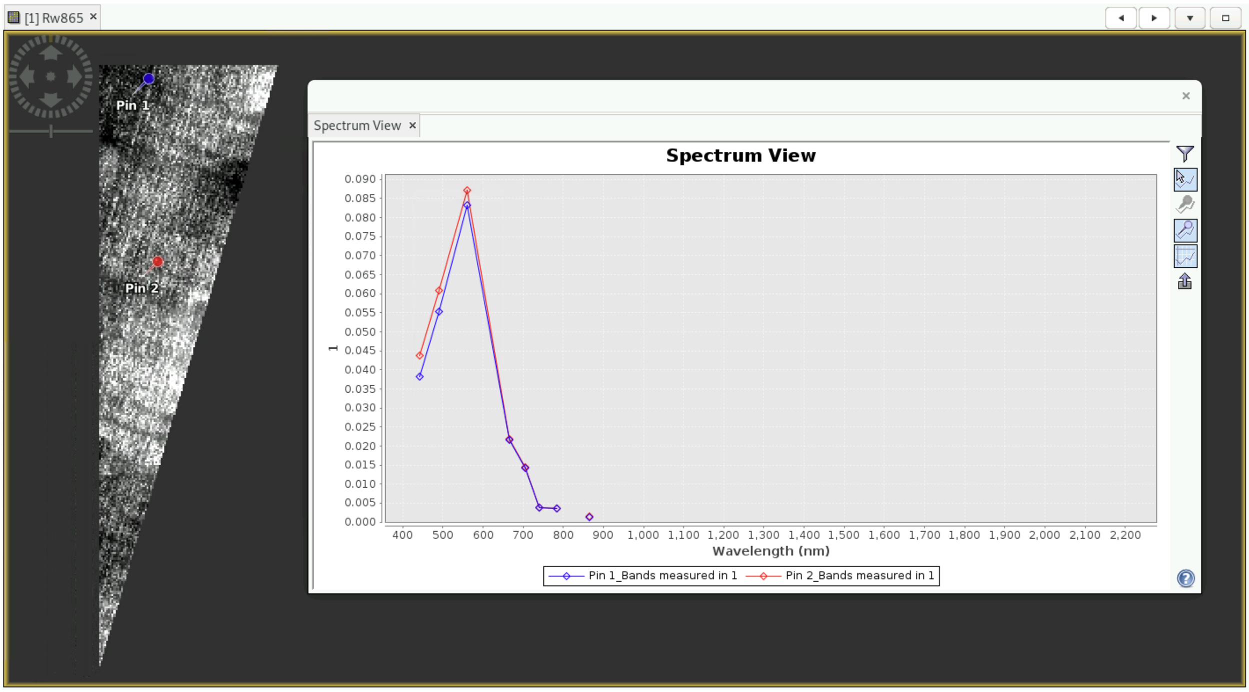

Figure 3-12: Sen2Water reflectance and spectra for two different points

h) Product S2B_MSIL1C_20240103T221939_N0510_R029_T01KAB_20240103T232410.SAFE

Product could not be processed (product located on both sides of the ante-meridian).

A repetition of the test with Sen2Water version v0.4.2 resolves the issue.

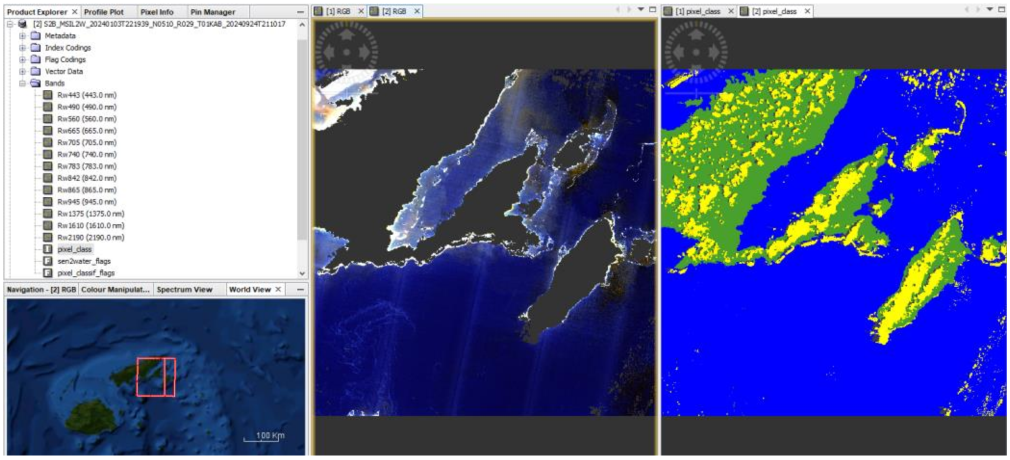

Figure 3-13: Granule of 01KAB without artefacts at ante-meridian (fixed in version 0.4.2)

i) Product S2A_MSIL1C_20210702T101031_N0500_R022_T32TNM_20230131T141414.SAFE

This product contains missing packets. Pixels classified as clear water were correctly processed.

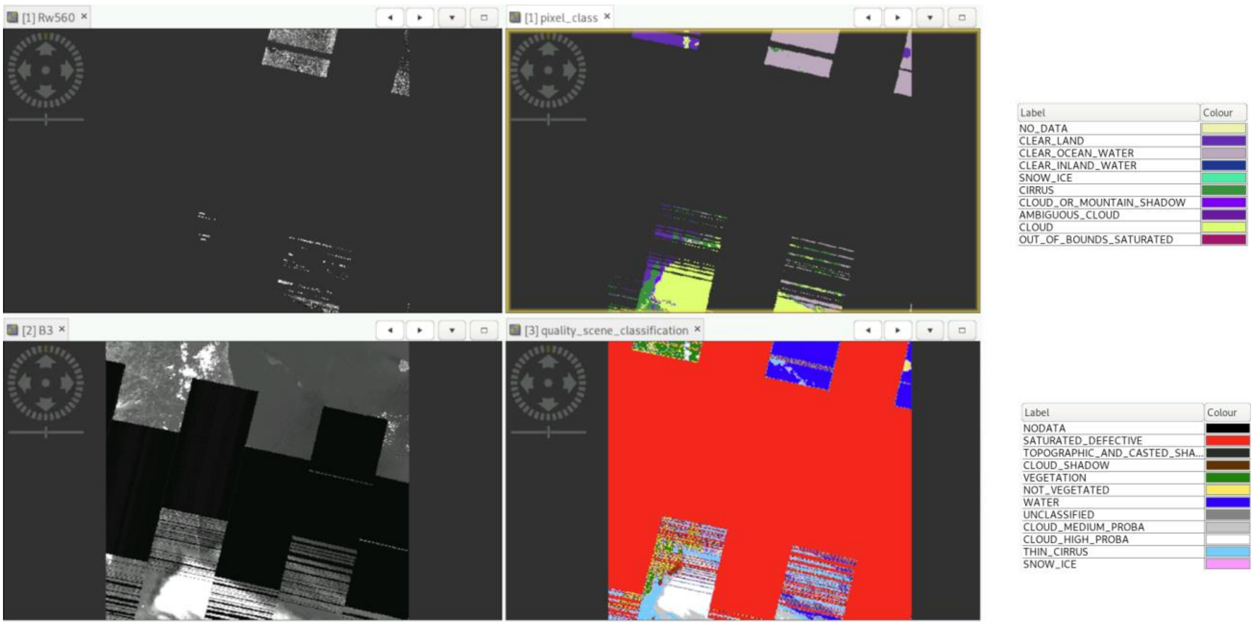

Figure 3-14: products with missing packets: not all clear pixels from Sen2Water pixel classification (upper right) have a reflectance in Sen2Water 560 nm band (upper left) and not all clear pixels from Sen2Cor pixel classification (lower right) are clear in Sen2Water pixel classification (upper right) – L1C reflectances are displayed (lower right) for context

One can notice that Sen2Water seem to use less pixels than Sen2Cor, according to the two pixel classifications. Moreover, not all pixels labelled as “clear land” in Sen2Water pixel classification have been computed in Sen2Water 560 nm band (see the top left part of Sen2Water reflectance at 560 nm), while all pixels labelled as “vegetation” or “not vegetated” are computed in Sen2Cor 560 nm band (not shown).

j) Product S2B_MSIL1C_20230806T100559_N0509_R022_T34WFT_20230806T104651.SAFE

This product has been sensed in Sweden, at a mean latitude of about 65° North. Sun zenith angle is thus high. However, no particular problem has been spotted. As in previous products, one can notice detector limits and stripes ; cloud shadows are maybe overestimated.

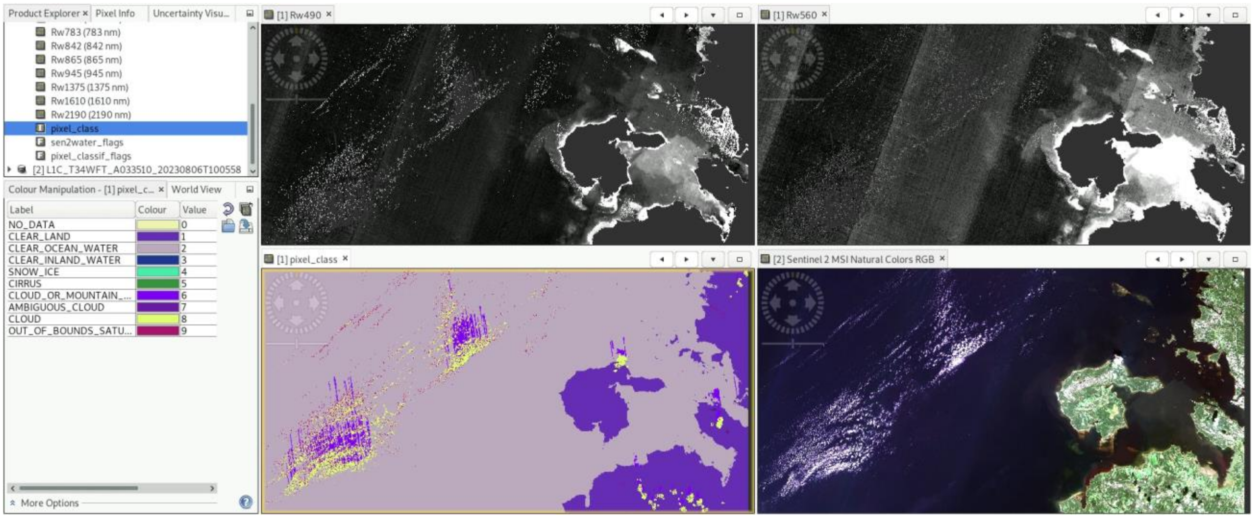

Figure 3-15: high latitude of the product has no clear impact on reflectances at 490 nm (top left), 560 nm (top right) nor on pixel classification (bottom left) ; L1C RGB reflectance is displayed for context (bottom right) ; cloud shadows seem overestimated

k) Product S2B_MSIL1C_20231226T105359_N0510_R051_T31SBD_20231226T114540.SAFE

This product contains pixels located on both sides of the Greenwich meridian. It has been processed with no difficulty. As for previous products, limits between detectors and stripes both in along and across track directions are visible.

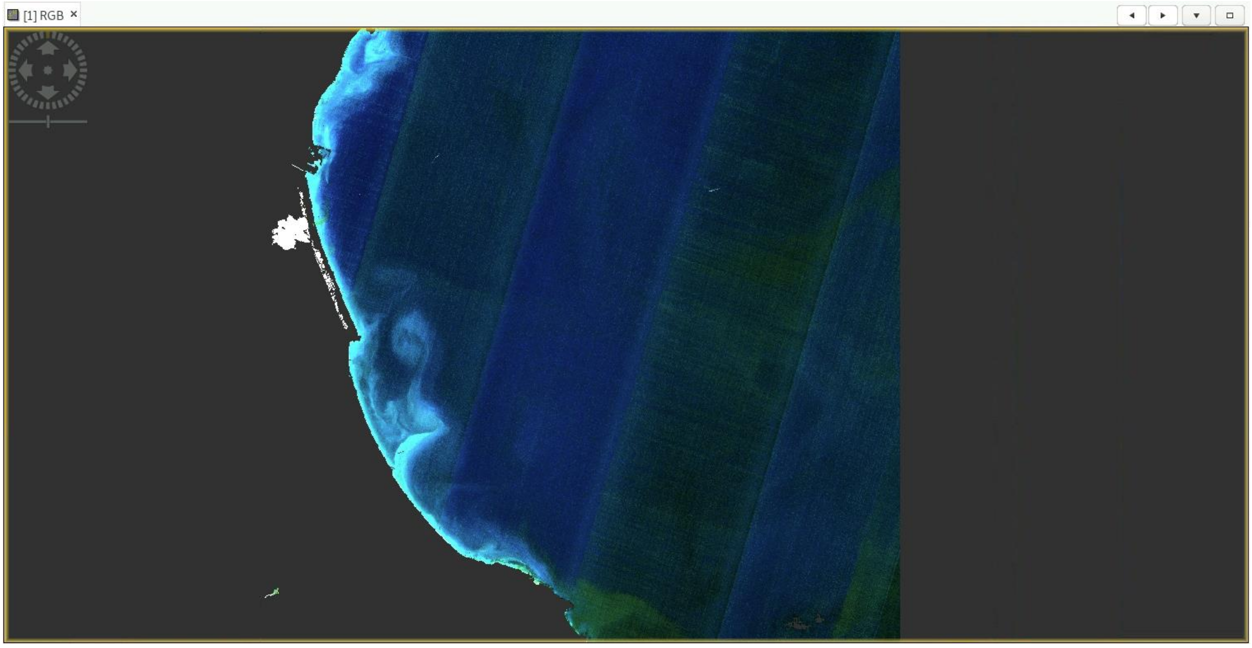

Figure 3-16: Sen2Water RGB reflectance (reflectance range is $1 \cdot 10^{-4}$ to $2 \cdot 10^{-2}$ for all bands), limits between detectors and along and across track stripes are visible

An area about 10 km South of Valencia, Spain, is made of lagoons and rice fields. This area is flagged as “clear ocean water” when the distance to the shoreline is closer than about 1 km, but when the distance to the shoreline is bigger than 1 km, the area is flagged as “out of bounds saturated”. Thus, one can notice two zones classified differently with no physical difference between them noticeable at the naked eye. No reflectance is available for products flagged as “out of bounds saturated”.

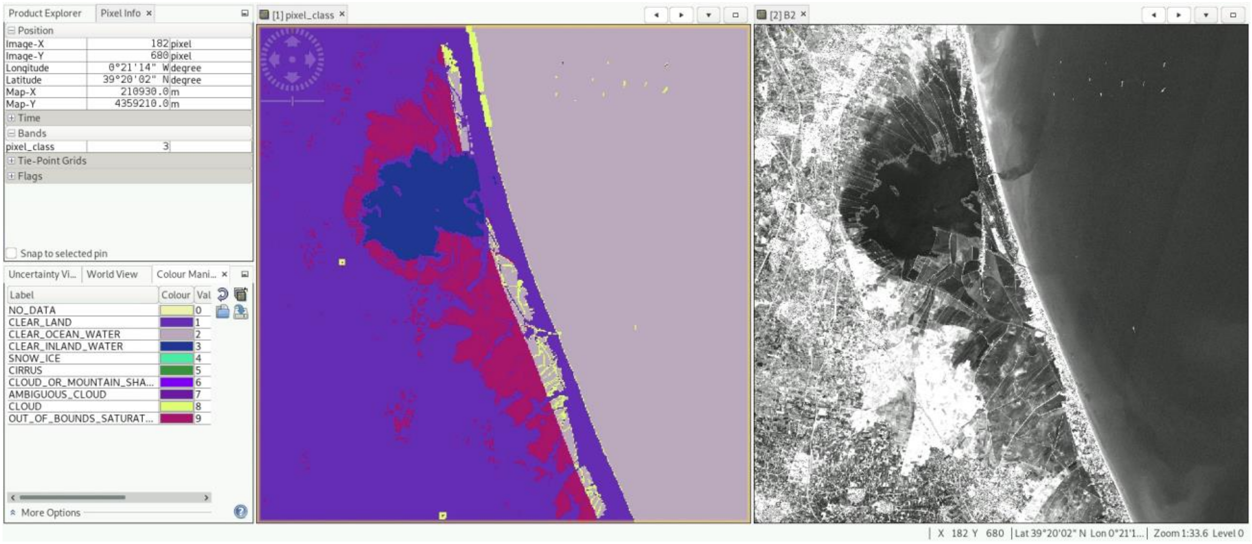

Figure 3-17: Sen2Water pixel classification on the left and L1C band 2 on the right: rice fields are correctly classified as “clear water” when distance with shoreline is lower than about 1 km, but they are incorrectly classified as "out of bound saturated" pixels otherwise

Water spectra are displayed in the following figure, for different points: point 1 is located in an area where reflectance is computed with POLYMER, point 2 with C2RCC and ACOLITE, point 3 with ACOLITE only and point 4 with C2RCC only. Spectra for pin 1 shows a strong and unexpected maximum of reflectance at

705 nm. There is also a less marked peak in the reflectance for this band for pins 2 and 3. Reflectance values above 900 nm are high for pin 1, which could be explained by a high turbidity or ground reflectance effects.

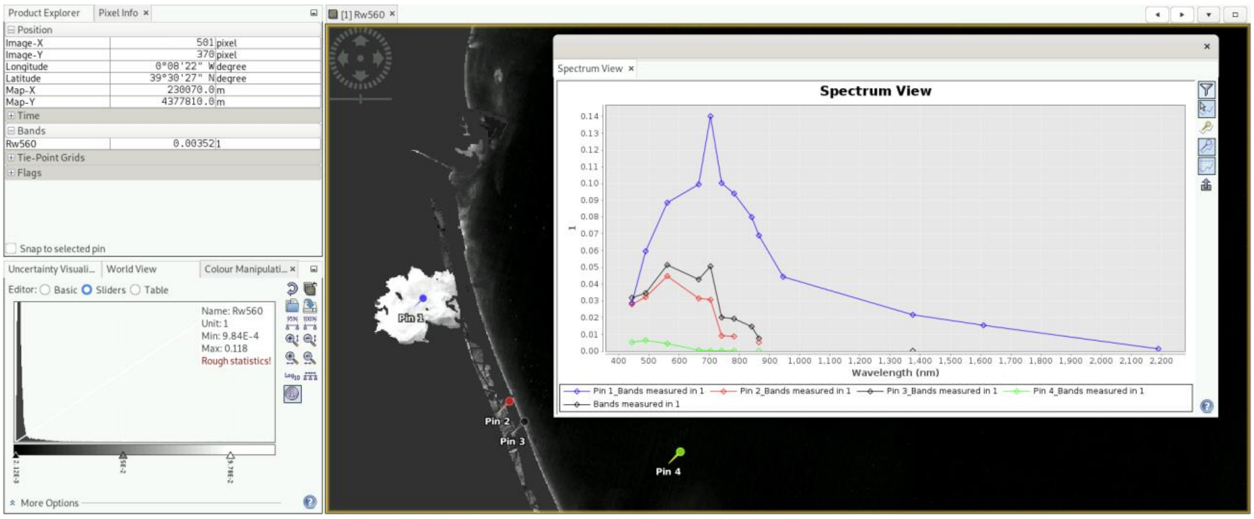

Figure 3-18: Sen2Water reflectance at 560 nm and spectra for four different points for which different algorithms are used to compute reflectance

l) Product S2A_MSIL1C_20240617T051231_N0510_R033_T42FXL_20240617T081319.SAFE

White caps are visible in this product. Most of white caps are flagged as clouds, surrounding water is flagged as “out of bounds saturated”. However, reflectance is computed even for pixels flagged as “out of bouds saturated”.

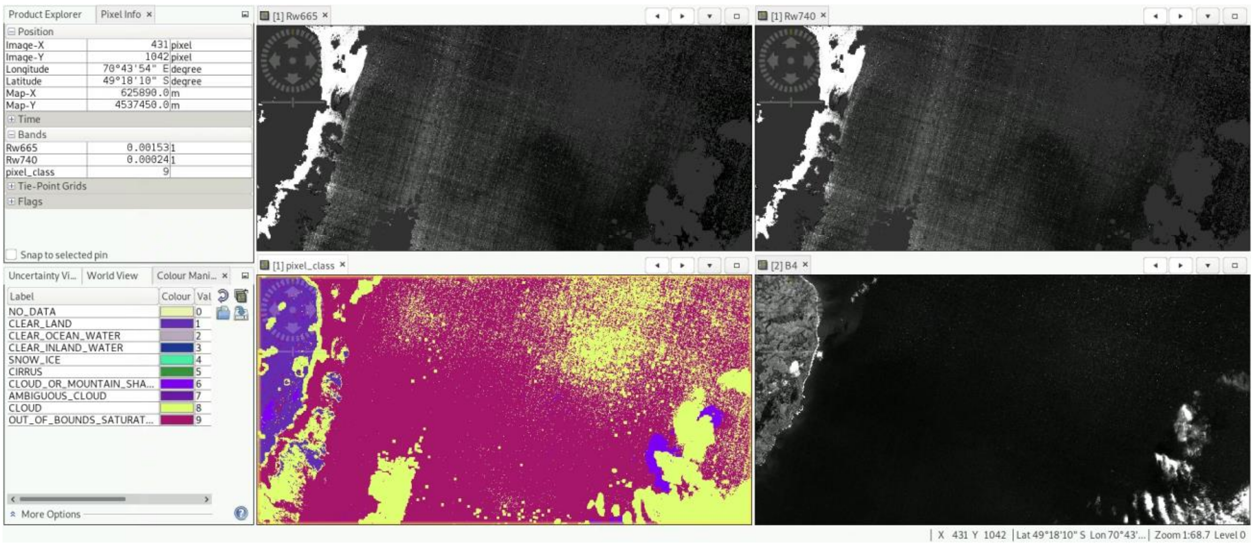

Figure 3-19: whitecaps are visible on the top right corner of this image and are not processed in Sen2Water reflectance at 665 nm (top left) and at 740 nm (top left), because they are flagged as “cloud” in Sen2Water pixel classification (bottom left) ; L1C reflectance at 665 nm (bottom right) for context

m) Product S2A_MSIL1C_20240330T140751_N0510_R053_T24VVR_20240330T174815.SAFE

Sea ice (ice floe) is visible in this product. Most of it is correctly labelled as “snow/ice”, however pixels near the shoreline are incorrectly labelled as “cloud” and thus some are also labelled as “cloud shadow”. As noted previously, noise, detectors’ limits and stripes can be observed on reflectances.

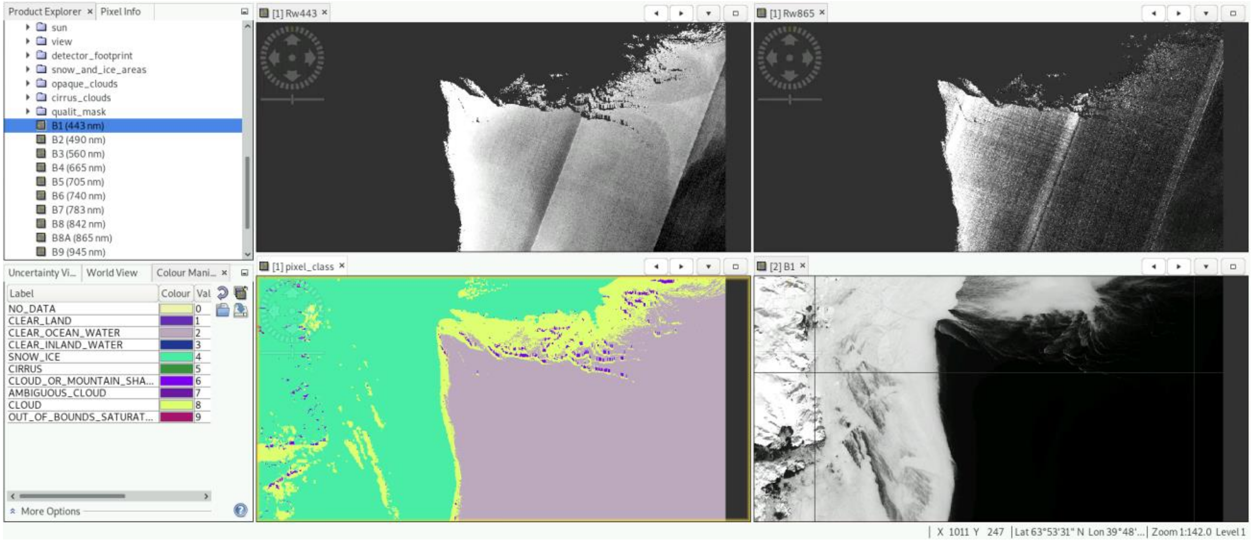

Figure 3-20: sea ice on Sen2Water reflectance at 440 nm (top left) and at 865 nm (top left), Sen2Water pixel classification (bottom left) and L1C reflectance at 440 nm (bottom right) – shoreline is flagged as “cloud”

Water spectra are presented for four different points located in the ocean in the figure below. The are consistent with a very pure water.

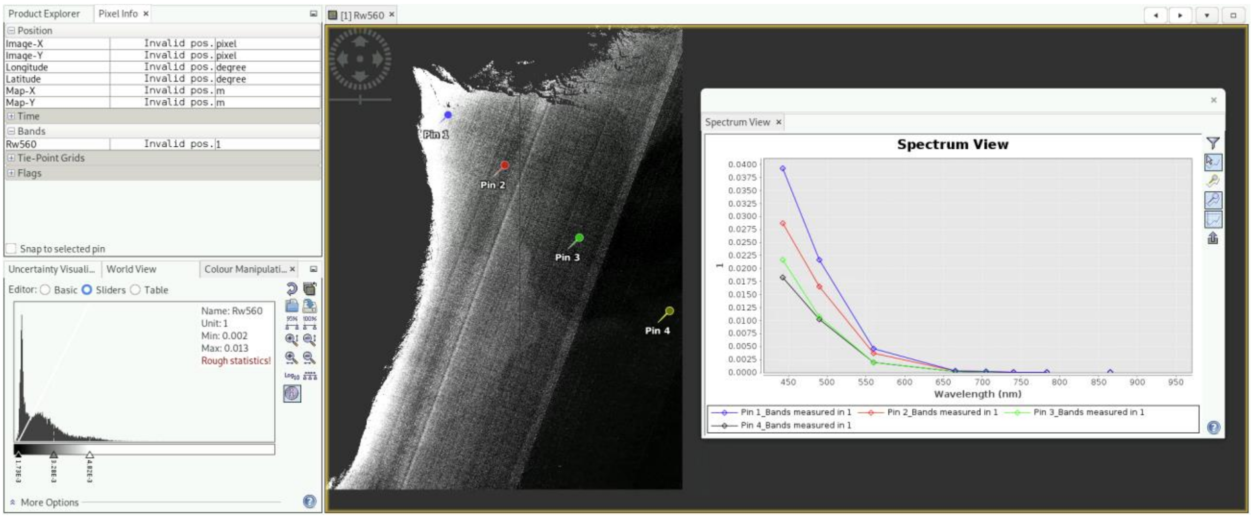

Figure 3-21: Sen2Water reflectance at 560 nm and water spectra for four different points

n) Product S2A_MSIL1C_20240601T173911_N0510_R098_T12QZJ_20240602T000646.SAFE

This product is affected by sun glint. No pixel is labelled as clear ocean water, however many pixels seem to be clear water. Most pixels are labelled either “cloud” or “ambiguous cloud”.

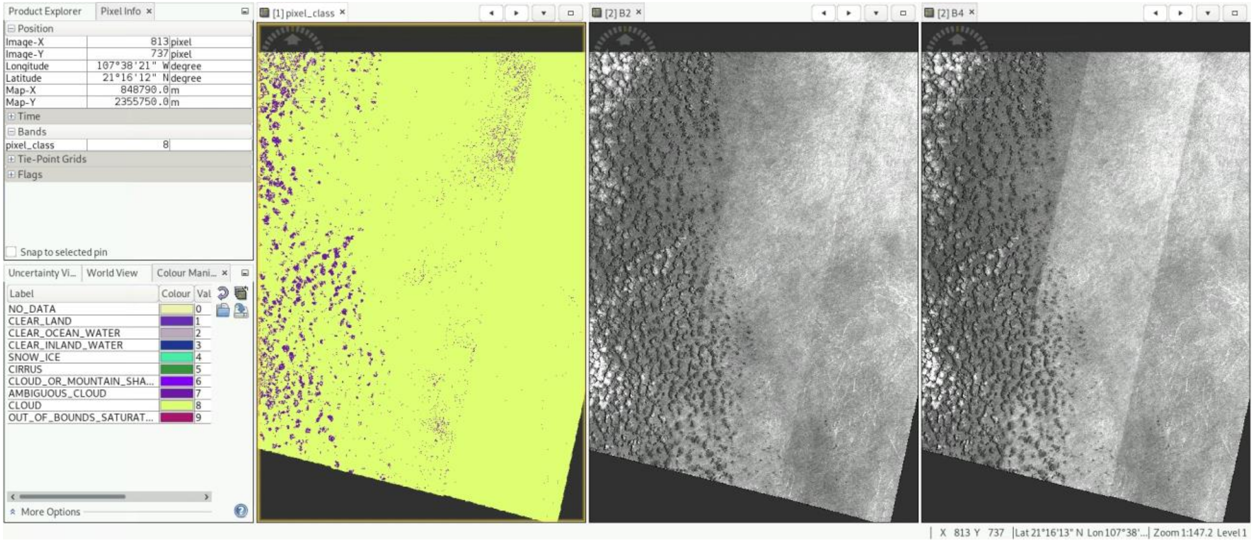

Figure 3-22: clear pixels flagged as “cloud” in a product in which sun glint is important ; Sen2Water pixel classification on the left, L1C reflectance at 490 nm on the middle, L1C reflectance at 665 nm on the right

o) Product S2A_MSIL1C_20240719T102021_N0510_R065_T32TNT_20240719T122006.SAFE

This product is located over the Constance Lake, Germany. Scene classification and reflectance look correct except over the Rhine river at the South-East corner of the lake, where water is very turbid. This river is classified as “out of bounds saturated”, “with polymer” and “polymer invalid” and no reflectance is computed. This may be an expected behaviour for highly turbid waters, in this case this should be explained to the user.

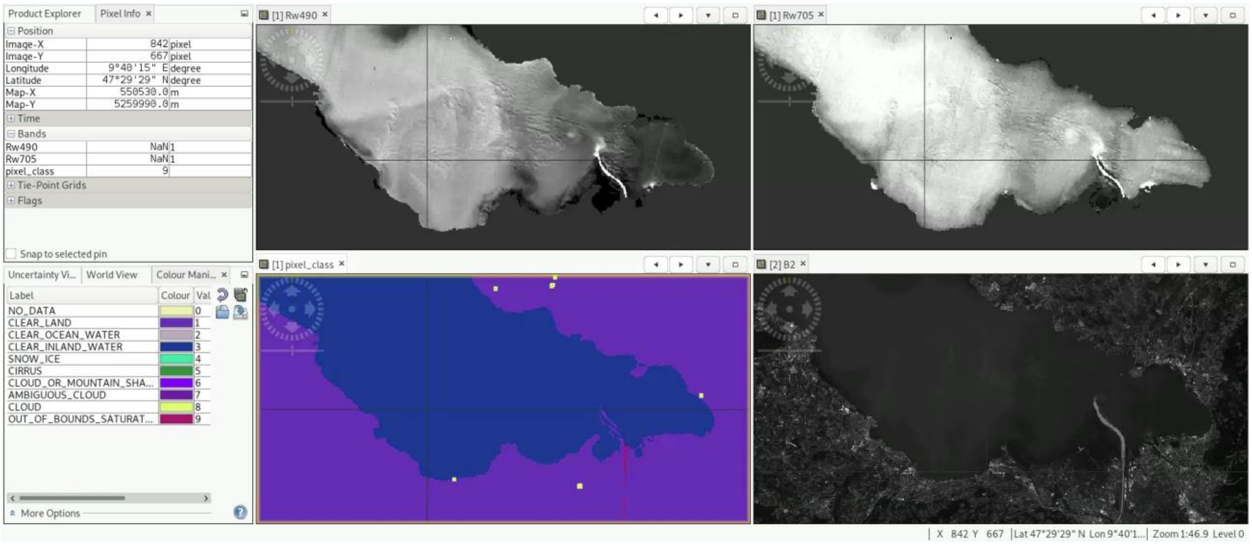

Figure 3-23: inland water over Lake Constance, Germany : L2W reflectance at 490 nm on the top left corner, L2W reflectance at 705 nm on the top right corner, Sen2Water pixel classification on the bottom left corner and L1C reflectance at 490 nm on the bottom right corner. Rhine river is labelled as “out of bounds saturated”

POLYMER processor is used to compute the reflectance over Lake Constance, Germany. Negative values are observed for highest wavelengths, such as 865 nm, for which a histogram is presented below.

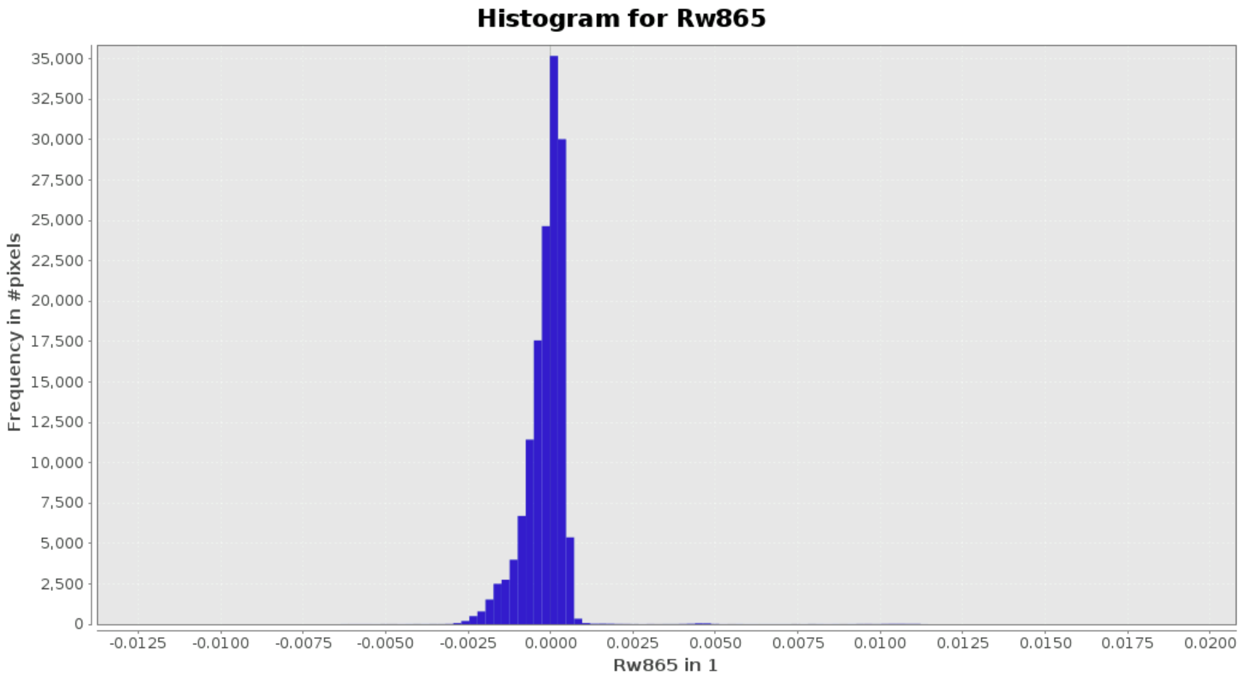

Figure 3-24: histogram of Sen2Water reflectance over Lake Constance, Germany, at 865 nm, with negative values

Water spectra are presented in figure below for five different points in the lake, with point number 3 located at the mouth of Rhine River. Negative reflectances are measured for all pins in the SWIR. Except for the negative reflectance on B09, the spectrum of pin 3 looks reasonable considering the very high water turbidity In any case this point is flagged as "out of bound - saturated".

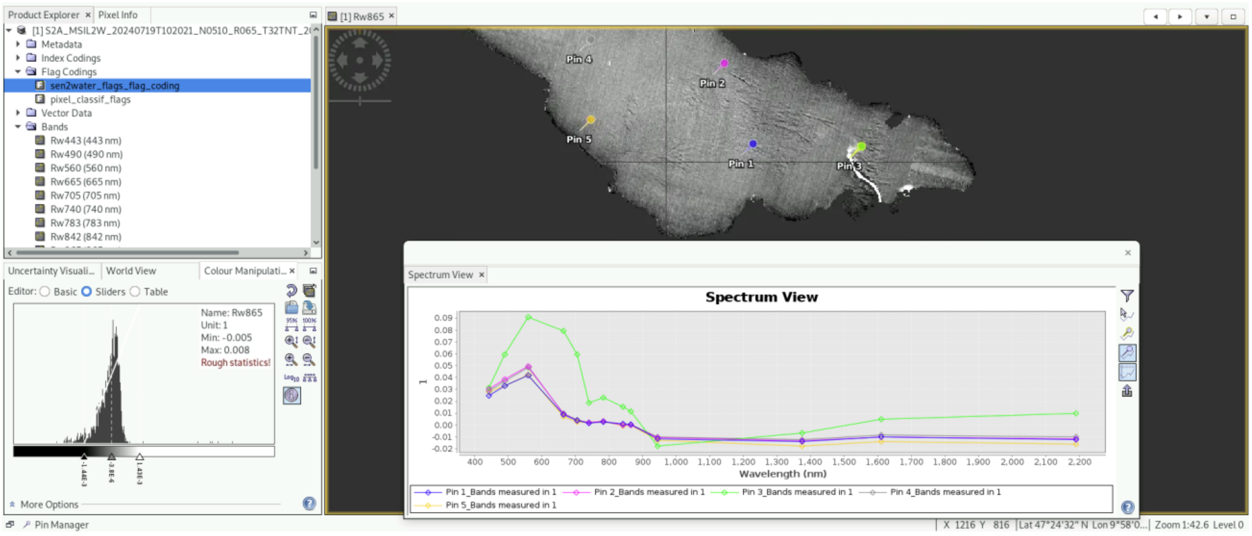

Figure 3-25: Sen2Water reflectance at 865 nm and reflectance spectra for 5 different points

3.3.2 In-situ: scatter plots and performance indicators for all water types

First of all, results are presented for all water types available (coastal oceans, lakes, rivers and other).

Scatter plots of satellite reflectances as a function of in-situ reflectances are displayed with data from products computed with both Sen2Cor and Sen2Water, for the two validation pipelines and for the four bands studied (band 1 at 440 nm, band 2 at 490 nm, band 3 at 560 nm and band 4 at 665 nm).

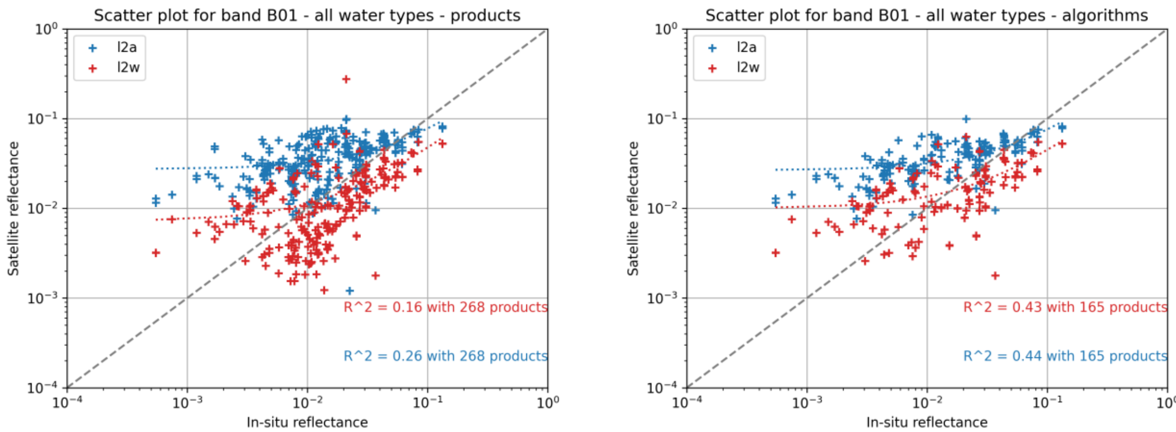

Figure 3-26: scatter plots of satellite reflectances computed with Sen2Cor (blue) and Sen2Water (red) as a function of in-situ reflectances for band 1 at 440 nm, for all water types, for the "products" validation pipeline on the left and the "algorithms" on the right

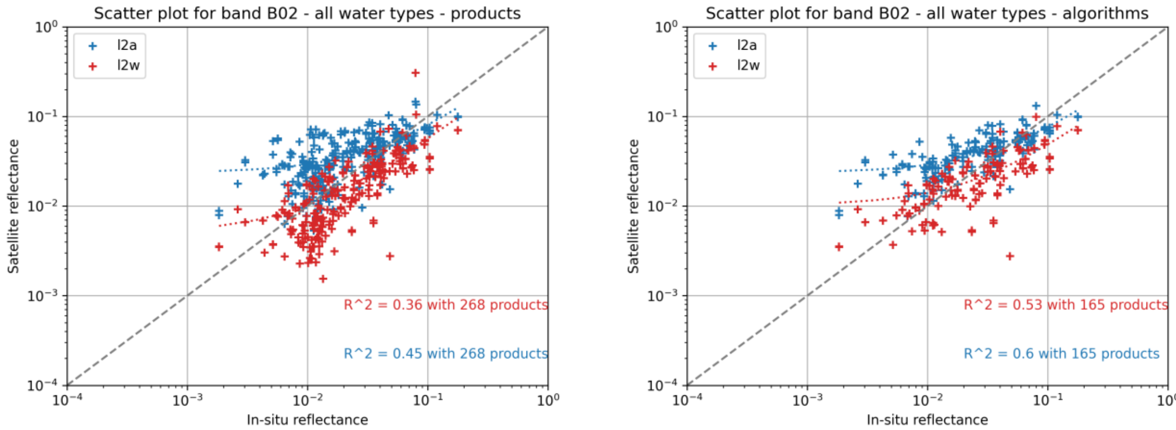

Figure 3-27: scatter plots of satellite reflectances computed with Sen2Cor (blue) and Sen2Water (red) as a function of in-situ reflectances for band 2 at 490 nm, for all water types, for the "products" validation pipeline on the left and the "algorithms" on the right

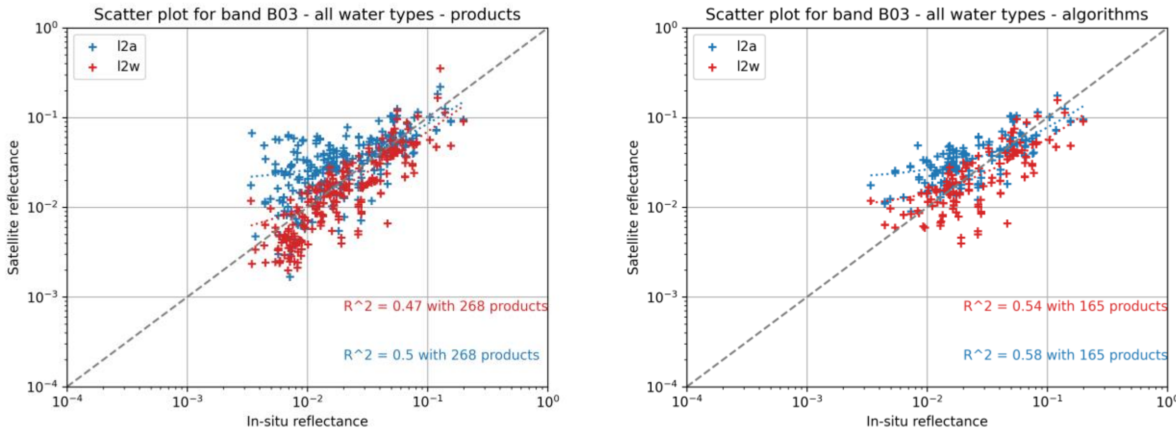

Figure 3-28: scatter plots of satellite reflectances computed with Sen2Cor (blue) and Sen2Water (red) as a function of in-situ reflectances for band 3 at 560 nm, for all water types, for the "products" validation pipeline on the left and the "algorithms" on the right

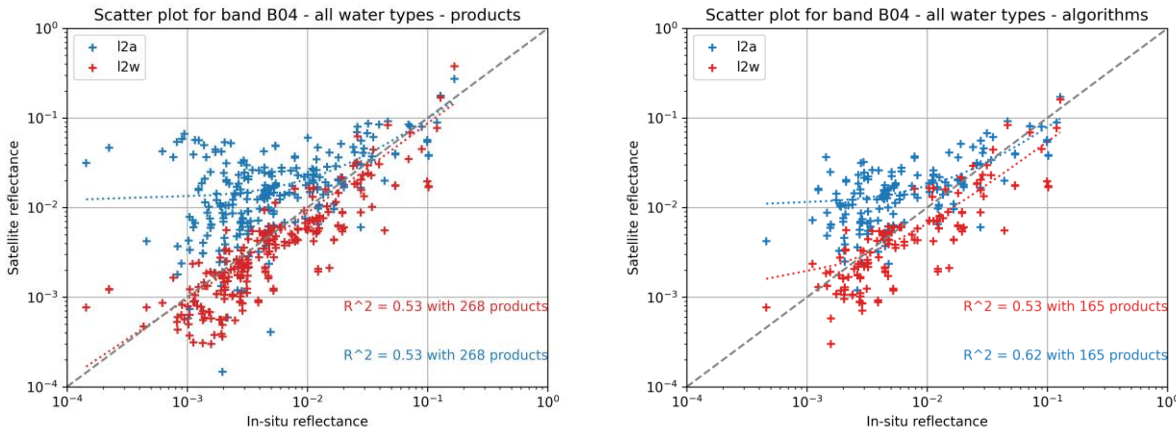

Figure 3-29: scatter plots of satellite reflectances computed with Sen2Cor (blue) and Sen2Water (red) as a function of in-situ reflectances for band 4 at 665 nm, for all water types, for the "products" validation pipeline on the left and the "algorithms" on the right

These scatter plots show that the Sen2Water processor tends to produce lower reflectances than the Sen2Cor processor. Overall, the points seem to be closer to the 1:1 line with the Sen2Water processor than with the Sen2Cor processor, however on one hand Sen2Cor reflectances seem to be often higher than in-situ reflectances, on the other hand Sen2Water reflectances tend to be lower than in-situ reflectances. The coefficients of determination are always lower with the Sen2Water processor than with the Sen2Cor processor. As seen below, the behaviour is however strongly different for the coastal ocean dataset.

It seems that the Sen2Water processor has a greater range of possible reflectances. Indeed, Sen2Water satellite reflectances seem to be spread over a wider range of values than Sen2Cor satellite reflectances. It is to be particularly visible for band 2 for the "products" validation pipeline scatter plot.

When one compares the scatter plots using data from the "products" validation pipeline and the "algorithms" validation pipeline, one first notices that fewer points are present. Indeed, more filters are implemented with the "algorithms" validation pipeline, outliers are removed. The coefficients of determination are always higher in the "algorithms" validation pipeline than in the "products" validation pipeline.

Then, we compare the results using performance indicators presented before.

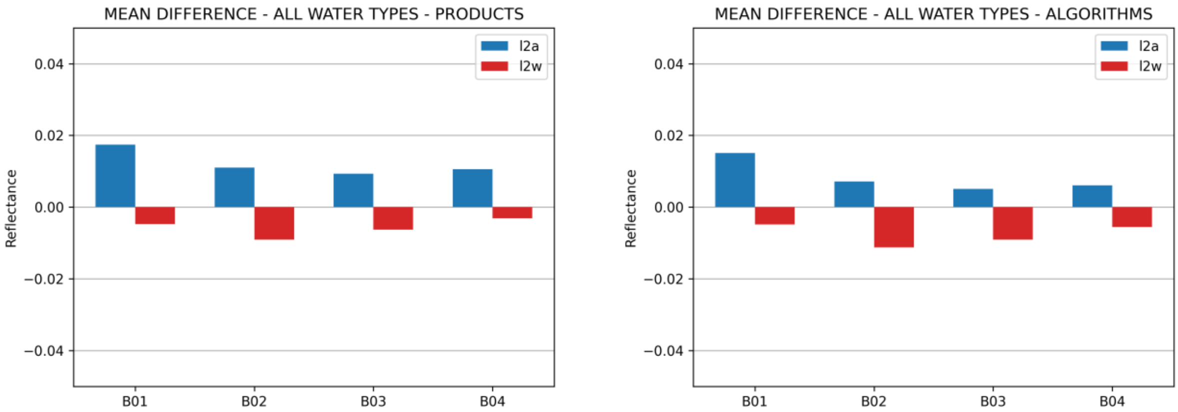

Figure 3-30: mean difference between satellite reflectances computed with Sen2Cor (blue) or Sen2Water (red) and in-situ reflectances for four bands at 440, 490, 560 and 665 nm, for points over all water types, for the "products" validation pipeline on the left and the "algorithms" on the right

First of all, one can notice that while Sen2Cor has a positive bias, Sen2Water has a negative bias : it tends to correct too much the reflectances. In the "products" validation pipeline, mean difference is always lower with Sen2Water than with Sen2Cor, which shows the good performance of Sen2Water. However, in the "algorithms" validation pipeline, mean difference is lower with Sen2Water for bands 1 and 4 but higher for bands 2 and 3.

Differences between satellite and in-situ reflectances can vary a lot, from an order of magnitude of 10^{-1} to 10^{-3}. Thus, the mean difference indicator can be not fully representative of all results. The beta coefficient looks at the relative difference between satellite and in-situ reflectances and moreover uses the median instead of the mean. It gives a different picture of the bias.

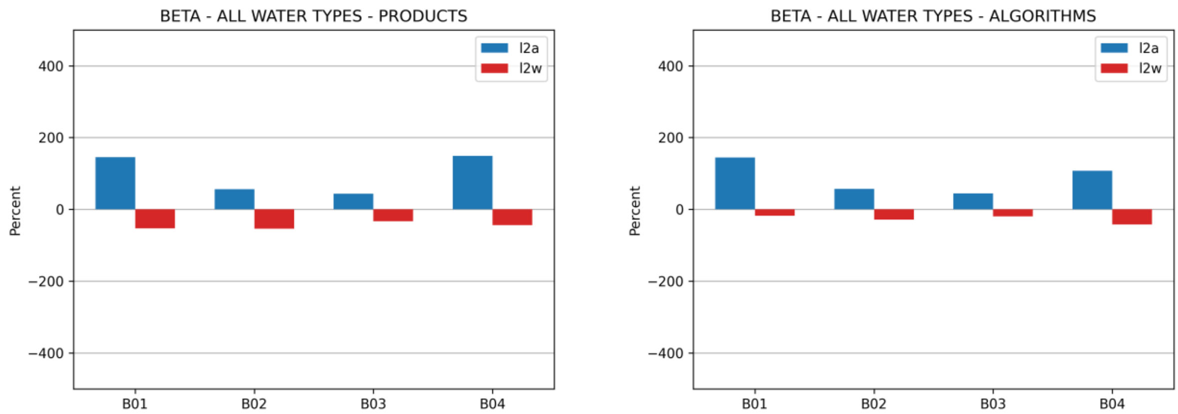

Figure 3-31: beta indicator between satellite reflectances computed with Sen2Cor (blue) or Sen2Water (red) and in-situ reflectances for four bands at 440, 490, 560 and 665 nm, for points over all water types, for the "products" validation pipeline on the left and the "algorithms" on the right

Looking at the beta indicator, one can notices that similarly as for the mean difference, the Sen2Water processor has a negative bias, while the Sen2Cor processor has a positive bias. However, contrary to the mean difference, one observes that the “algorithms” validation pipeline has lower bias than the “products” one for all wavelengths. For both pipelines, Sen2Water processor has a lower bias than Sen2Cor processor.

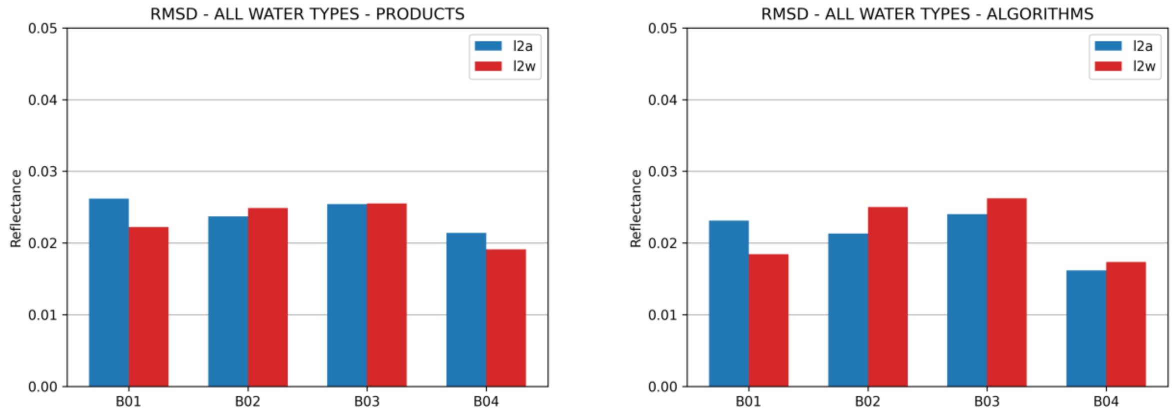

Figure 3-32: RMSD between satellite reflectances computed with Sen2Cor (blue) or Sen2Water (red) and in-situ reflectances for four bands at 440, 490, 560 and 665 nm, for points over all water types, for the “products” validation pipeline on the left and the “algorithms” on the right

RMSD indicates that the two processors behave similarly, for both “products” and “algorithms” validation pipelines. For the “products” validation pipeline, Sen2Water has better RMSD than Sen2Cor in bands 1 and 4 but worse results in bands 2 and 3. For the “algorithms” validation pipeline, Sen2Water has better RMSD than Sen2Cor for band 1 but worse results for bands 2 to 4.

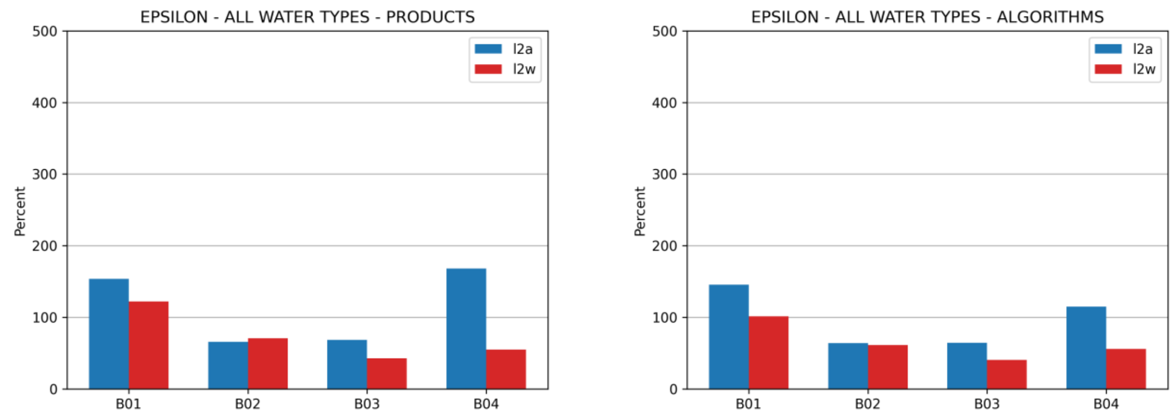

Figure 3-33: epsilon indicator between satellite reflectances computed with Sen2Cor (blue) or Sen2Water (red) and in-situ reflectances for four bands at 440, 490, 560 and 665 nm, for points over all water types, for the “products” validation pipeline on the left and the “algorithms” on the right

Epsilon indicator shows that for almost both pipelines and all bands, Sen2Water has a lower spread than Sen2Cor, except for “product” validation pipeline band 2, for which indicators are very close.

Thus, when using matchups over all water types, it seems that Sen2Water has a lower bias than Sen2Cor, and a spread similar or slightly lower than Sen2Water.

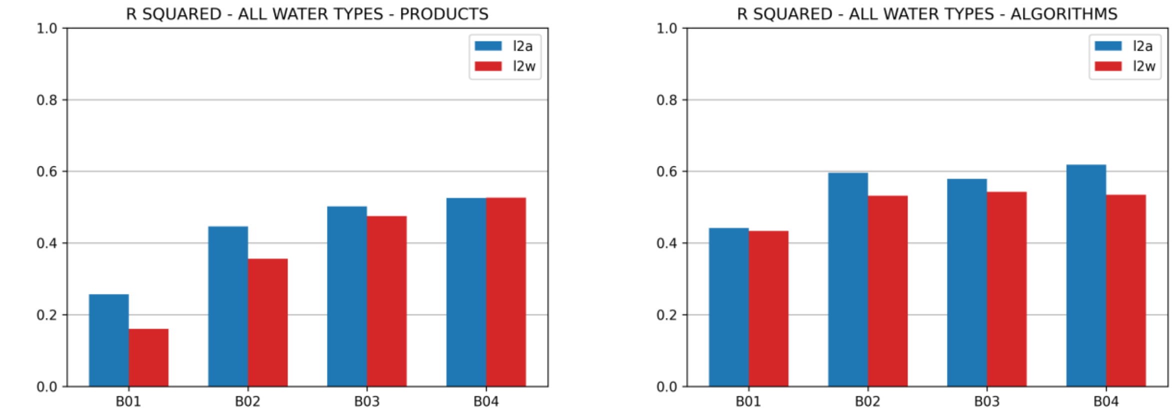

Figure 3-34: squared coefficients of determination between satellite reflectances computed with Sen2Cor (blue) or Sen2Water (red) and in-situ reflectances for four bands at 440, 490, 560 and 665 nm, for points over all water types, for the "products" validation pipeline on the left and the"algorithms" on the right

Coefficients of determination are always lower with Sen2Water processor than with Sen2Cor processor, yet this behaviour is strongly different for the open ocean dataset. One can notice that coefficients of determination increase for all bands and for the two processors in the "algorithms" validation pipeline compared to the "products" validation pipeline.

3.3.3 In-situ: scatter plots and performance indicators for coastal oceans

Same scatter plots as those presented before are displayed below, but this time for data over coastal oceans.

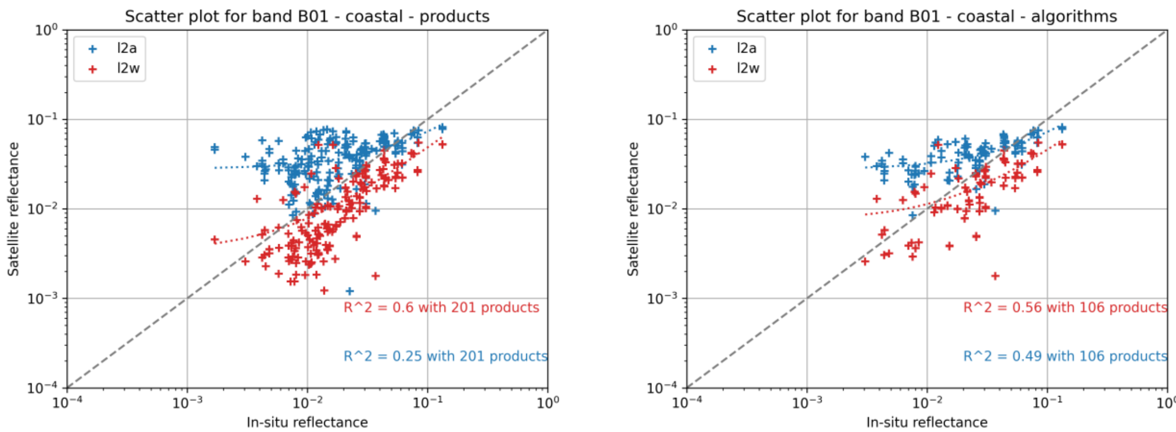

Figure 3-35: scatter plots of satellite reflectances computed with Sen2Cor (blue) and Sen2Water (red) as a function of in-situ reflectances for band 1 at 440 nm, for points over coastal oceans, for the "products" validation pipeline on the left and the "algorithms" on the right

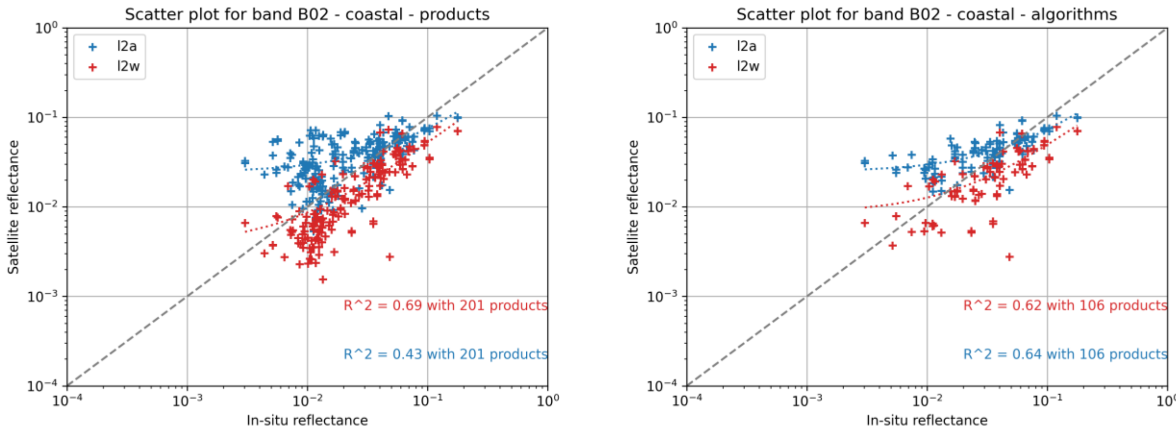

Figure 3-36: scatter plots of satellite reflectances computed with Sen2Cor (blue) and Sen2Water (red) as a function of in-situ reflectances for band 2 at 490 nm, for points over coastal oceans, for the "products" validation pipeline on the left and the "algorithms" on the right

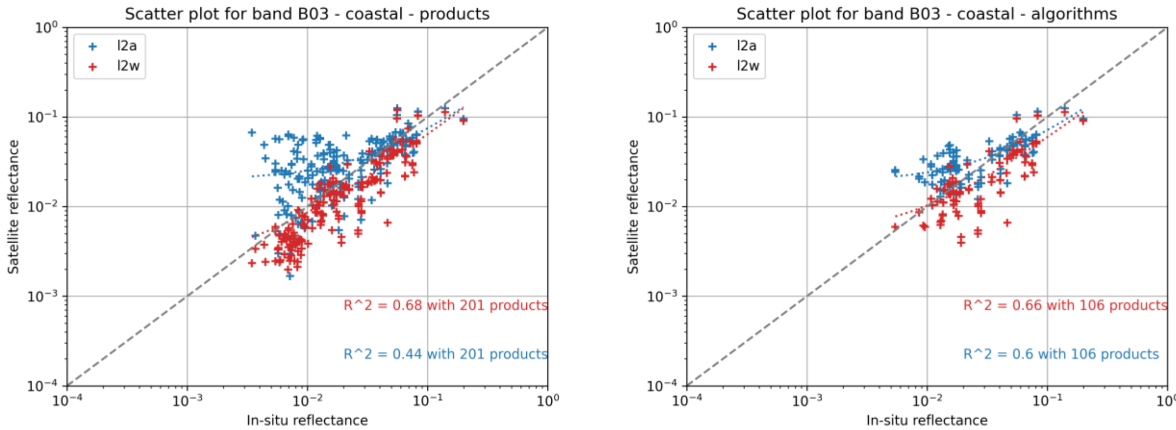

Figure 3-37: scatter plots of satellite reflectances computed with Sen2Cor (blue) and Sen2Water (red) as a function of in-situ reflectances for band 3 at 560 nm, for points over coastal oceans, for the "products" validation pipeline on the left and the "algorithms" on the right

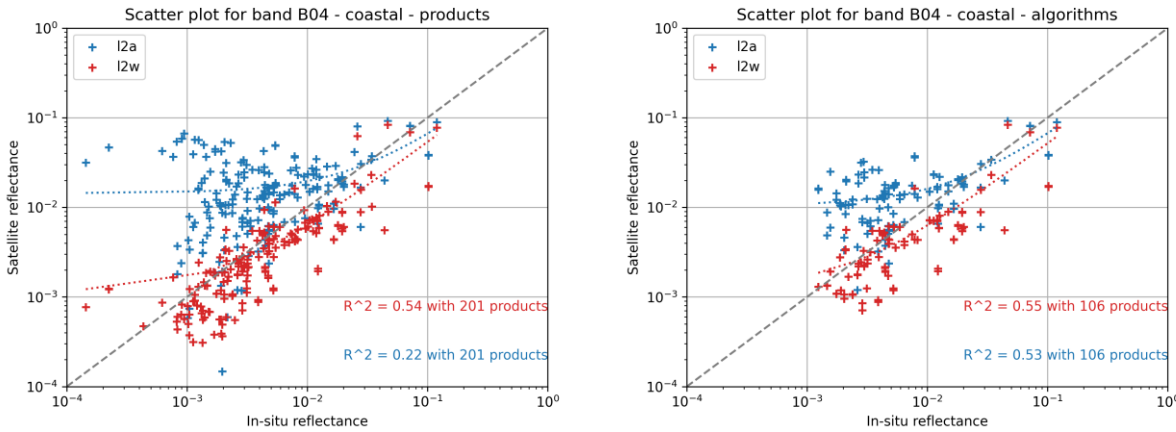

Figure 3-38: scatter plots of satellite reflectances computed with Sen2CorSen2Cor (blue) and Sen2Water (red) as a function of in-situ reflectances for band 4 at 665 nm, for points over coastal oceans, for the "products" validation pipeline on the left and the "algorithms" on the right

Similarly as for the scatter plots displayed with all available points, one can notice here that the Sen2Water processing tends to provide smaller reflectances than the Sen2Cor processing. From a positive bias with the Sen2Cor processing, the Sen2Water processing seem to produce here reflectances with a negative bias. This is clearly visible in the scatter plot of band 2 for the "products" validation pipeline. As observed before, the dynamic range seem to be higher with the Sen2Water processor than with the Sen2Cor processor.

Coefficients of determination tend to be higher with only coastal oceans points than with all points. Contrary to what has been observed for the scatter plots obtained with all water types, coefficients of determination are often higher with the Sen2Water processor than with Sen2Cor. Similarly as with all water types, coefficients of determination are often higher in the "algorithms" validation pipeline than in the "products" validation pipeline.

Then, we compare the results using performance indicators presented before.

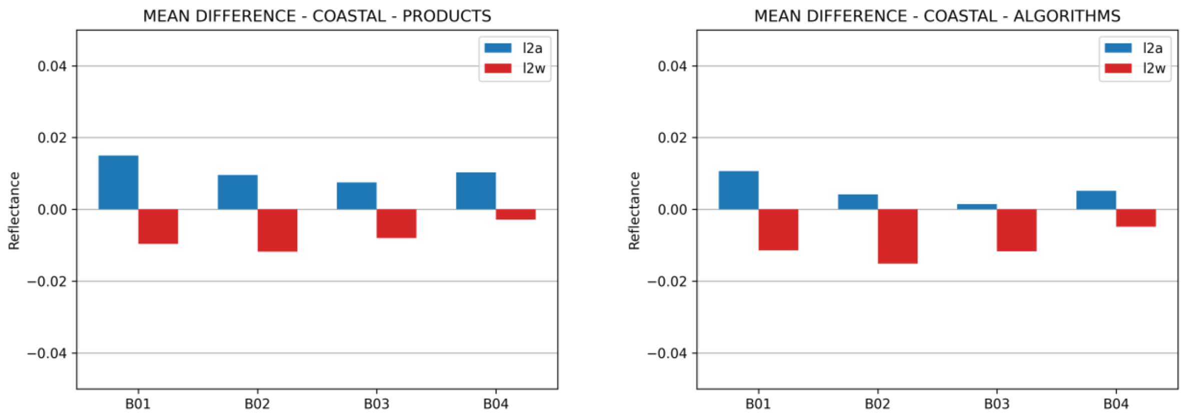

Figure 3-39: mean difference between satellite reflectances computed with Sen2Cor (blue) or Sen2Water (red) and in-situ reflectances for four bands at 440, 490, 560 and 665 nm, for points over coastal oceans, for the "products" validation pipeline on the left and the "algorithms" on the right

As noted previously, one can note in the figure above that while Sen2Cor processor tends to produce reflectances higher than those measured in-situ, Sen2Water produces reflectances lower than those measured in-situ. Regarding the distance between satellite and in-situ measurements, while Sen2Water performs better or similar to Sen2Cor for all bands in the "products" validation pipeline, in the "algorithms" validation pipeline Sen2Water performs better for bands 1 and 4 but Sen2Cor performs better for bands 2 and 3.

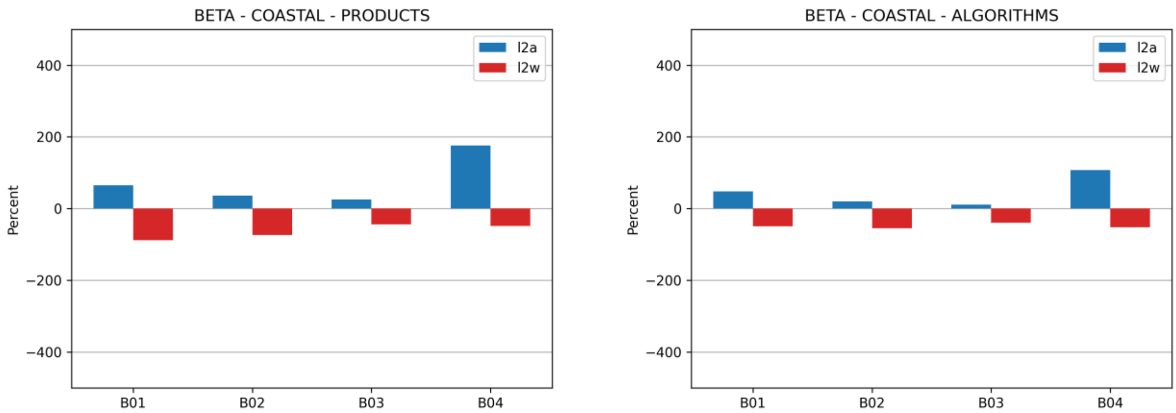

Figure 3-40: beta indicator between satellite reflectances computed with Sen2Cor (blue) or Sen2Water (red) and in-situ reflectances for four bands at 440, 490, 560 and 665 nm, for points over coastal oceans, for the "products" validation pipeline on the left and the "algorithms" on the right

Again, while Sen2Cor is biased positively, one observes here that Sen2Water is biased negatively. While beta indicator seems closer to zero for Sen2Water than Sen2Cor for bands 1 and 4, it seems that Sen2Cor has better results for bands 2 and 3, for the two validation pipelines.

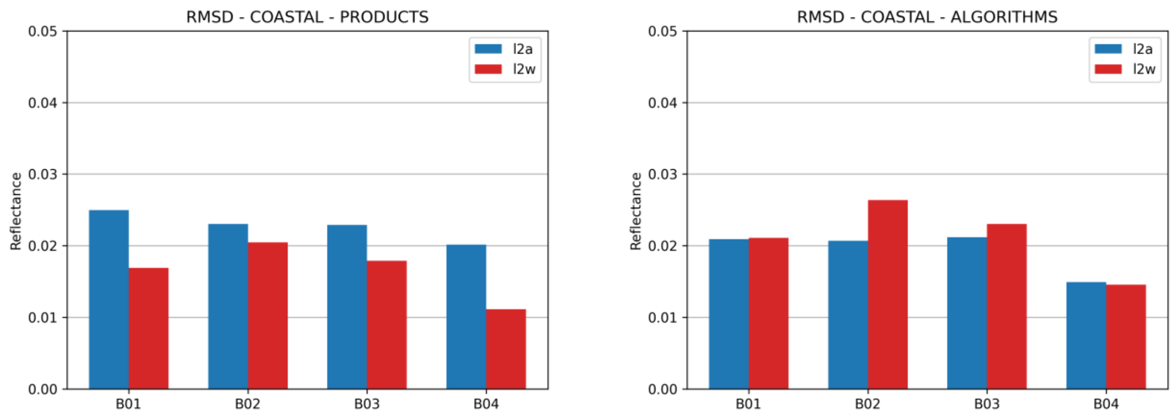

Figure 3-41: RMSD between satellite reflectances computed with Sen2Cor (blue) or Sen2Water (red) and in-situ reflectances for four bands at 440, 490, 560 and 665 nm, for points over coastal oceans, for the "products" validation pipeline on the left and the "algorithms" on the right

While the RMSD is always lower with the Sen2Water processor than with the Sen2Cor processor for the "products" validation pipeline, it is the opposite with the "algorithms" validation pipeline. No clear conclusion can be drawn here.

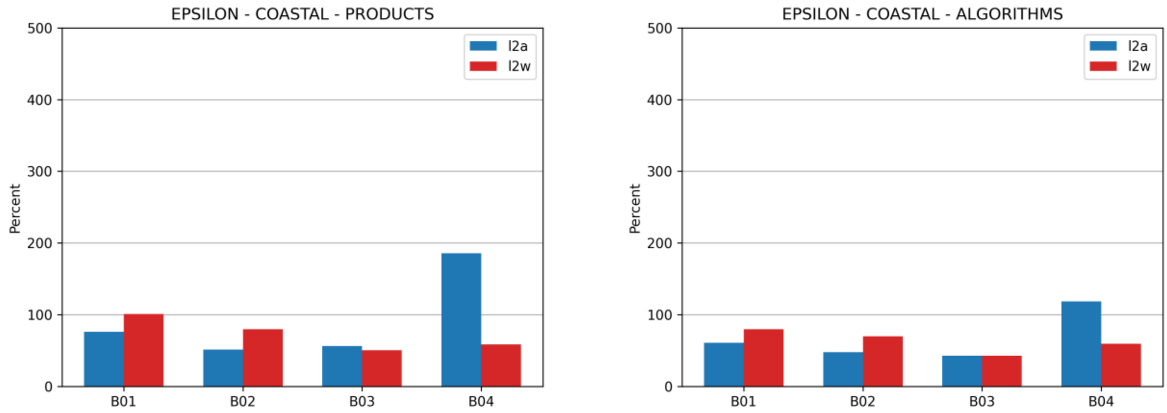

Figure 3-42: epsilon indicator between satellite reflectances computed with Sen2Cor (blue) or Sen2Water (red) and in-situ reflectances for four bands at 440, 490, 560 and 665 nm, for points over coastal oceans, for the "products" validation pipeline on the left and the "algorithms" on the right

The epsilon indicator shows that for bands 1 and 2, the Sen2Cor processor tends to have a lower value for both validation pipelines, while bands 3 and 4 it is the Sen2Water processor that tends to have a higher value.

Thus, over coastal oceans, while band 4 has both a lower bias and a lower spread with the Sen2Water processor than with the Sen2Cor processor, bands 2 and 3 have worse results with Sen2Water than with Sen2Cor. For band 1, results are mixed, with no clear conclusion.

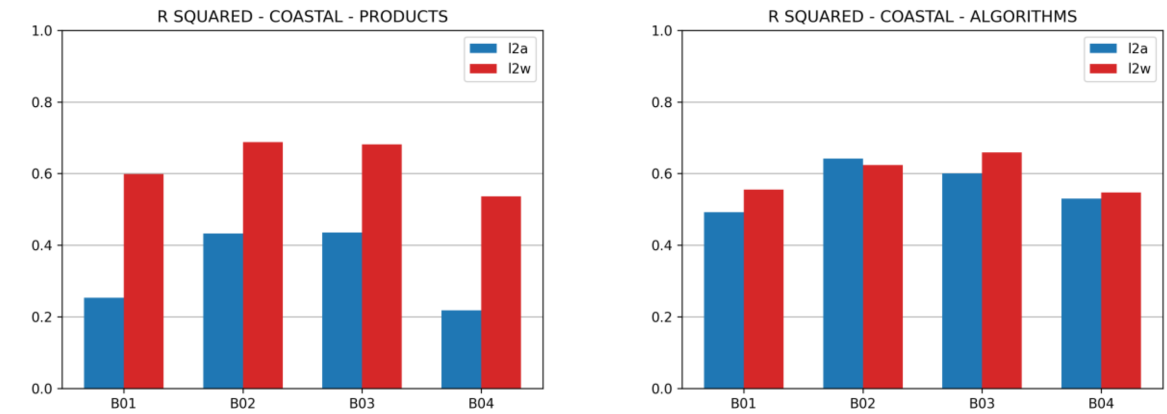

Figure 3-43: squared coefficients of determination between satellite reflectances computed with Sen2Cor (blue) or Sen2Water (red) and in-situ reflectances for four bands at 440, 490, 560 and 665 nm, for points over coastal oceans, for the "products" validation pipeline on the left and the "algorithms" on the right

Coefficients of determination are always higher with Sen2Water than with Sen2Cor, except for band 2 in the "algorithms" validation pipeline.

3.3.4 In-situ: scatter plots and performance indicators for lakes

Same scatter plots as those presented before are displayed below, but this time for data over lakes.

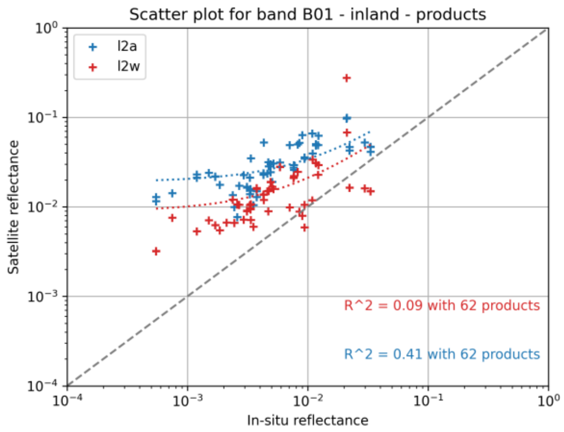

Figure 3-44 : scatter plots of satellite reflectances computed with Sen2Cor (blue) and Sen2Water (red) as a function of in-situ reflectances for band 1 at 440 nm, for points over lakes, for the "products" validation pipeline on the left and the "algorithms" on the right

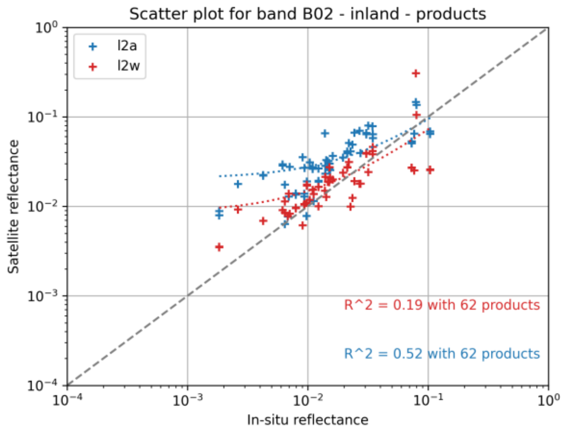

Figure 3-45: scatter plots of satellite reflectances computed with Sen2Cor (blue) and Sen2Water (red) as a function of in-situ reflectances for band 2 at 490 nm, for points over lakes, for the "products" validation pipeline on the left and the "algorithms" on the right

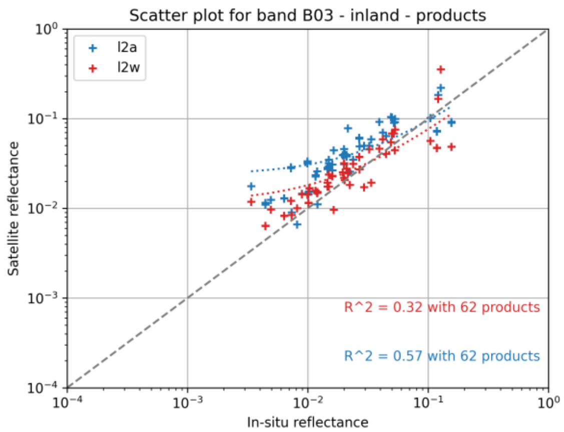

Figure 3-46: scatter plots of satellite reflectances computed with Sen2Cor (blue) and Sen2Water (red) as a function of in-situ reflectances for band 3 at 560 nm, for points over lakes, for the "products" validation pipeline on the left and the "algorithms" on the right

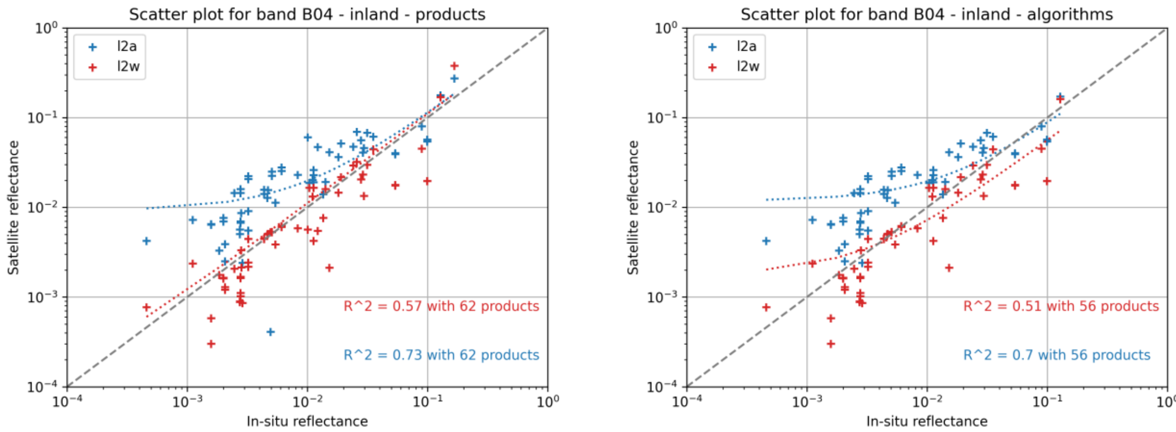

Figure 3-47: scatter plots of satellite reflectances computed with Sen2Cor (blue) and Sen2Water (red) as a function of in-situ reflectances for band 4 at 665 nm, for points over lakes, for the "products" validation pipeline on the left and the "algorithms" on the right

Similarly as previously, reflectances provided by the Sen2Water processor are lower than those from Sen2Cor processor. Contrary to the reflectances over coastal oceans, it seems that the reflectances over lakes provided by Sen2Water have a small bias compared to that of Sen2Cor reflectances.

As noted before, coefficients of determination are often higher in the "algorithms" validation pipeline than in the "products" validation pipeline. As with all water types matchups, but opposite to open ocean matchups, coefficients of determination tend to be lower with the Sen2Water processor than with Sen2Cor. Sen2Water coefficients of determination are much lower with lakes matchups than with open oceans matchups.

Then, we compare the results using performance indicators presented before.

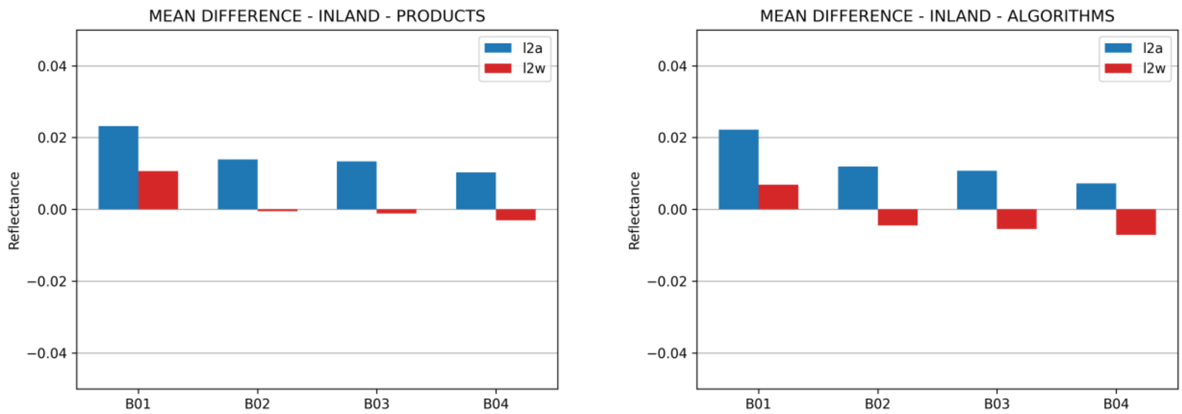

Figure 3-48: mean difference between satellite reflectances computed with Sen2Cor (blue) or Sen2Water (red) and in-situ reflectances for four bands at 440, 490, 560 and 665 nm, for points over lakes, for the "products" validation pipeline on the left and the "algorithms" on the right

Contrary to what has been observed for all water types and for coastal oceans, biases measured through the mean difference can be positive or negative for the Sen2Water processor. Performance is always better with the Sen2Water processor than with the Sen2Cor processor.

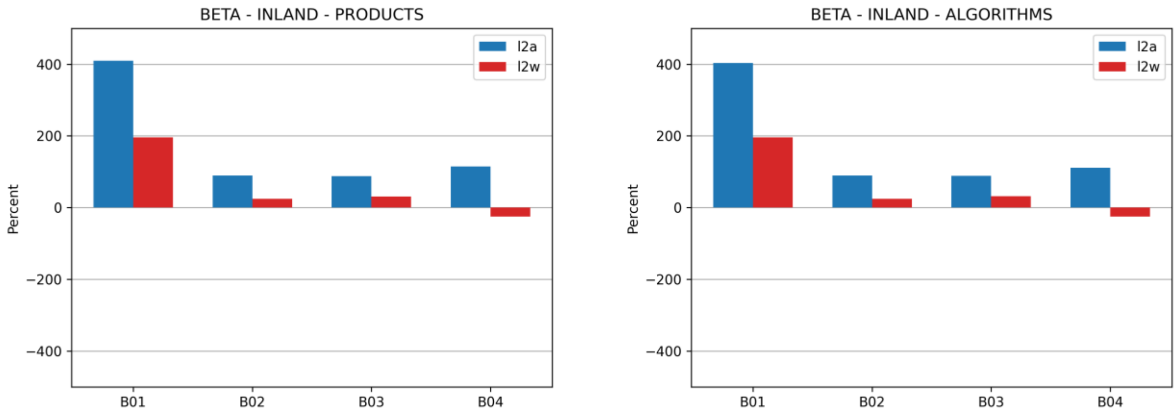

Figure 3-49: beta indicator between satellite reflectances computed with Sen2Cor (blue) or Sen2Water (red) and in-situ reflectances for four bands at 440, 490, 560 and 665 nm, for points over lakes, for the "products" validation pipeline on the left and the "algorithms" on the right

Similarly as what is observed with the mean difference, bias measured with the beta indicator is always lower with Sen2Water than with Sen2Cor. Biases for bands 1 to 3 are positive for the two validation pipelines, while they are negative for band 4.

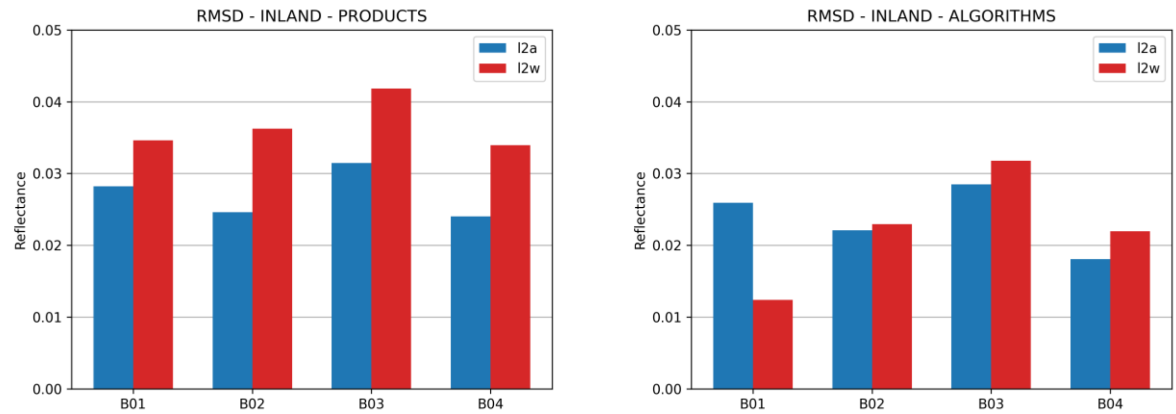

Figure 3-50: RMSD between satellite reflectances computed with Sen2Cor (blue) or Sen2Water (red) and in-situ reflectances for four bands at 440, 490, 560 and 665 nm, for points over lakes, for the "products" validation pipeline on the left and the "algorithms" on the right

RMSD is higher for reflectances computed with the Sen2Water processor than for those computed with Sen2Cor, except for band 1 for the "algorithm" validation pipeline.

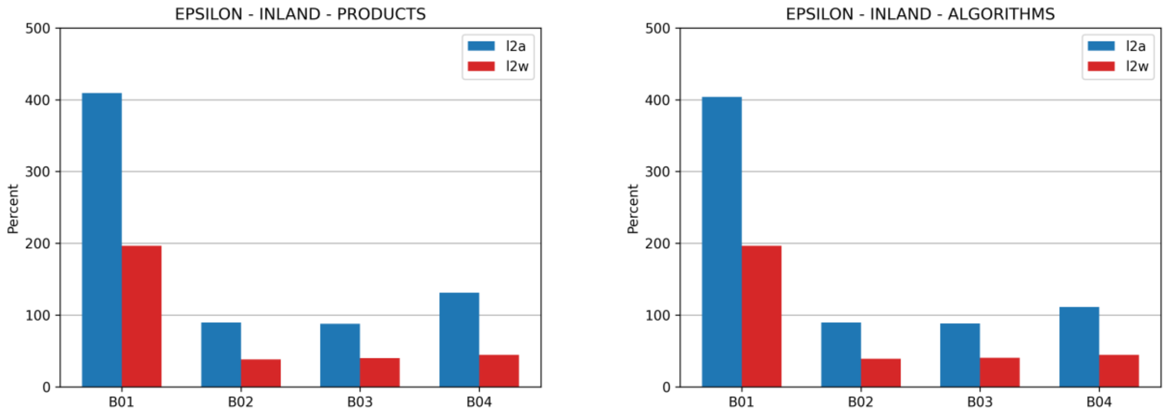

Figure 3-51: epsilon indicator between satellite reflectances computed with Sen2Cor (blue) or Sen2Water (red) and in-situ reflectances for four bands at 440, 490, 560 and 665 nm, for points over lakes, for the "products" validation pipeline on the left and the "algorithms" on the right

Contrary to what is observed with the RMSD, the epsilon indicator shows that all bands for both validation pipelines have a lower spread when computed with Sen2Water as compared to when computed with Sen2Cor.

Thus, over lakes, satellite reflectances computed with Sen2Water have a lower bias than those computed with Sen2Cor, for all bands and for the two validation pipelines. The spread is higher for reflectances computed with Sen2Water, compared to those computed with Sen2Cor, if one uses the RMSD, but lower if one uses the epsilon indicator.

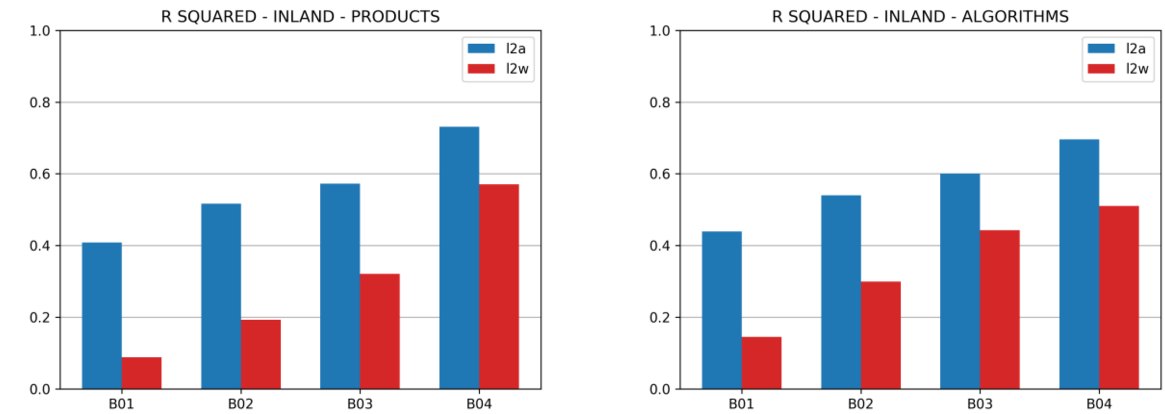

Figure 3-52: squared coefficients of determination between satellite reflectances computed with Sen2Cor (blue) or Sen2Water (red) and in-situ reflectances for four bands at 440, 490, 560 and 665 nm, for points over lakes, for the "products" validation pipeline on the left and the "algorithms" on the right

Finally, coefficients of determination are always lower with Sen2Water than with Sen2Cor, for all bands and validation pipelines. Sen2Water coefficients of determination are also lower over lakes than over coastal oceans.

3.3.5 Summary of the performance indicators

Figures summarizing the results obtained for each metric (mean difference, beta indicator, RMSD, epsilon indicator, squared coefficient of determination) are presented hereafter.

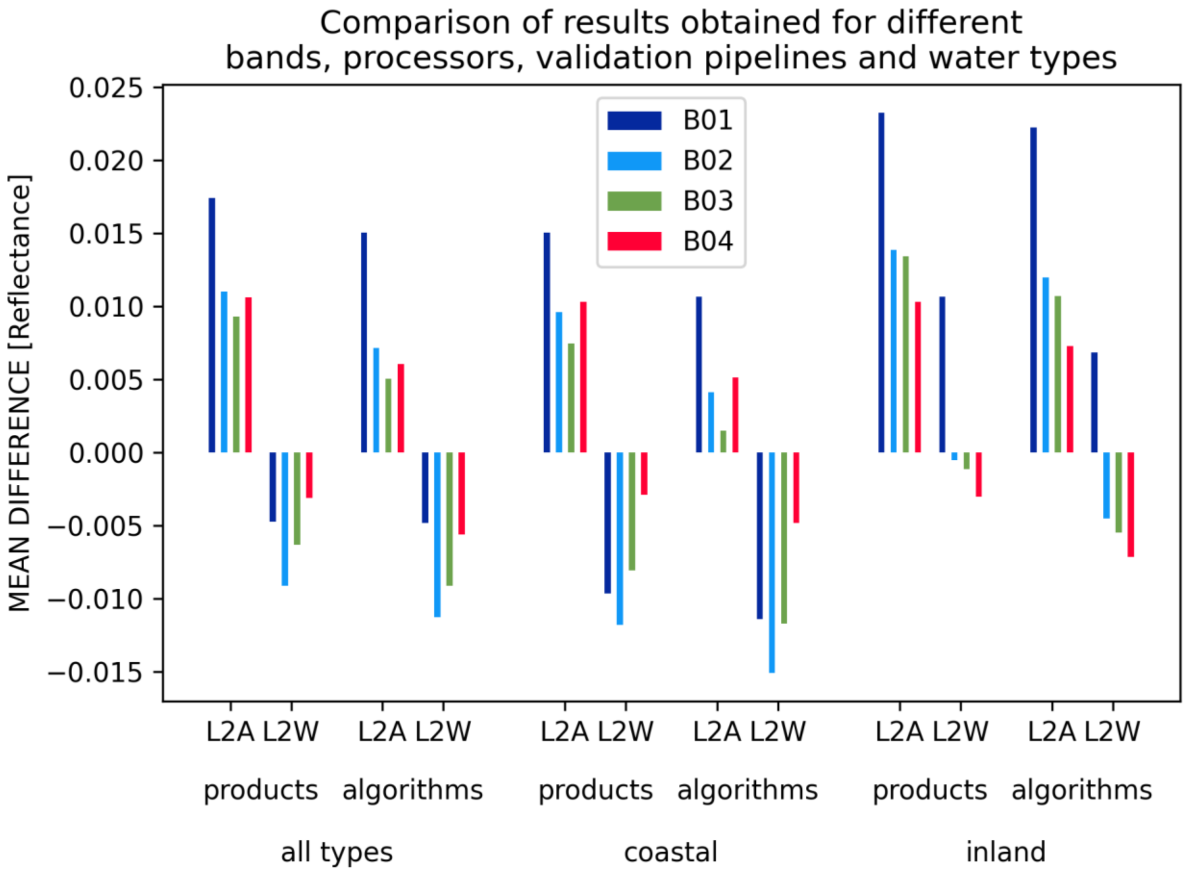

Figure 53: comparison of mean differences obtained with the satellite/in-situ matchups for the four bands, two processors, two validation pipelines and three water types analysed

Figure above shows a summary of all the results obtained for the mean difference metric. As mentioned before, while Sen2Core presents a positive bias, Sen2Water is negatively biased. Performance of Sen2Water is better over inland waters than over coastal waters.

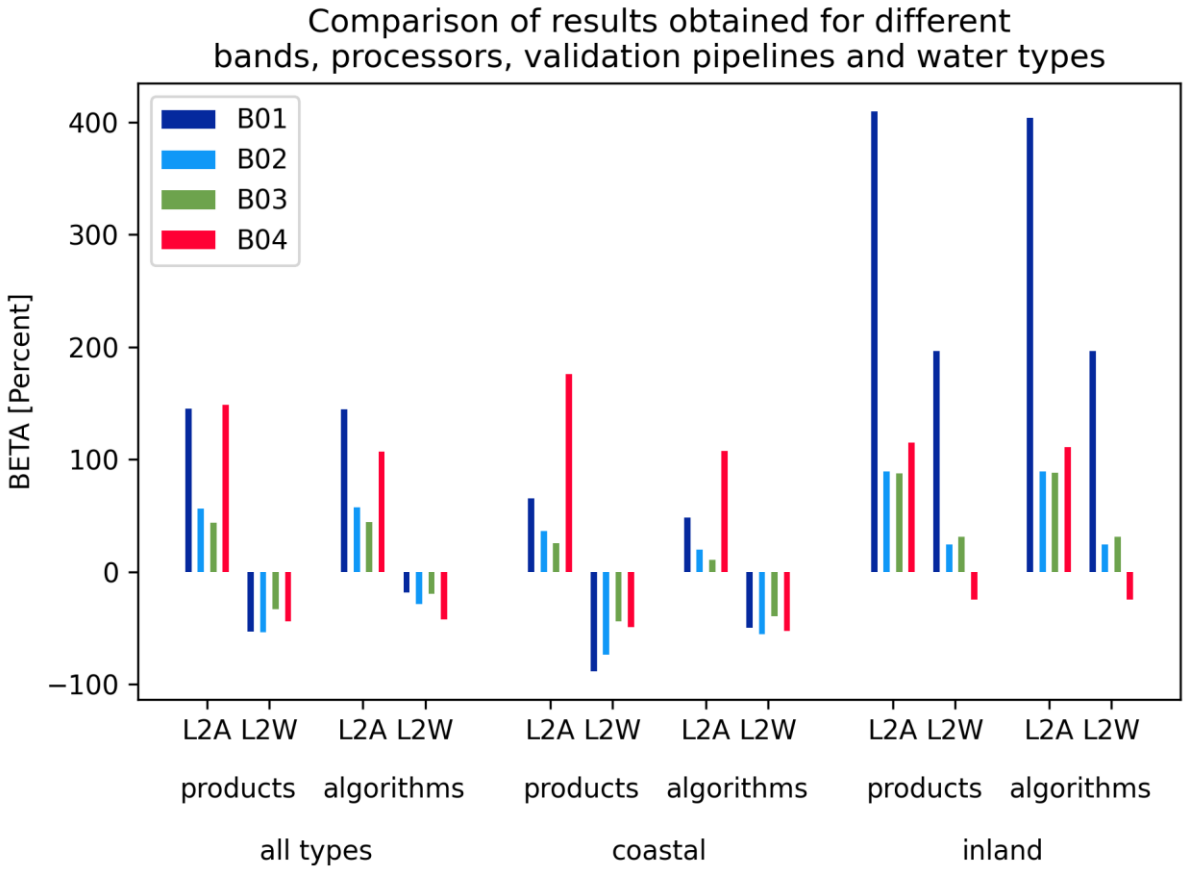

Figure 54: comparison of beta indicators obtained with the satellite/in-situ matchups for the four bands, two processors, two validation pipelines and three water types analysed

Figure above shows a summary of all the results obtained for the mean difference metric. As mentioned before, while Sen2Core presents a positive bias, Sen2Water tends to be negatively biased, except over inland waters. Performance of Sen2Water is better over inland waters than over coastal waters, except for band one.

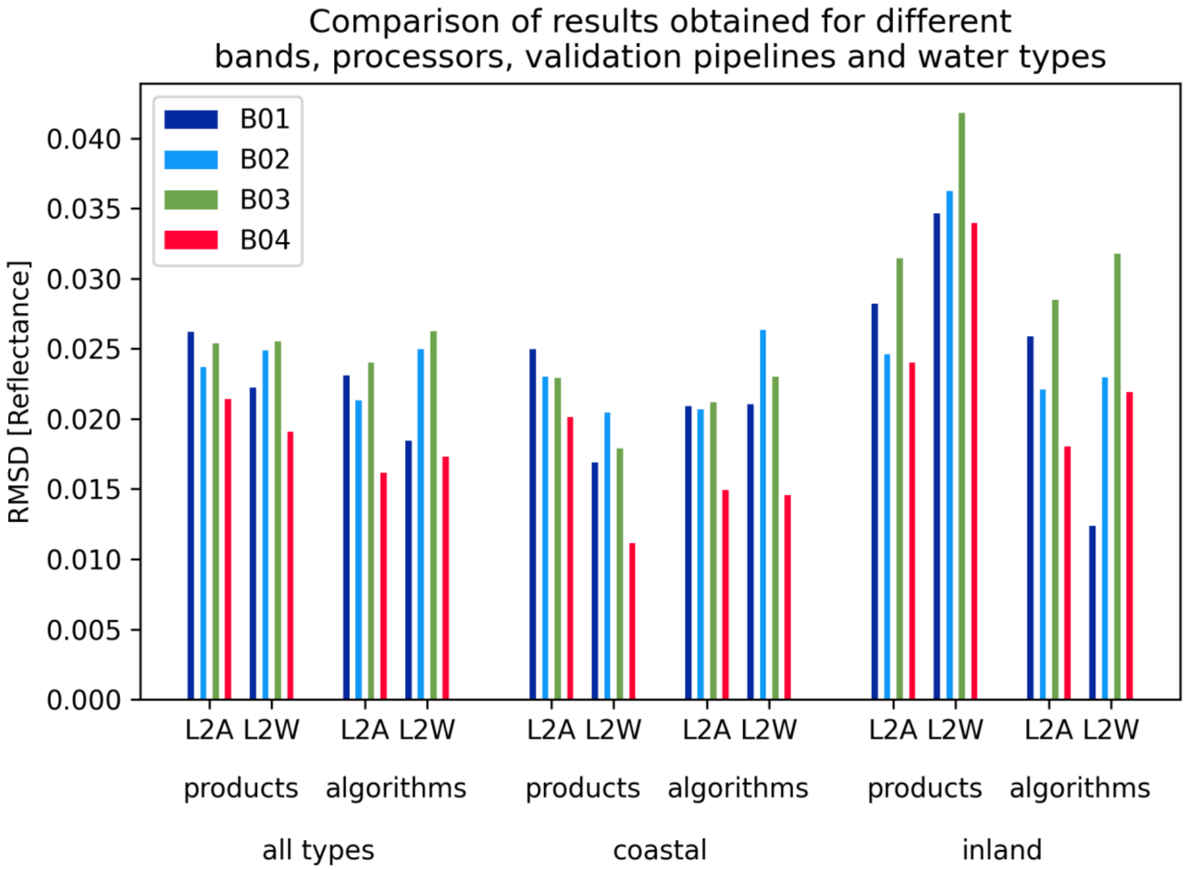

Figure 55: comparison of RMSD obtained with the satellite/in-situ matchups for the four bands, two processors, two validation pipelines and three water types analysed

Figure above shows a summary of all the results obtained for the RMSD metric. Sen2Water tends to present less spread over coastal waters than over inland waters.

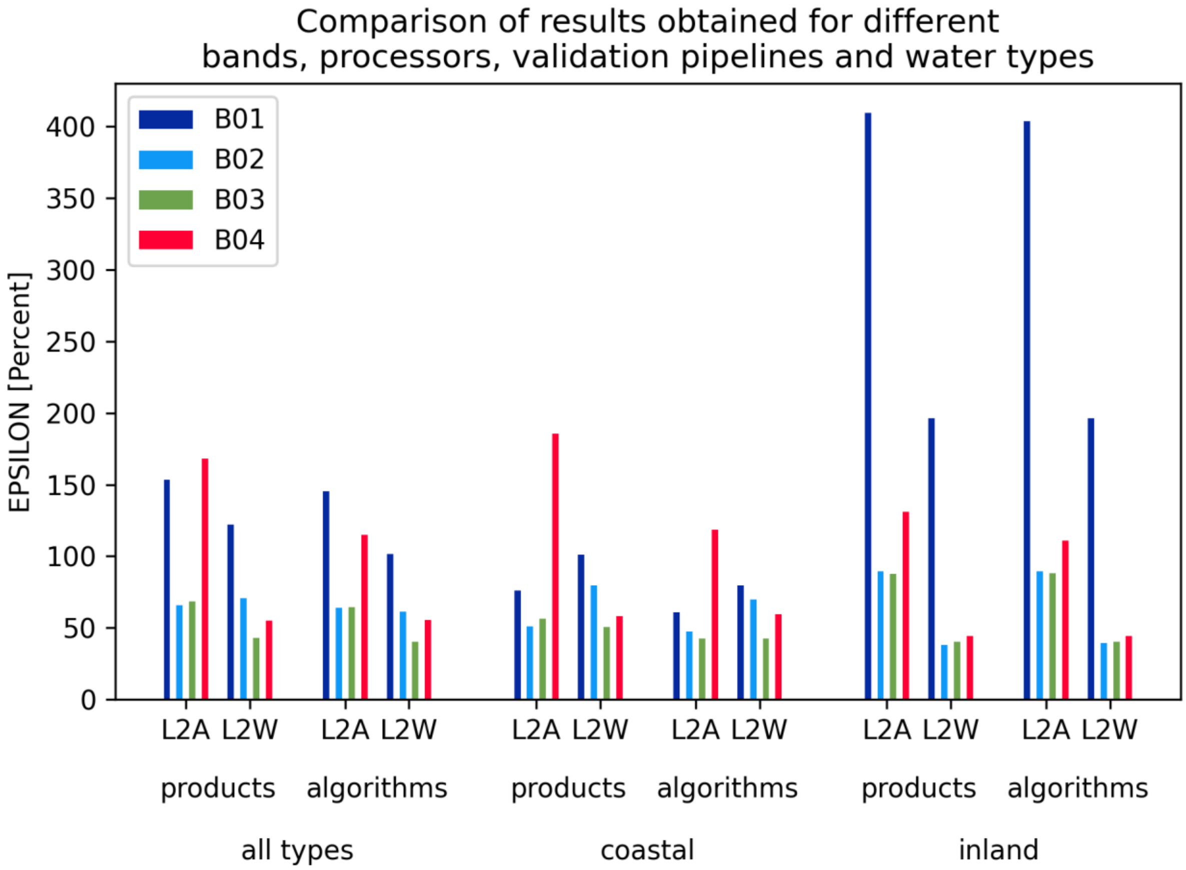

Figure 56: comparison of epsilon indicators obtained with the satellite/in-situ matchups for the four bands, two processors, two validation pipelines and three water types analysed

Figure above shows a summary of all the results obtained for the epsilon indicator metric. Contrary to what is observed with the RMSD metric, Sen2Water tends to present more spread over coastal waters than over inland waters, except for band one.

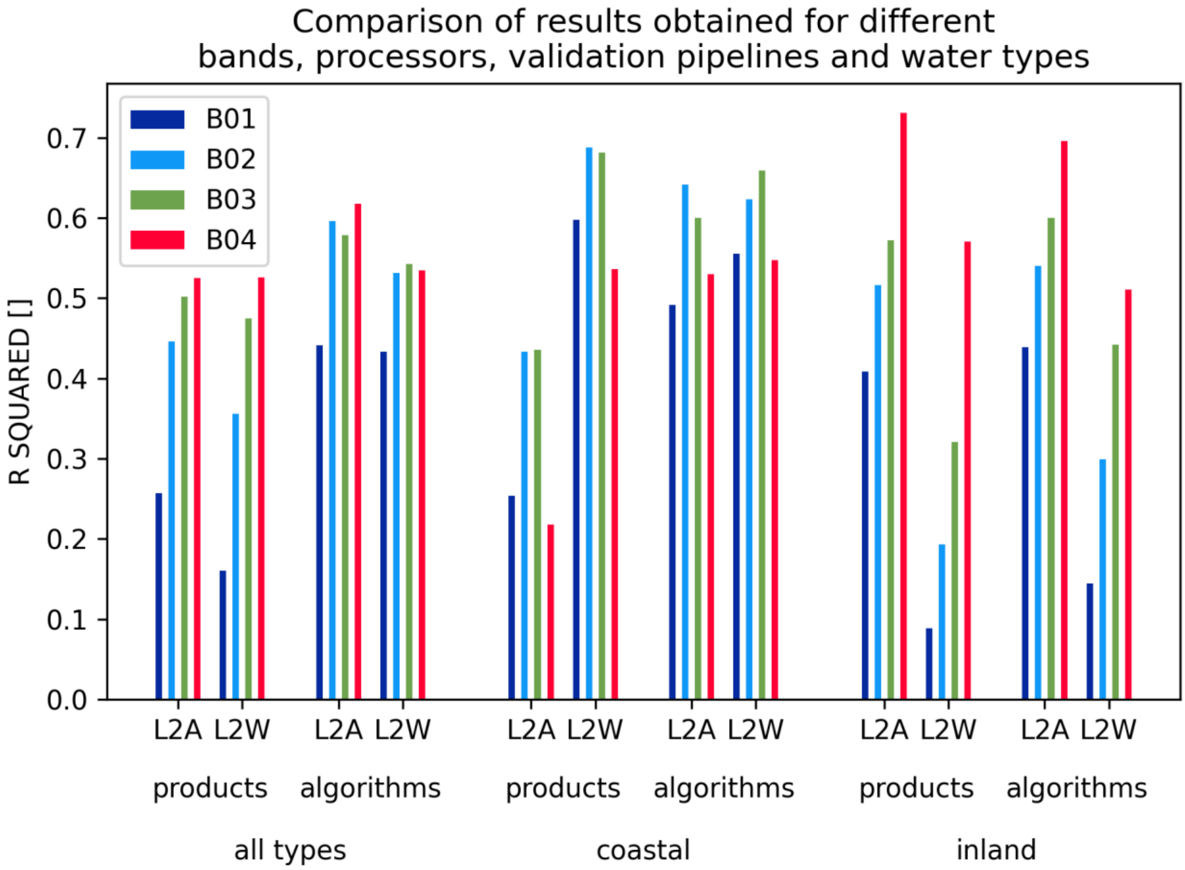

Figure 57: comparison of squared coefficients of determination obtained with the satellite/in-situ matchups for the four bands, two processors, two validation pipelines and three water types analysed

Figure above shows a summary of all the results obtained for the squared coefficients of determination. Squared coefficients of determination are always lower over inland water than over coastal waters, except for band four for the algorithms validation pipeline.

Exact figures obtained for each performance indicator are given below.

Table 1: mean differences obtained with the satellite/in-situ matchups for the four bands, two processors, two validation pipelines and three water types analysed

Mean difference	All water types				Coastal waters				Inland waters			
	Products		Algorithms		Products		Algorithms		Products		Algorithms	
	L2A	L2W	L2A	L2W	L2A	L2W	L2A	L2W	L2A	L2W	L2A	L2W
B01	0,017	-0,005	0,015	-0,005	0,015	-0,010	0,011	-0,011	0,023	0,011	0,022	0,007
B02	0,011	-0,009	0,007	-0,011	0,010	-0,012	0,004	-0,015	0,014	-0,001	0,012	-0,004
B03	0,009	-0,006	0,005	-0,009	0,007	-0,008	0,001	-0,012	0,013	-0,001	0,011	-0,005
B04	0,011	-0,003	0,006	-0,006	0,010	-0,003	0,005	-0,005	0,010	-0,003	0,007	-0,007

Table 2: beta indicators obtained with the satellite/in-situ matchups for the four bands, two processors, two validation pipelines and three water types analysed

Beta indicator	All water types				Coastal waters				Inland waters			
	Products		Algorithms		Products		Algorithms		Products		Algorithms	
	L2A	L2W	L2A	L2W	L2A	L2W	L2A	L2W	L2A	L2W	L2A	L2W
B01	145,2	-53,0	144,8	-18,1	65,3	-88,6	48,4	-49,8	409,4	196,2	403,7	196,3
B02	56,5	-53,7	57,4	-28,6	36,6	-73,6	19,7	-55,2	89,4	24,4	89,4	24,4
B03	43,5	-33,2	44,3	-19,4	25,4	-44,1	10,6	-39,2	87,6	31,1	88,1	31,5
B04	148,8	-43,7	107,1	-42,5	176,1	-48,9	107,5	-52,6	115,0	-24,7	111,0	-24,7

Table 3: RMSD obtained with the satellite/in-situ matchups for the four bands, two processors, two validation pipelines and three water types analysed

RMSD	All water types				Coastal waters				Inland waters			
	Products		Algorithms		Products		Algorithms		Products		Algorithms	
	L2A	L2W	L2A	L2W	L2A	L2W	L2A	L2W	L2A	L2W	L2A	L2W
B01	0,026	0,022	0,023	0,018	0,025	0,017	0,021	0,021	0,028	0,035	0,026	0,012
B02	0,024	0,025	0,021	0,025	0,023	0,020	0,021	0,026	0,025	0,036	0,022	0,023
B03	0,025	0,026	0,024	0,026	0,023	0,018	0,021	0,023	0,031	0,042	0,028	0,032
B04	0,021	0,019	0,016	0,017	0,020	0,011	0,015	0,015	0,024	0,034	0,018	0,022

Table 4: epsilon indicators obtained with the satellite/in-situ matchups for the four bands, two processors, two validation pipelines and three water types analysed

Epsilon indicator	All water types				Coastal waters				Inland waters			
	Products		Algorithms		Products		Algorithms		Products		Algorithms	
	L2A	L2W	L2A	L2W	L2A	L2W	L2A	L2W	L2A	L2W	L2A	L2W
B01	153,6	122,0	145,5	101,4	76,2	101,0	60,7	79,6	409,4	196,2	403,7	196,3
B02	65,8	70,8	63,8	61,2	51,2	79,6	47,6	69,6	89,4	38,0	89,4	39,2
B03	68,2	42,8	64,2	40,4	56,3	50,5	42,7	42,5	87,6	40,1	88,1	40,4
B04	168,1	55,0	115,0	55,5	185,6	58,3	118,6	59,3	131,2	44,3	111,0	44,3

Table 5: squared coefficients of determination obtained with the satellite/in-situ matchups for the four bands, two processors, two validation pipelines and three water types analysed

Squared coeff. of determination	All water types				Coastal waters				Inland waters			
	Products		Algorithms		Products		Algorithms		Products		Algorithms	
	L2A	L2W	L2A	L2W	L2A	L2W	L2A	L2W	L2A	L2W	L2A	L2W
B01	0,257	0,160	0,441	0,433	0,254	0,598	0,492	0,555	0,408	0,088	0,439	0,144
B02	0,446	0,356	0,596	0,532	0,433	0,688	0,642	0,623	0,516	0,193	0,540	0,299
B03	0,502	0,475	0,578	0,543	0,435	0,681	0,600	0,659	0,572	0,321	0,600	0,442
B04	0,525	0,526	0,618	0,535	0,218	0,536	0,530	0,547	0,731	0,571	0,696	0,510

3.3.6 Product inter-comparison

i. Products S2A_MSIL1C_20240719T102021_N0510_R065_T32TNT_20240719T122006 and S3B_OL_2_WFR____20240719T100805_20240719T101105_20240720T165702_0179_095_236_2160_MAR_O_NT_003

Products over Lake Constance, Germany, are compared, both measured on the 19/07/2024 at 10:20 UTC by MSI and at 10:08 UTC by OLCI.

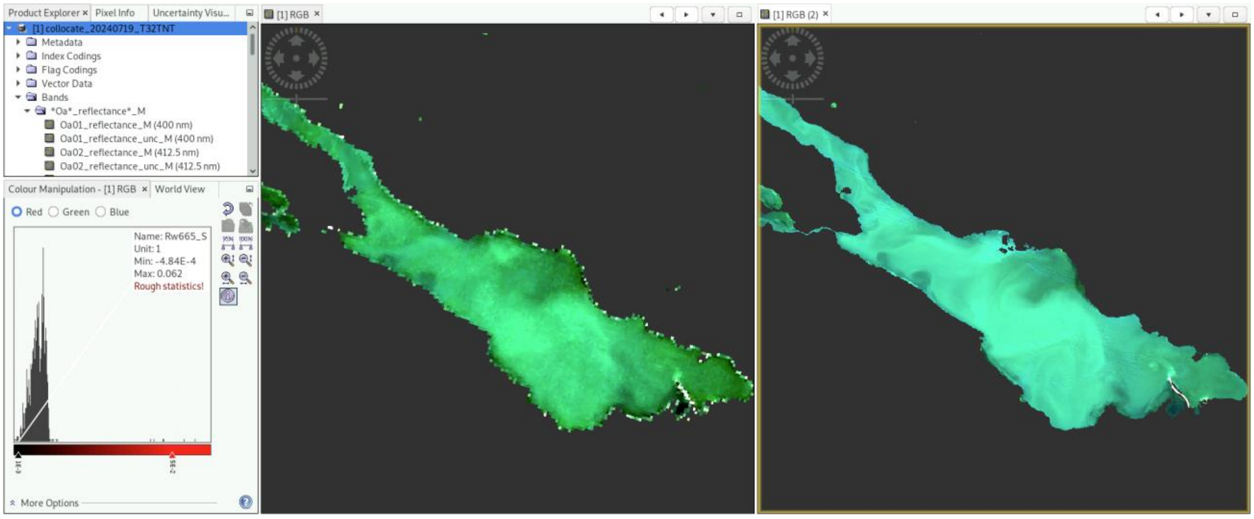

Figure 3-58: OLCI level 2 ocean colour RGB reflectance (left) and Sen2Water RGB reflectance (right), reflectance range is $1 \cdot 10^{-3}$ to $5 \cdot 10^{-2}$ for the three colors, over Lake Constance, Germany

Figure above is presented to understand the context of the figures presented below.

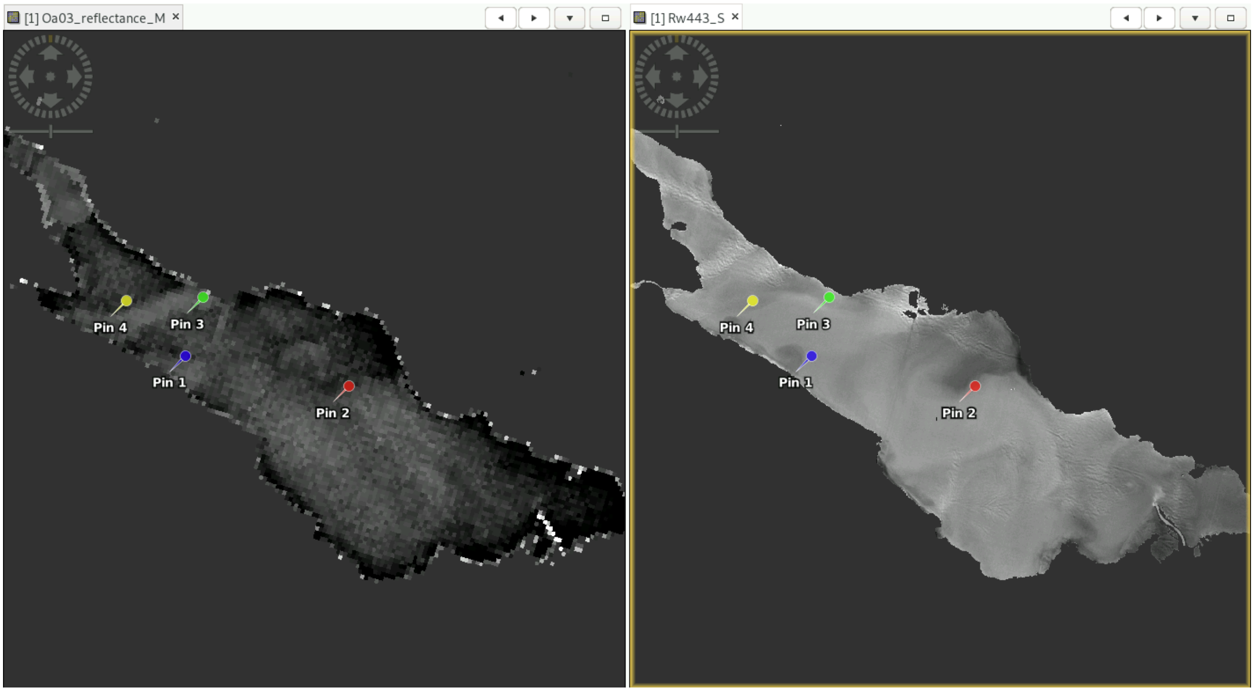

Figure 3-59: on the left, OLCI level 2 ocean colour at 440 nm, on the right Sen2Water reflectances at 440 nm, both collocated over Lake Constance, Germany (reflectance range is $1 \cdot 10^{-3}$ to $5 \cdot 10^{-2}$)

Similar structures can be observed in the two products, for example on both sides of pin 1 (in blue). North-West to pin 1, lower (darker) reflectances can be observed in both products, whereas higher (clearer) reflectances can be noted South-East to pin 1 (in blue). Similarly, pin 2 (in red) seem to separate two areas, a darker one North-West and a clearer one South-East, in the two products analysed.

However, whereas a strip of high reflectances crossing the lake is noticeable between pins 3 (in green) and 4 (in yellow) in the OLCI product, this is not the case in Sen2Water product.

It seems that Sen2Water reflectances are on average higher (clearer) than OLCI level 2 reflectances, by 0% to 100%, depending on the band.

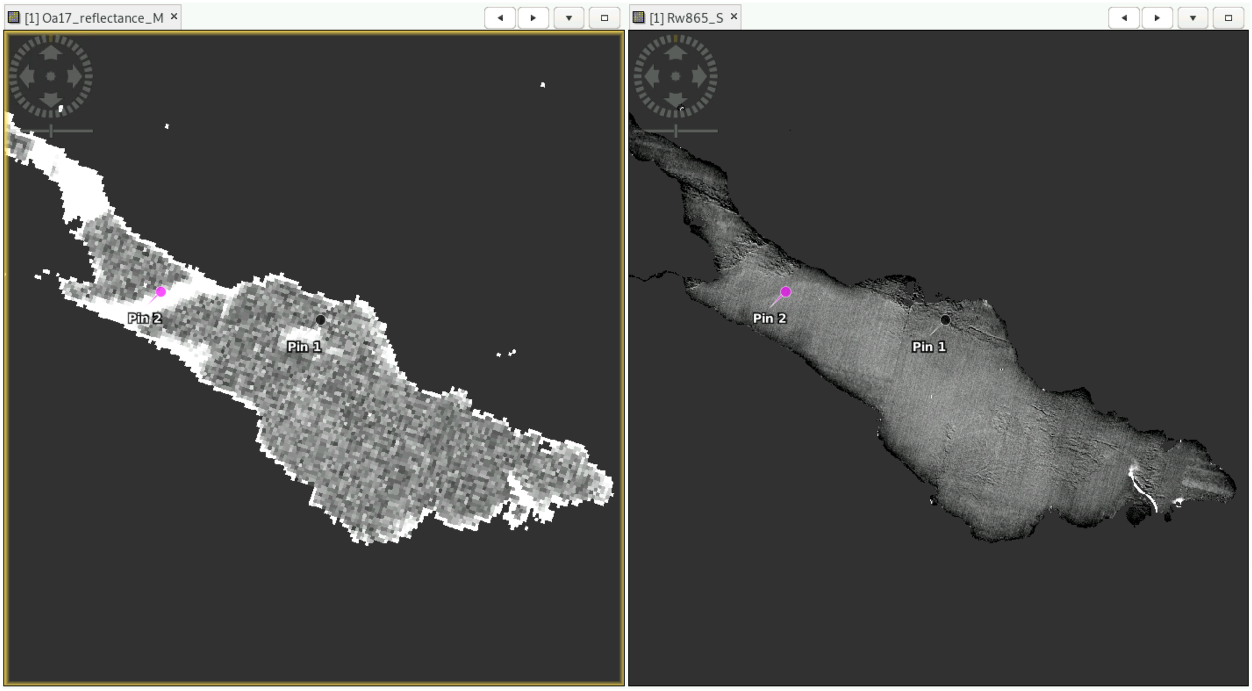

Figure 3-60: on the left, OLCI level 2 ocean colour at 865 nm, on the right Sen2Water reflectances at 865 nm, both collocated over Lake Constance, Germany (reflectance range is $-1 \cdot 10^{-3}$ to $1.5 \cdot 10^{-3}$)

As noted previously, a strip of bright reflectances under pin 2 (in purple) is clearly noticeable in the OLCI product, whereas it is not in the Sen2Water product. Additionally, a bright zone under pin 1 (in dark) can be observed in the OLCI product, whereas it seems to be absent in the Sen2Water product.

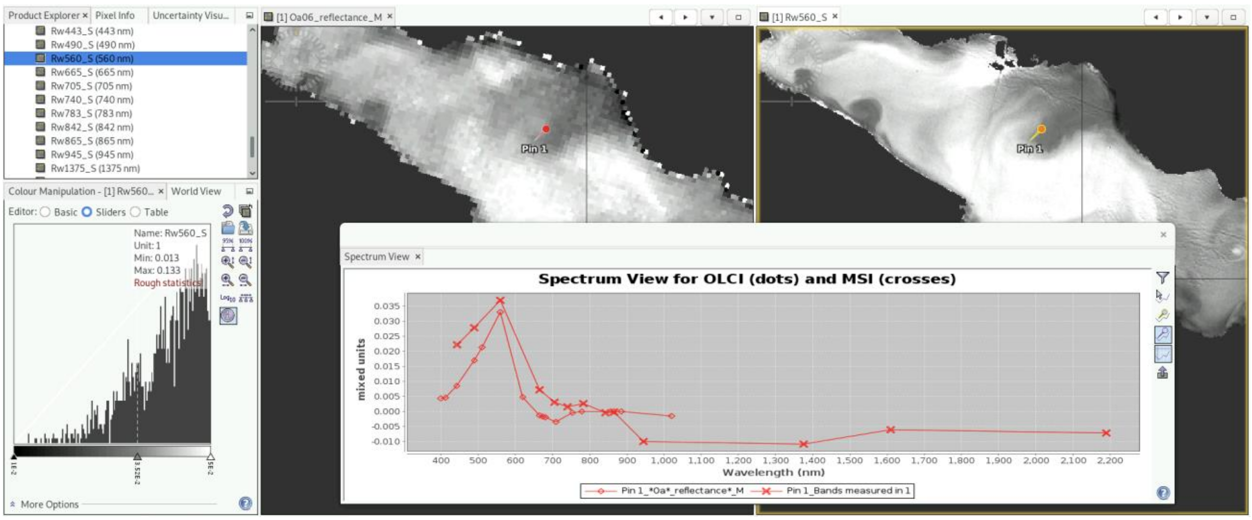

Figure 3-61: on the left, OLCI level 2 ocean colour at 560 nm, on the right Sen2Water reflectances at 560 nm, both collocated over Lake Constance, Germany, in the middle spectrum view of OLCI and Sen2Water products (reflectance range is $1 \cdot 10^{-2}$ to $5 \cdot 10^{-2}$)

Spectral shape is similar between the two products; however, values are different. In the VNIR spectral range, Sen2Water reflectances are higher than those from OLCI level 2. For instance, differences can be higher than 100% for bands at 440 nm or at 665 nm for example. Negative values can be observed for bands above 900 nm in Sen2Water products as mentioned previously.

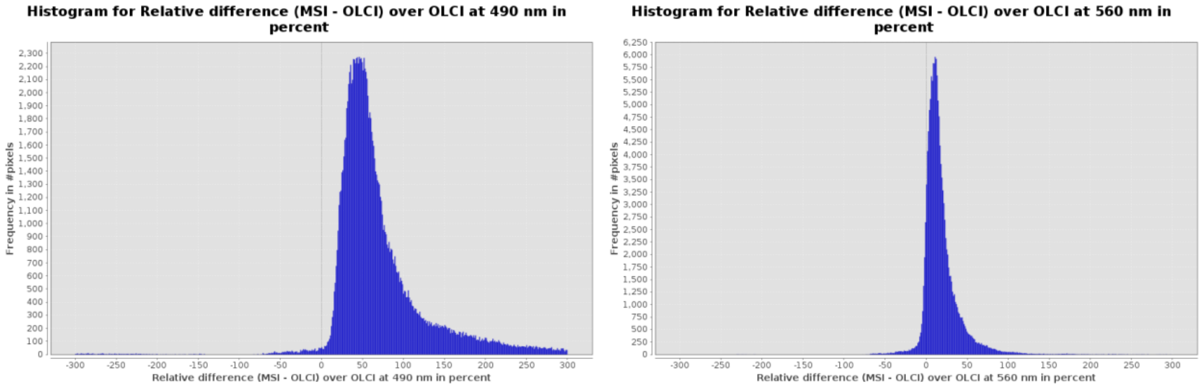

Figure 3-62: Histograms of the relative difference between Sen2Water reflectance and OLCI level 2 ocean colour over Lake Constance, Germany, at 490 nm (left) and 560 nm (right)

Histograms of relative difference between MSI and OLCI reflectances have their maximum around +50 percent at 490 nm and +20 percent at 560 nm.

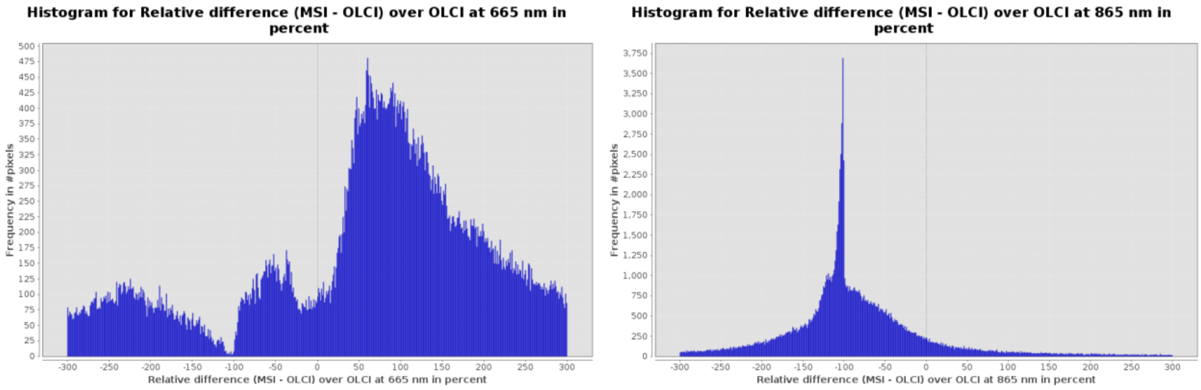

Figure 3-63: Histograms of the relative difference between Sen2Water reflectance and OLCI level 2 ocean colour over Lake Constance, Germany, at 665 nm (left) and 865 nm (right)

Histograms of relative difference between MSI and OLCI reflectances have their maximum around +80 percent at 665 nm and -100 percent at 865 nm.

Up to 665 nm, Sen2Water's reflectances are higher than those from OLCI level 2 ocean colour product, however at 865 nm OLCI has higher values.

ii. Products S2A_MSIL1C_20240104T022321_N0510_R103_T51PWN_20240104T032345 and S3B_OL_2_WFR____20240104T015920_20240104T020220_20240105T093953_0179_088_117_2700_MAR_O_NT_003

Products over Bantayan Island, Philippines, are compared, both measured on the 04/01/2024 at 02:23 UTC by MSI and at 01:59 UTC by OLCI.

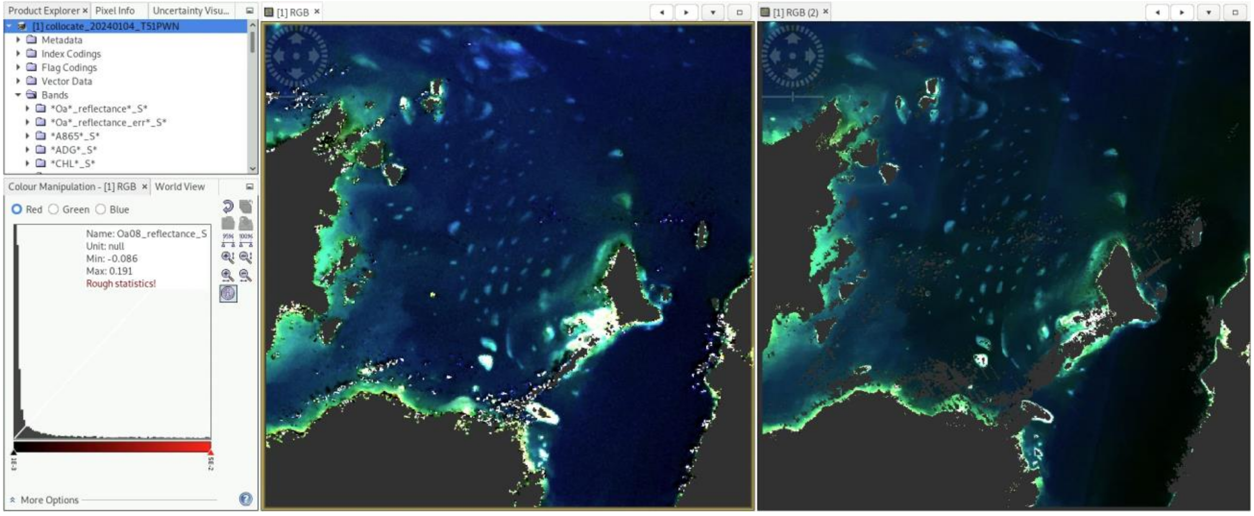

Figure 3-64: OLCI level 2 ocean colour RGB reflectance (left) and Sen2Water RGB reflectance (right), reflectance range is $1 \cdot 10^{-3}$ to $5 \cdot 10^{-2}$ for the three colors, over Bantayan Island, Philippines

Figure above is presented to understand the context of the figures presented below.

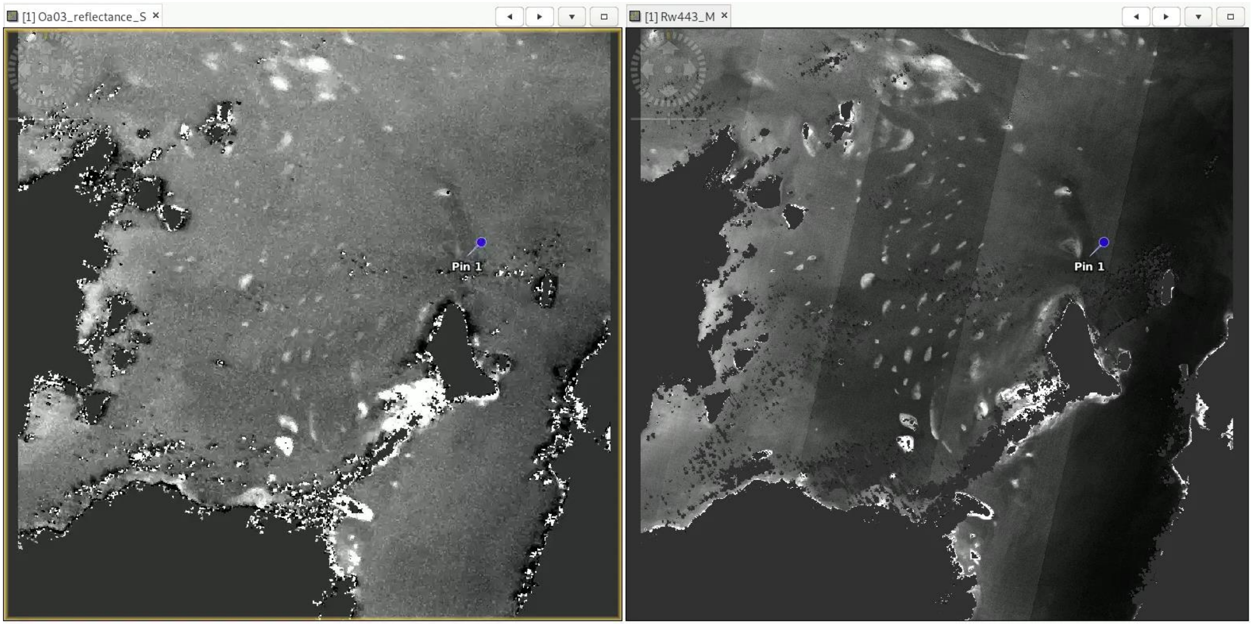

Figure 3-65: on the left, OLCI level 2 ocean colour at 440 nm, on the right Sen2Water reflectances at 440 nm, both collocated over Bantayan Island, Philippines (reflectance range is 0 to $3 \cdot 10^{-2}$)

Footprint of detectors can be clearly seen in the Sen2Water product, and reflectances seem to vary notably between the detectors. Similar structures can be seen in the two products, for example above pin 1 (in blue) with a banana-shaped darker area. Multiple sandbanks can also be observed in the two products in the center of the image.

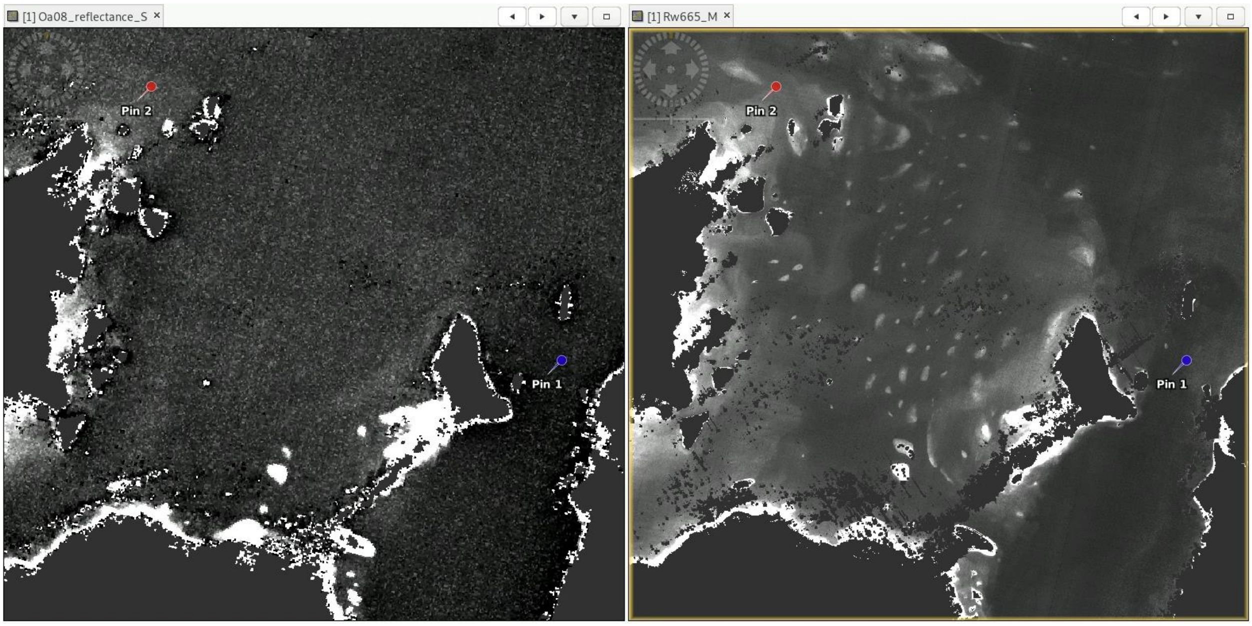

Figure 3-66: on the left, OLCI level 2 ocean colour at 665 nm, on the right Sen2Water reflectances at 665 nm, both collocated over Bantayan Island, Philippines (reflectance range is $-1 \cdot 10^{-3}$ to $7 \cdot 10^{-3}$)

Similar structures can be seen in the two products, for example a darker area around pin 1 (in blue), with a round shape limit with Northern waters. Around pin 2 (in red) another example can be seen, with brighter reflectances. Sandbanks in the middle of the image are visible in the Sen2Water image, however they are not in the OLCI image.

Reflectances look less noisy for Sen2Water; as expected, more details can be seen in the Sen2Water product due to the better resolution of MSI compared to OLCI.

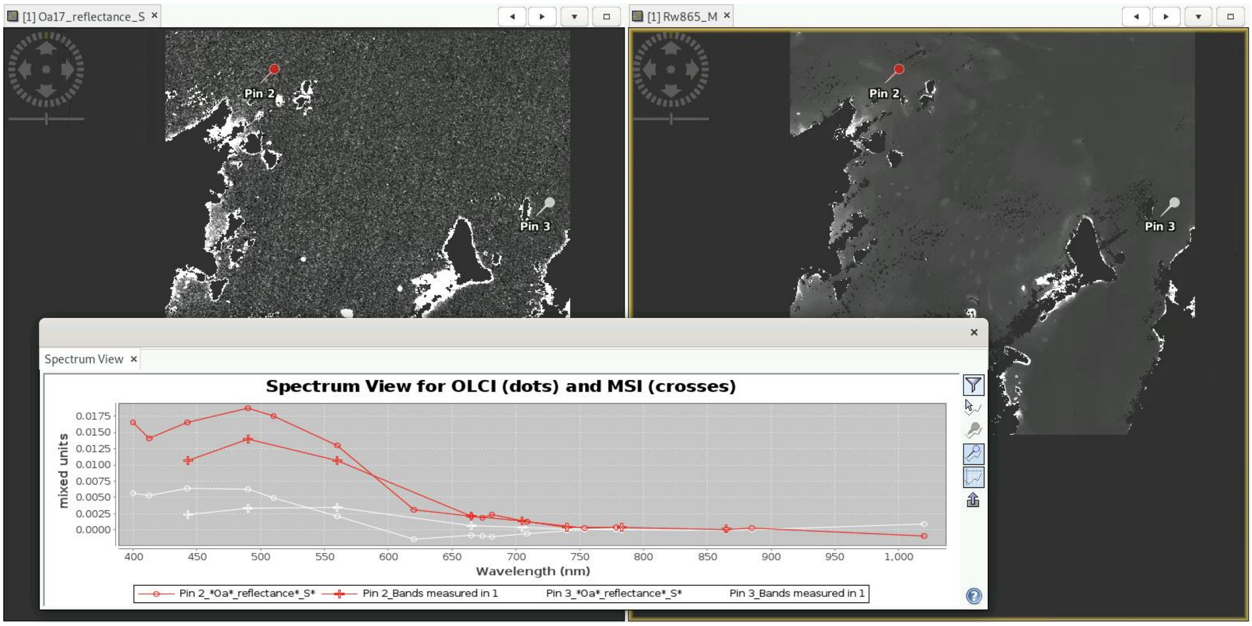

Figure 3-67: on the left, OLCI level 2 ocean colour at 865 nm, on the right Sen2Water reflectances at 865 nm, both collocated over Bantayan Island, Philippines, in the middle spectrum view of OLCI and Sen2Water products (reflectance range is $-5 \cdot 10^{-4}$ to $1.5 \cdot 10^{-3}$)

For the two spectra presented, OLCI level 2 reflectances are higher than Sen2Water reflectances. Up to 500 nm, the two spectra present important absolute differences, up to 100 %, and above 560 nm as reflectances are much smaller, absolute differences seem to be much smaller. Negative reflectances occur in the OLCI product between 600 nm and 700 nm around pin 3.

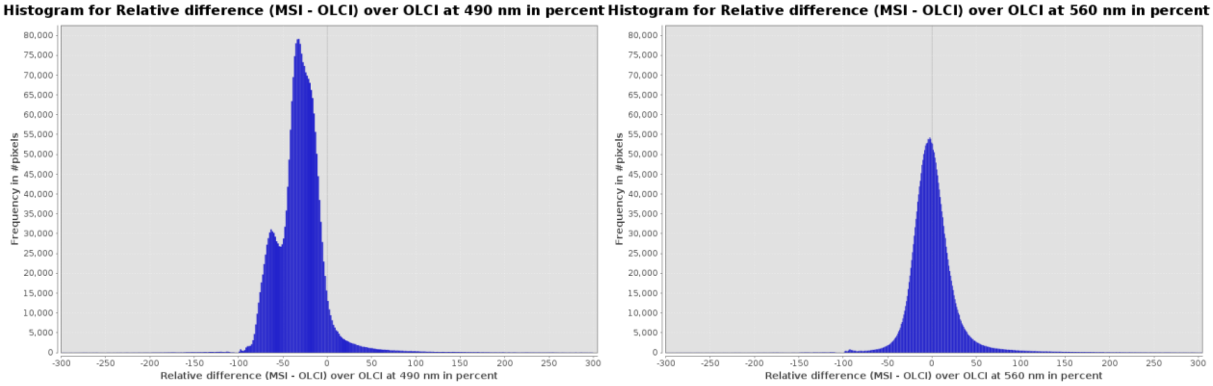

Figure 3-68: Histograms of the relative difference between Sen2Water reflectance and OLCI level 2 ocean colour over Bantayan Island, Philippines, at 490 nm (left) and 560 nm (right)

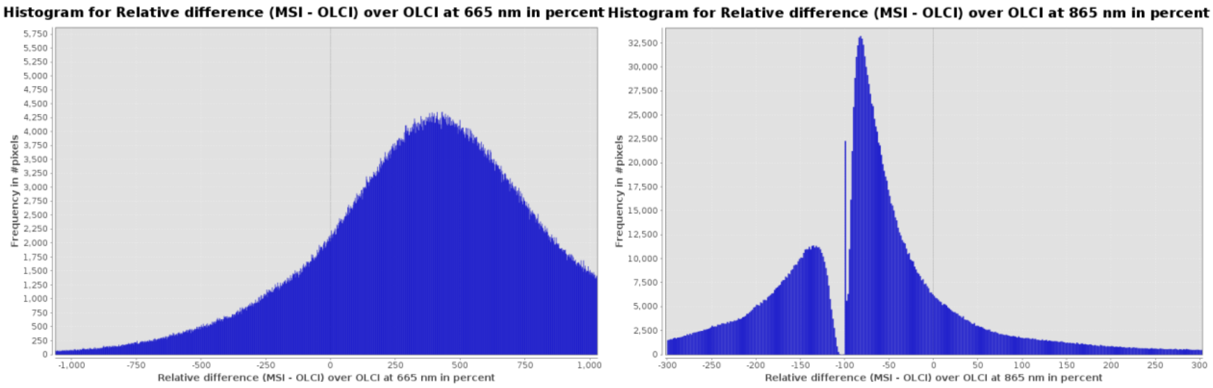

Figure 3-69: Histograms of the relative difference between Sen2Water reflectance and OLCI level 2 ocean colour over Bantayan Island, Philippines, at 665 nm (left) and 865 nm (right)

iii. Products S2B_MSIL1C_20230806T100559_N0509_R022_T34WFT_20230806T104651 and S3A_OL_2_WFR____20230806T092211_20230806T092511_20230807T221544_0179_102_036_1800_MAR_O_NT_003

Products over Bothnian Bay, between Sweden and Finland, are compared, both measured on the 06/08/2023 at 10:05 UTC by MSI and at 09:22 UTC by OLCI.

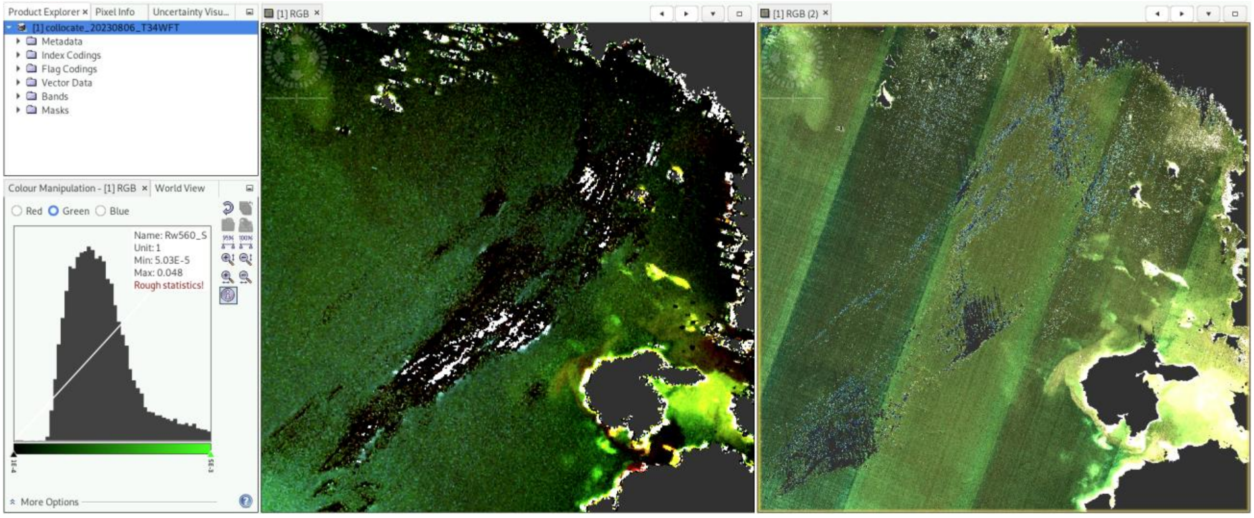

Figure 3-70: OLCI level 2 ocean colour RGB reflectance (left) and Sen2Water RGB reflectance (right), reflectance range is $1 \cdot 10^{-4}$ to $5 \cdot 10^{-3}$ for the three colors, over Bothnian Bay, between Sweden and Finland

Figure above is presented to understand the context of the figures presented below.

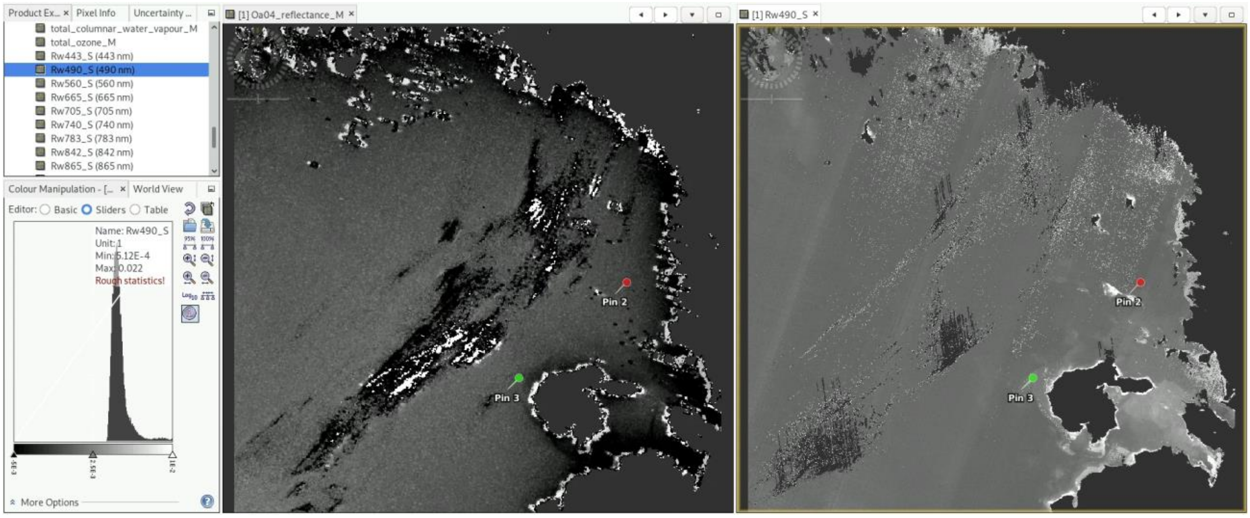

Figure 3-71: on the left, OLCI level 2 ocean colour at 665 nm, on the right Sen2Water reflectances at 490 nm, both collocated over Bothnian Bay, between Sweden and Finland (reflectance range is $-0.5 \cdot 10^{-3}$ to $1 \cdot 10^{-2}$)

Sen2Water reflectances look higher (clearer) than OLCI level 2 reflectances. Under pin 2 (in red), a sandbank is clearly noticeable in the Sen2Water product, but barely visible in the OLCI level 2 product. A structure clearly visible under pin 3 (in green) in the Sen2Water reflectance is not visible in the OLCI level 2 product.

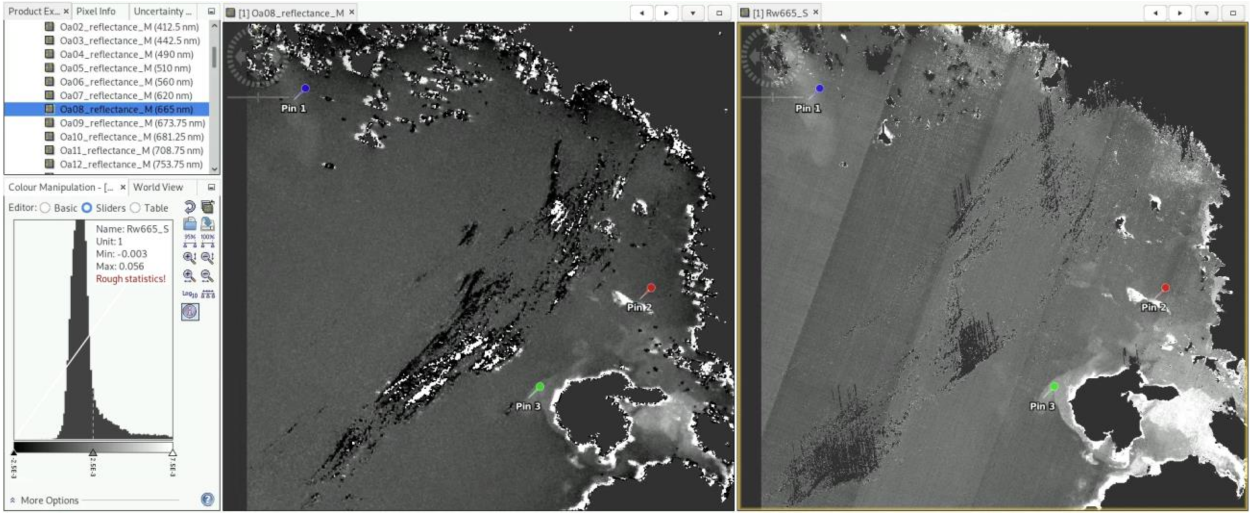

Figure 3-72: on the left, OLCI level 2 ocean colour at 665 nm, on the right Sen2Water reflectances at 665 nm, both collocated over Bothnian Bay, between Sweden and Finland (reflectance range is $-2.5 \cdot 10^{-3}$ to $7.5 \cdot 10^{-3}$)

Similar structures can be observed between the two products over points 1 (in blue), 2 (in red) and 3 (in green). Under 2 is likely positioned a sandbank.

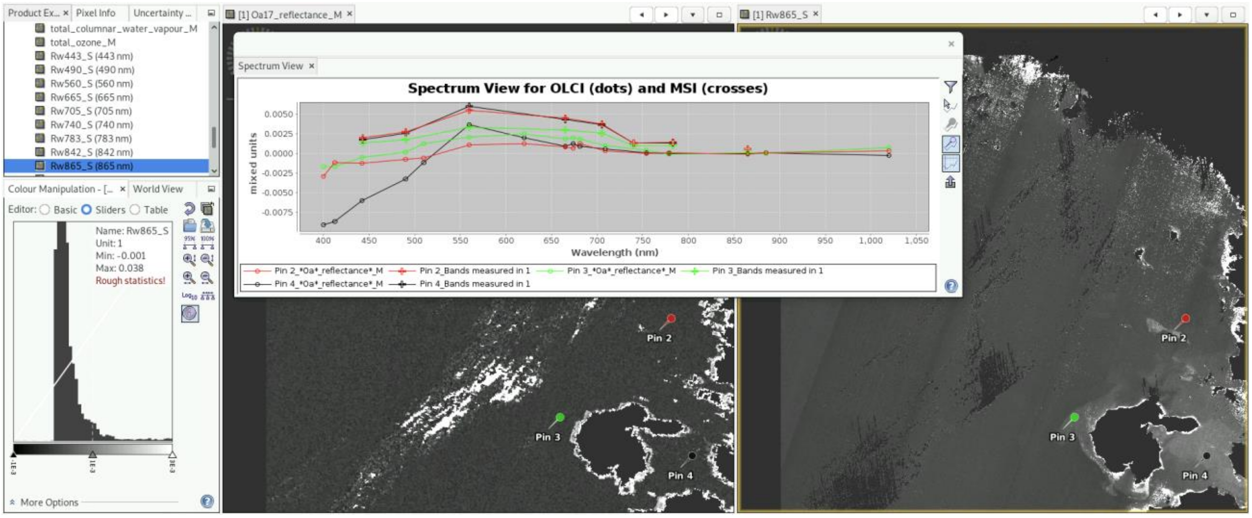

Figure 3-73: on the left, OLCI level 2 ocean colour at 865 nm, on the right Sen2Water reflectances at 865 nm, both collocated over Bothnian Bay, between Sweden and Finland, in the middle spectrum view of OLCI and Sen2Water products (reflectance range is $-1 \cdot 10^{-3}$ to $3 \cdot 10^{-3}$)

Sandbanks clearly visible in the Sen2Water product under pins 2 and 3 (in red and green) are not visible in the OLCI level 2 product. The bay located under pin 4 (in black) has higher reflectances (is brighter) in the Sen2Water product than in the OLCI level 2 product.

One can notice in the spectrum view that under pin 4 (in black), OLCI level 2 reflectances are negative for short wavelength but positive for Sen2Water reflectances. Overall, Sen2Water spectra are above those from OLCI level 2, for all wavelengths and pins.

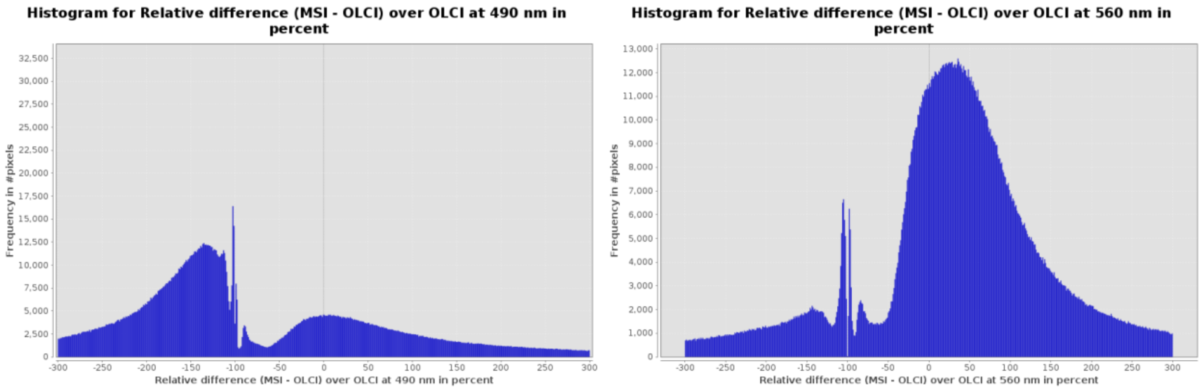

Figure 3-74: Histograms of the relative difference between Sen2Water reflectance and OLCI level 2 ocean colour over Bothnian Bay, between Sweden and Finland, at 490 nm (left) and 560 nm (right)

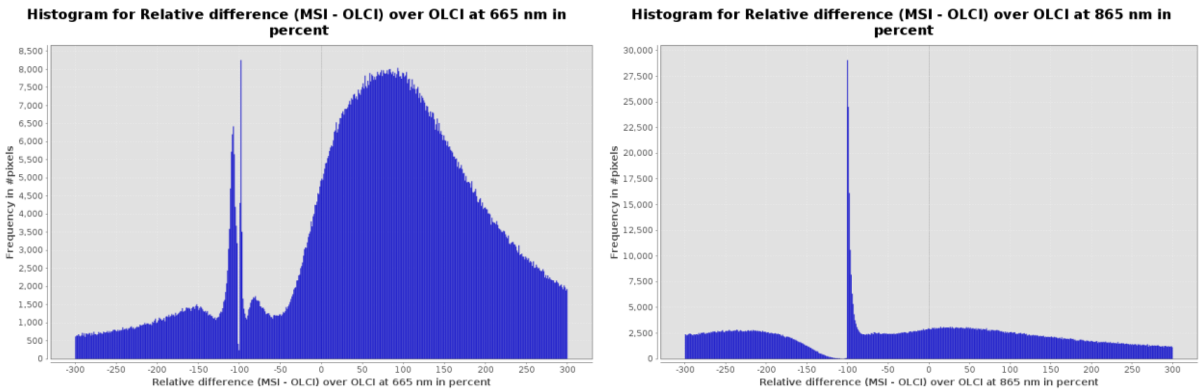

Figure 3-75: Histograms of the relative difference between Sen2Water reflectance and OLCI level 2 ocean colour over Bothnian Bay, between Sweden and Finland, at 665 nm (left) and 865 nm (right)

iv. Products S2A_MSIL1C_20240704T074611_N0510_R135_T36NZJ_20240704T093938 and S3A_OL_2_WFR____20240704T072541_20240704T072841_20240705T145535_0179_114_163_2880_MAR_O_NT_003

Products over Lake Turkana, Kenya and Ethiopia, are compared, both measured on the 04/07/2024 at 07:46 UTC by MSI and at 07:28 UTC by OLCI.

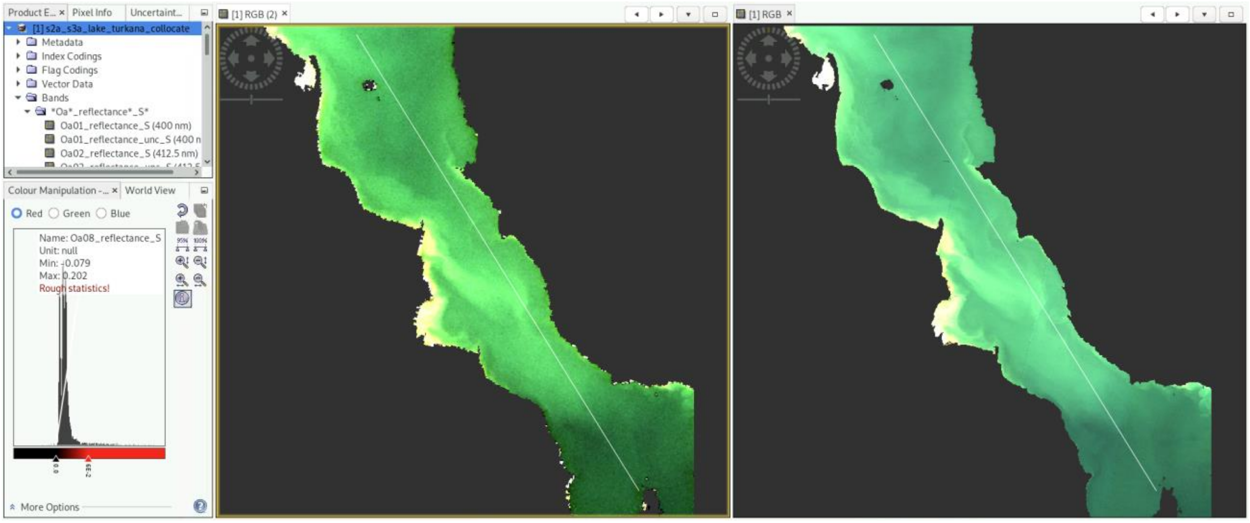

Figure 3-76: OLCI level 2 ocean colour RGB reflectance (left) and Sen2Water RGB reflectance (right), reflectance range is 0 to $4 \cdot 10^{-2}$ for the three colors, over Lake Turkana, between Kenya and Ethiopia

Figure above is presented to understand the context of the figures presented below. The white line is the transect from which are extracted pixels. Those pixels are compared between OLCI level 2 ocean colour and Sen2Water in figure below.

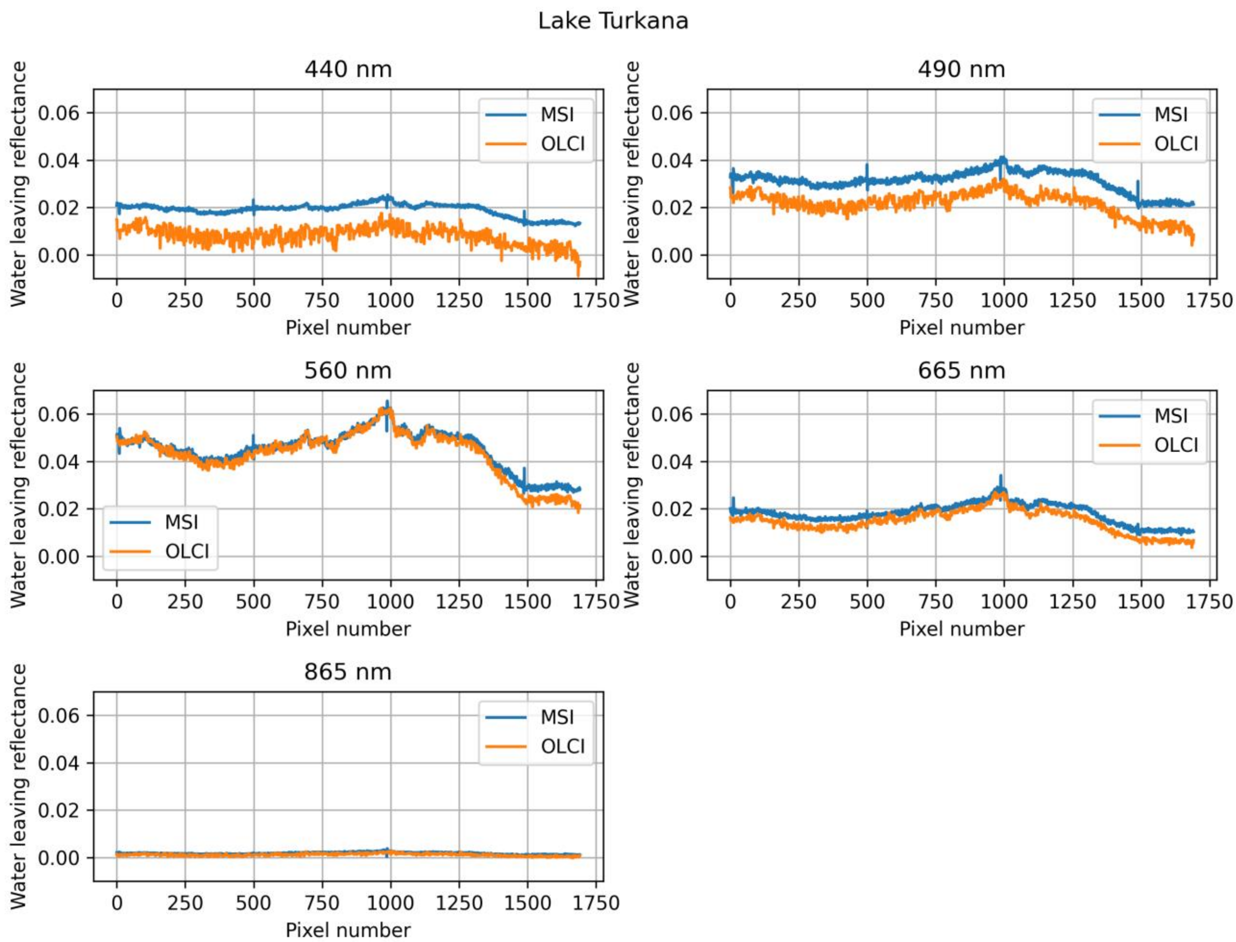

Figure 3-77: Profiles over a transect in two products, a Sen2Water product and OLCI level 2 ocean colour product, for five bands at 440, 490, 560, 665 and 865 nm. Pixels profile over a transect are presented in figure above. For bands at 440 and 490 nm, differences between OLCI level 2 ocean colour product and Sen2Water product can be higher than 100%. For bands 560 and 665 nm, difference is much smaller (maximum of about 50%). For band at 865 nm, water leaving reflectance are so small that no difference is noticeable. For all profiles presented, shapes are very similar between OLCI level 2 ocean colour and Sen2Water.

v. Products S2B_MSIL1C_20240515T101559_N0510_R065_T32UQE_20240515T140423 and S3B_OL_2_WFR____20240515T094959_20240515T095259_20240516T171106_0179_093_079_1980_MAR_O_NT_003

Products over Lake Müritz, Germany, are compared, both measured on the 15/05/2024 at 14:04 UTC by MSI and at 079:49 UTC by OLCI.

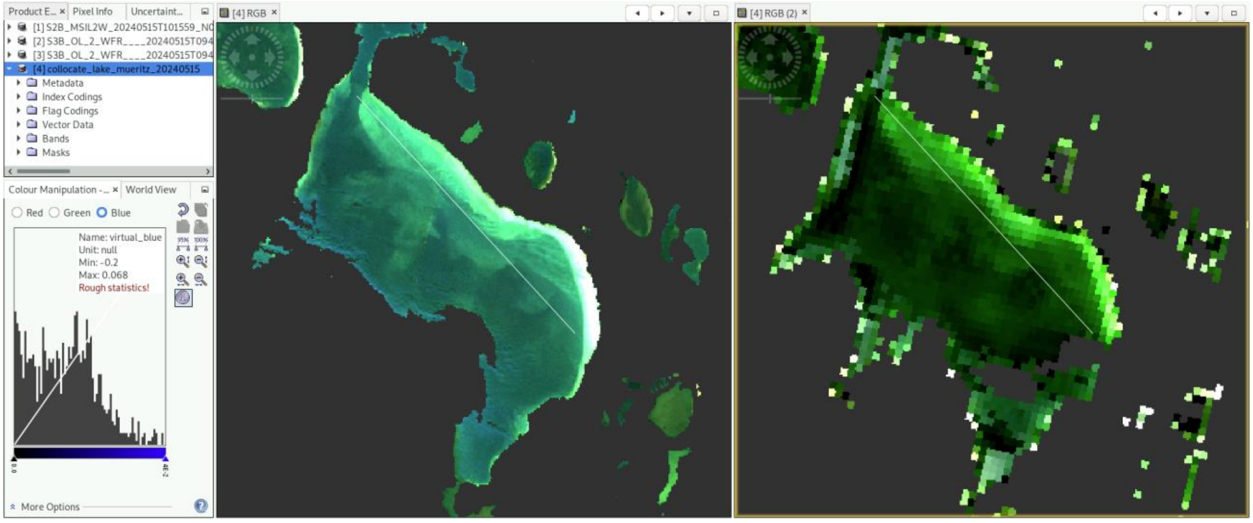

Figure 3-78: OLCI level 2 ocean colour RGB reflectance (left) and Sen2Water RGB reflectance (right), reflectance range is 0 to $4 \cdot 10^{-2}$ for the three colors, over Lake Müritz, Germany

Figure above is presented to understand the context of the figures presented below. The white line is the transect from which are extracted pixels. Those pixels are compared between OLCI level 2 ocean colour and Sen2Water in figure below.

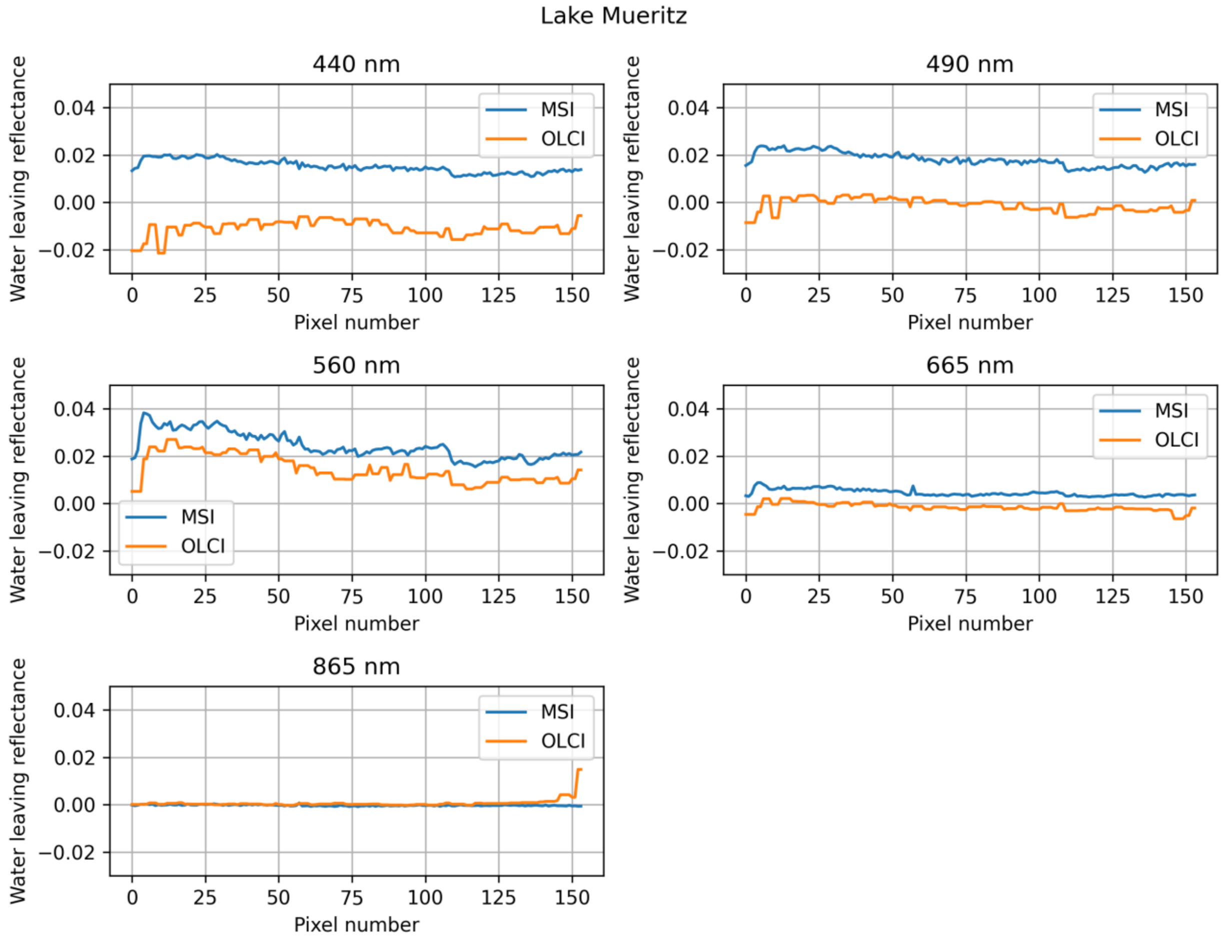

Figure 3-79: Profiles over a transect in two products, a Sen2Water product and OLCI level 2 ocean colour product, for five bands at 440, 490, 560, 665 and 865 nm

Pixels profile over a transect are presented in figure above. For bands at 440, 490 and 665 nm, differences between OLCI level 2 ocean colour product and Sen2Water product are high. Indeed, OLCI reflectance is almost the opposite of MSI reflectance for band at 440 nm; OLCI reflectance is about zero at 490 and 665 nm but MSI reflectance is not zero for these same bands (reflectance of about 0.02 and 0.005 respectively). For bands at 560 nm, difference between the two products is smaller: the two curves having a similar shape and limited relative difference.

3.4 Conclusions and way forward

3.4.1 Validation status

The validation shows that the processor performs reasonably well over various types of scenes.

Scatter plots show a reasonably good agreement, with a slope close to one and small offsets. The performance is less good for in-land waters, especially for the 443 nm band which shows a significant bias and reduced correlation coefficient.

The results in line with those published in the open literature (e.g. ACIX-AQUA benchmark), although somewhat less positive than those reported by Copernicus Services. However the latter are based on different data sets and validation methodology and therefore not directly comparable. More precisely:

- Mean difference results are significantly higher than bias results presented in CMEMS validation report published in June 2022, which also uses AERONET-OC data. RMSD results are one order of magnitude higher than RMSD results in the same CMEMS validation report.
- Mean difference results are one to two orders of magnitude lower than bias results presented in CGLOPS validation report published in February 2020. RMSD results are one order of magnitude higher than RMSE results presented in the same CGLOPS validation report.
- Beta and epsilon indicators are of the same order of magnitude than those presented in the ACIX-AQUA validation report.

Comparisons with OLCI products revealed an overall consistency spectrally and spatially, but reflectances are globally over-estimated.

The performance over in-land waters is noticeably less good than for coastal waters, but due to adjacency effects and aerosol contamination a higher uncertainty is expected.

Observed reflectance spectra seem reasonable. Negative reflectances are sometimes observed especially in the NIR, but this is a common problem for atmospheric correction over dark surfaces.

SWIR reflectances are provided over in-land water but not over coastal waters. This feature may cause concern to users and should at least be clearly explained in the user documentation. It could also be questioned if the provision of SWIR bands over in-land water is really useful, in so far as the values are often not physical (negative) and difficult to validate due to a lack of reference data.

Visual inspection did not highlight major issues. Regarding over image quality:

- Limits between detectors can be clearly seen in the reflectances. This could be mitigated by implementing a better inter-detector strategy at Level 1C processing.
- Sun-glint has a very clear impact on results, with a characteristic odd/even detector pattern. A sun-glint correction method, if efficient, would significantly improve the performance of processor.
- Sen2Water images are often affected with visible effects such as high noise, along-track and across-track stripes. These effects, which are already visible at L1C on low reflectance areas are not due the Sen2Water processing but are limitations of the sensor. There is little perspective for improvements on this aspect for the current Sentinel-2 mission, but more stringent performance requirements could be expressed for Sentinel-2 Next Generation to support aquatic applications.

Regarding pixel classification:

- Cloud detection is generally conservative, with several instances of commission errors.
- Cloud shadows look somewhat over-estimated in some cases.
- Seasonal lakes, white caps, sun glint-affected pixels or turbid waters seem to be classified as “out of bounds saturated” or “cloud”; a reflectance is sometimes computed, sometimes not. The definition of “out of bounds saturated”, as well as in which conditions a reflectance is provided nevertheless should be clearly explained in users documentation.

3.4.2 Limitations and open issues

- The meaning of "out of bound saturated" needs to be clarified in user documentation
- Test product located on both sides of the ante-meridian could not be processed with Sen2Water v0.4.1, but it was fixed in v0.4.2.

3.4.3 Conclusion and recommendations

To further improve the quality of Sen2Water products, it is recommended to:

- Implement an improved inter-detector management strategy in the L1C processor.
- Implement a sun-glint correction if possible.

3.4.4 Way forward

A delta validation could be performed for the version 0.5 of the Sen2Water processor.

The current test data set and validation procedure should be used for the validation of the future re-engineered version of the processor.

4 Lessons learned and recommendations for future operational validation of Sen2Water operational products

For the future, a robust routine validation strategy for operational products could rely on:

- Scene classification validation over randomly selected sites over ocean and in-land waters. The methodology used by DLR for Sen2cor SCL validation should be fully applicable.
- Visual inspection on the selected products to detect potential image artefacts.
- Systematic match-up processing using AERONET-OC measurements, and Hypernets (as they become available).

5 Bibliography

CODDINGTON, O. M., RICHARD, E. C., HARBER, D., *et al.* Version 2 of the TSIS-1 Hybrid solar reference spectrum and extension to the full spectrum. *Earth and Space Science*, 2023, vol. 10, no 3, p. e2022EA002637.

LEHMANN, Moritz K., GURLIN, Daniela, PAHLEVAN, Nima, et al. GLORIA-A globally representative hyperspectral in situ dataset for optical sensing of water quality. Scientific data, 2023, vol. 10, no 1, p. 100.

PAHLEVAN, Nima, MANGIN, Antoine, BALASUBRAMANIAN, Sundarabalan V., et al. ACIX-Aqua: A global assessment of atmospheric correction methods for Landsat-8 and Sentinel-2 over lakes, rivers, and coastal waters. Remote Sensing of Environment, 2021, vol. 258, p. 112366.

SMITH, Brandon. GitHub - BrandonSmithJ/band-adjustment : Spectral Band Adjustments for Remote Sensing Reflectance Spectra in Coastal/Inland Waters. *GitHub* [online]. [accessed July 30th, 2024]. Available at: https://github.com/BrandonSmithJ/band-adjustment

ZIBORDI, Giuseppe, MÉLIN, Frédéric, BERTHON, Jean-François, et al. AERONET-OC: a network for the validation of ocean color primary products. Journal of Atmospheric and Oceanic Technology, 2009, vol. 26, no 8, p. 1634-1651.

End of the document